**Thermal, Density, Seismological, and Rheological
Structure of the Lithospheric-Sublithospheric
Mantle From Combined Petrological-Geophysical
Modelling: Insights on Lithospheric Stability and
the Initiation of Subduction**

Submitted by

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To my parents. . .

Abstract

This thesis presents a first-of-its-kind combined geophysical-petrological methodology to study the thermal, compositional, density, rheological, and seismological structure of different lithospheric domains. The methodology is incorporated in a finite-element code (LitMod) that solves simultaneously the heat transfer, thermodynamical, geopotential, isostasy, and rheological equations for a particular lithospheric structure with any given composition.

LitMod has been applied to a number of synthetic and real transects in both oceanic and continental domains. It is found that the highly depleted composition typically assumed for Archean lithosphere cannot be representative of the whole lithospheric thickness. A model in which the cratonic keel is composed of at least two boundary layers (i.e. a thick thermal boundary layer including a chemical boundary layer in its upper part) is a necessary condition for reconciling petrological and geophysical data. The observed S-wave anomalies at depths of 350 - 400 km beneath cratons can be explained by allowing a slightly depleted composition down to the bottom of the thermal boundary layer, which is also consistent with other geophysical observables.

In continental compressional settings, the inclusion of compositional and compressibility effects suggest that mechanisms other than pure lithospheric thickening (e.g. eclogitization of injected melts and/or metasomatism) are necessary to destabilize the root of a thickened lithosphere.

In the oceanic domain, a plate model with an asymptotic thermal thickness (depth to the 1300 °C isotherm) of 110 ± 5 km is consistent with all the available geophysical and petrological data. Although the compositional (density) structure of mature oceanic lithosphere makes it gravitationally unstable with respect to the sublithospheric mantle after $\gtrsim 30 - 80$ Ma, the density contrast $\Delta\rho$ never exceeds values of $\sim 40 \text{ kg m}^{-3}$. Thus,

the role of $\Delta\rho$ in triggering/assisting subduction initiation is less critical than previously thought.

A new model for spontaneous initiation of subduction triggered by a Rayleigh-Taylor instability is presented. This model is consistent with density and lithospheric strength estimations in oceanic plates. It is shown that the finite growth of the instability provides the necessary forces to produce whole lithospheric failure, bend the elastic part of the plate, and initiate subduction.

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Original Contribution

This thesis contains only the results of the research conducted by the candidate during the period 2002 - 2006, under the guidance of his supervisor. Some of the material has been published elsewhere in a slightly different form. Most of the material comprising Chapter 3 has been published in two papers (Afonso & Ranalli, 2005; Afonso et al., 2005). Selected parts of Chapters 2, 3, and 4 have been also published elsewhere (Afonso & Ranalli, 2004). Parts of Chapter 5 have been published in an abstract format (Afonso et al., 2006). In all of the above publications, the candidate is the senior author.

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CHAPTER 1

Introduction

Ever since the inception of plate tectonics scientists have been trying to elucidate the fundamental driving mechanisms for the Earth's surface motions. It is now widely accepted that the release of gravitational potential energy by subsolidus mantle convection is the energy source behind plate tectonics and its wide range of geological and geophysical phenomena (e.g. volcanism, orogenesis, earthquakes, subduction, etc). However, a comprehensive picture of how sublithospheric convection and lithospheric plates interact, mechanically and geochemically, is still far from complete. The rich variety of processes that take place simultaneously makes the problem as fascinating as complex. In particular, topics such as lithospheric stability with respect to mantle convection and the initiation of subduction remain poorly understood.

A detailed modelling of the thermophysical properties of the lithospheric - sublithospheric mantle is of primary importance, since they ultimately control the response of the system to perturbations arising from mantle convection. Besides their dependence on temperature and pressure, system properties depend in turn on the crystal structure and chemical composition of its constitutive minerals, which varies considerably among lithospheres of different nature (i.e. oceanic versus continental) and ages. Thus, lithospheric-sublithospheric models should include these factors accordingly. Unfortunately, direct observation of the lithospheric-sublithospheric mantle is highly limited, and extrapolations of thermophysical properties and compositions from one particular location to another carries implicitly unquantifiable uncertainties. Therefore, indirect methods need to be used as constraints when modelling large sections of the Earth. These methods include the study of seismic waves, potential fields (gravity and magnetic fields), surface heat flow, and isostasy. Since each of these geophysical fields is affected to a different degree by thermal and compositional heterogeneities, an integrated modelling

approach that includes all of these in a self-consistent manner is desirable.

The primary goals of this thesis are: (a) to present an integrated modelling technique that permits to give constraints on possible compositional fields for any lithospheric-sublithospheric model; (b) to evaluate the effects that compositional heterogeneities among different lithospheric domains may have on their relative stability upon the convective sublithospheric mantle; and (c) to study the implications of the results on the initiation of a subduction zone.

Chapter 2 provides a brief review of the evidence for compositional heterogeneities in the lithosphere. Processes responsible for changing the average undepleted upper mantle composition, as well as the mean compositions that characterize different lithospheric domains, are examined.

Chapter 3 introduces a new model to estimate the elastic parameters of rocks and seismic velocities within the upper mantle. This method rests exclusively on the mineral physics of composites. Rigorous comparisons with many different types of rocks and synthetic composites are presented. The fundamentals of important thermodynamic parameters, and the methods to estimate them as a function of pressure, temperature, and composition, are introduced.

Chapter 4 presents a new finite-element code (LitMod), used throughout this thesis to model two-dimensional lithospheric-sublithospheric sections. LitMod integrates mineral physics, geochemical, petrological, and geophysical information into one single model using predictions of seismic velocities, surface heat flow, elevation, and gravity and geoid anomalies as constraints. All the relevant concepts and methods applied in the development of the code are discussed.

LitMod is applied in Chapter 5 to study both synthetic and real sections of oceanic and continental lithosphere. Synthetic models include a section of oceanic lithosphere

perpendicular to a mid-ocean ridge, thickened Phanerozoic continental lithosphere, and Archean continental lithosphere. Their density, seismic, compositional, and thermal structure are presented and compared with previous competing models to assess their validity. Estimations of the relative stability of the lithosphere with respect to a reference adiabatic mantle are also given and discussed. Real sections (i.e. based on actual geological-geophysical transects) include a 500 km-long transect across the Namibian volcanic margin, and a 140 km-long transect across the Slave Craton. The modelling results are used to evaluate previously proposed models for their evolution, composition, and structure.

Chapter 6 deals with the topic of oceanic lithosphere buoyancy and the initiation of subduction by gravitational instabilities. Previous models for subduction initiation are discussed and evaluated in terms of the evidence presented in this thesis. A two-dimensional analytical theory for the initiation of subduction by a Rayleigh-Taylor instability is presented. The problems of elastic bending, available negative buoyancy, and whole-lithospheric failure are discussed in detail.

Final discussion and conclusions about the proposed process for subduction initiation form the main part of Chapter 7. Predictions from the model in terms of geophysical observables are discussed and used to evaluate favourable sites at which a new subduction zone may be initiated in the present-day Earth.

CHAPTER 2

Composition and lateral heterogeneities of the lithospheric and sublithospheric mantle

2.1 Introduction

The lithosphere is the long-term rigid outer layer of the Earth, which comprises the crust and a portion of the uppermost upper mantle. It is a chemical, mechanical, and thermal boundary layer composed of a number of plates that translate coherently over a hotter and much less viscous material, active in the convection process. In detail, although the concept of a lithosphere is straightforward, it can be defined in different ways depending on what particular property is under study. This gives rise to a debate over which definition is best, and whether different definitions are consistent among themselves.

In a seismological sense, the *seismic lithosphere*, or LID, has been classically defined as the high-velocity material that overlies the upper mantle Low Velocity Zone (LVZ) (e.g. Anderson, 1989). In ocean basins the LVZ is marked by a strong decrease in S-wave velocities, typically at depths $\lesssim 100$ km. In stable continental regions, the LVZ is much less evident, or entirely absent, and usually thinner than beneath oceans (e.g. Carlson et al., 2005; Thybo, 2006). Although there is some evidence suggesting that the LVZ is a global feature (Thybo, 2006), the base of the LID in continental areas is not always well defined by seismological data (Anderson, 1989, Carlson et al., 2005), making the definition of the seismological lithosphere rather ambiguous.

From a mantle convection point of view, the *thermal lithosphere* is defined as the thermal boundary layer within which heat is transferred primarily by conduction. Its base is typically taken as the depth at which the conductive geotherm intersects a particular adiabat (usually the 1300 - 1315 °C adiabat). On the other hand, since the

temperature changes continuously from the convective interior to the surface, sometimes the base of the lithosphere is defined as the depth at which the temperature reaches a certain fraction of the difference $(T_m - T_s)$, where T_s and T_m are the surface temperature and the mantle temperature beneath the boundary layer, respectively (Schubert et al., 2001).

Since the strength of silicate rocks is strongly dependent on temperature, a *mechanical lithosphere* can be defined as the material above a certain isotherm that is effectively isolated (mechanically) from the underlying convective mantle over geological time scales. This isotherm is typically around 800 - 900 °C, since olivine-rich rocks at temperatures lower than this value cannot be deformed by more than 1 % in time scales of 100 Ma (Schubert et al., 2001). The above definition implies then that the thermal lithosphere includes the mechanical lithosphere. Accordingly, there is an upper layer that takes no active part in convection, underlain by the lower part of the thermal boundary layer which, under some circumstances, can become unstable and convect.

Due to its long-term rigidity, the lithosphere flexes when subjected to vertical loading (cf. e.g. Watts, 2001). This approach considers the lithosphere to be an elastic plate with a characteristic elastic thickness, T_e , resting on an inviscid or viscous fluid. The thickness T_e is one of the main parameters defining the strength of the plate, and in the pure elastic assumption (i.e. the whole lithosphere is elastic) it should coincide with the mechanical thickness. However, the elastic assumption is not consistent with respect to the bending stresses that it predicts, and a yield criterion must be applied in order to constrain them to realistic values. An effective elastic thickness, T_e' is defined then as the thickness that makes the bending moment in an elastic plate equal to that arising from the actual stress distribution in the plate, considering the depth-dependent rheology (Watts, 2001). The term *elastic lithosphere* is usually cited when referring to this load-supporting layer. In principle, when the dependence of the elastic thickness on

plate curvature (i.e. rheology) is accounted for, the mechanical thickness and T_e (not T_e') can be matched.

If the mechanical lithosphere is indeed isolated from the homogenizing process of convection, it should accumulate and preserve distinct geochemical and isotopic signatures for longer periods than the underlying convecting mantle. Although testing of this concept started only in relatively recent times due to the improvement of analytical methods, it has been clearly shown that this is actually the case in both oceanic and continental lithosphere (e.g. Hawkesworth et al., 1999; Griffin et al., 1999b; O'Reilly et al., 2001, and references therein). Since the continental lithospheric mantle is usually older, this geochemical and isotopic signature seems to be more obvious in continental areas. In this way, a *geochemical lithosphere* can be defined. Griffin et al. (1999b), for example, have shown that the lithosphere-asthenosphere boundary (LAB) in continental regions can be defined as the maximum depth from which low-Y (< 10 ppm) garnets, characteristic of depleted lithosphere, are derived. Using thermobarometric techniques, these authors have estimated that the geochemical LAB coincides with temperatures of 1250 - 1300 °C, establishing then a close correlation with the thermal definition of the lithosphere.

When a certain minimum volatile content (mainly C + H + O) is introduced into the upper mantle composition, a *petrological lithosphere* is defined as the uppermost portion of the upper mantle where amphibole (magnesian pargasite) is stable (Green & Falloon, 1998). Below the pargasite stability field, the mantle begins to experience partial melting. The total amount of melt generated in this region depends strongly on the total volatile content. For a geotherm representative of mature oceanic lithosphere (age > 80 Ma), the base of the petrological lithosphere should be at depths of $\sim 80 - 95$ km, according to the dehydration solidus of Green and Falloon (1998). This definition provides a petrological basis for the LVZ in oceanic lithosphere, as well as a correlation

with the thermal definition in the same domain. On the other hand, besides being strongly dependent on the local volatile content, this definition is highly ambiguous for continental domains. For instance, in continental areas with thermal thickness > 200 km, the petrological lithosphere does not have a lower boundary at all, while in continental domains with thermal thickness between 120 - 150 km, the petrological lithosphere is not thicker than ~ 100 km (see Fig. 7.6 in Green & Falloon, 1998).

In this thesis, unless indicated otherwise, the term lithosphere will be used as a synonym of thermal lithosphere. This definition is preferred over others for the following reasons: (a) there is a close correlation between the geochemical and thermal definitions, (b) there is a simple functional relationship between the thermal and the mechanical definitions, and (c) the thermal definition eliminates ambiguities between different lithospheric domains, since it must exist everywhere (i.e. there is always an intermediate isotherm between the convective interior and the surface temperatures). In what follows, the evidence for compositional heterogeneities in the lithosphere, as well as the mean compositions that characterize different lithospheric domains, will be examined.

2.2 The composition of distinct lithospheric domains

Although the bulk composition of the lithospheric mantle can be represented as that of a peridotite *sensu lato*, tectonothermal processes characteristic of different lithospheric domains can change this average composition considerably. There is now abundant evidence from xenoliths and geochemical studies on volcanic suites that the lithospheric mantle is highly heterogeneous in composition, both vertically and horizontally (e.g. Boyd et al., 1997; Griffin et al., 1998; Wang et al., 1998; Griffin et al., 1999a, 1999b, 1999c; Peccerillo & Panza, 1999; Hawkesworth et al., 1999; Kopylova & Russell, 2000; Poudjom-Djomani et al., 2001; O'Reilly et al., 2001; Yu et al., 2003; Walter, 2003,

Anderson and Thybo, 2006, and references therein).

The terms “depleted” and “fertile” are commonly used to describe the degree to which the composition of a peridotite has been modified by melt extraction. In terms of major-element composition, calcium and aluminum are easily removed from the solid phase when melting occurs (i.e. incompatible elements), while magnesium selectively remains behind in the solid residue (i.e. compatible element). Iron is equally partitioned between both liquid and solid phases at relatively low pressures during anhydrous melting, leading to little change in iron content over a wide range of magnesium content in mantle residues. However, at pressures > 3 GPa, iron content drops in the residue with increasing degrees of melt extraction (Carlson et al., 2005). Therefore, element ratios involving Al, Ca, Mg [$\text{mg\#} = (\text{Mg}/\text{Mg}+\text{Fe})$], and Fe are normally used to quantify the degree of depletion (e.g. Poudjom-Djomani et al., 2001). Another incompatible “element” that greatly affects the physical properties of the mantle is water. Water is two to three orders of magnitude more soluble in melt than in mantle minerals (Hirth & Kohlstedt, 1996). Consequently, melt extractions of $\sim 20 - 30 \%$ can effectively produce a “dry-type” mantle, which will have a higher solidus temperature and viscosity than its fertile counterpart.

From a mineralogical point of view, the expression of depletion is the loss first of clinopyroxene and garnet (for garnet peridotites), which are also the primary hosts for incompatible elements, through a melting reaction of the type (Walter, 2003)

where A , B , C , D , and E are factors obtained experimentally. Orthopyroxene begins to disappear with increasing melt extraction, resulting in the transition from lherzolite (olivine + orthopyroxene + clinopyroxene + garnet or spinel) to harzburgite (olivine +

orthopyroxene) and to dunite (> 90 % olivine).

The systematic depletion in clinopyroxene, aluminous phases (plagioclase, spinel, or garnet), and incompatible trace elements found in samples from both oceanic and continental uppermost mantle strongly point towards melt extraction as the main process responsible for their mineralogical-geochemical heterogeneity (Walter, 2003). Moreover, a secular evolution from depleted Mg-rich low-density Archean domains to more fertile, more dense Phanerozoic domains seems to be a well established fact in the continental lithospheric mantle (e.g. Hawkesworth et al., 1999; Gaul et al., 2000; Zheng et al., 2001; O'Reilly et al., 2001; Poudjom-Djomani et al., 2001; O'Reilly & Griffin, 2006). As a consequence, lithospheric domains with different tectonothermal histories are expected to have distinctive physical properties and they should be modelled accordingly.

As a first approximation, four major lithospheric domains will be distinguished in this thesis based on their distinctive petrological and geochemical features: (a) oceanic lithosphere, (b) Archean continental lithosphere, (c) Proterozoic continental lithosphere, and (d) Phanerozoic continental lithosphere. Besides interfacial effects (e.g. stress transfer between constituent phases), which will be treated in detail in Chapter 3, the thermophysical properties of a rock (strictly a composite) depend mainly on two factors: (i) the volumetric fractions of the phases that make up the rock, and (ii) the particular composition of each phase, since different compositions translate into different thermophysical properties of the same phase. These two factors are a direct consequence of the major-element composition of the rock. Hence, although the trace-element signatures are vital in understanding the long-term evolution of mantle reservoirs and the origin of specific magmatic rocks, this thesis will only deal with the major-element composition of different lithospheric domains. Since the processes that occur in a mid-ocean ridge (MOR) system provide information not only on the evolution of the oceanic lithosphere, but also on the composition of the undepleted upper mantle, this domain will

be discussed first.

2.2.1 Oceanic lithosphere

Typical samples of oceanic lithospheric mantle include (e.g. Bodinier & Godard, 2003):

- (a) Abyssal peridotites: These are fragments of upper mantle that have been most frequently dredged from walls of oceanic fracture zones or rift mountains of slow-spreading MORs (Dick, 1989).
- (b) Ophiolites: Tectonically emplaced slivers of ancient oceanic lithosphere obducted onto continental or oceanic crust in all major orogenic belts. Their composition usually ranges between ophiolitic lherzolites and ophiolitic harzburgites.
- (c) Exhumed peridotites: Mantle rocks that were exhumed above sea level by normal faults associated with rifting or by transcurrent movements along transform faults.
- (d) Alpine or “orogenic” peridotites: Tectonically emplaced peridotitic massifs. Although the term “orogenic” usually implies a subcontinental origin, a few examples have been identified as oceanic in origin.

Of the above, abyssal peridotites are the most important for an understanding of the evolution and composition of the oceanic lithospheric mantle, since they are widely accepted as being residues of mid-ocean ridge basalts (MORB) generation (Dick et al., 1984; Dick, 1989; Boyd, 1989; Baker & Beckett, 1999). The occurrence of tectonic windows necessary to expose suboceanic upper mantle is most common at slow-spreading mid-ocean ridges. As a result, the majority of the abyssal peridotites have been sampled in the slow-spreading Mid-Atlantic and Indian Ocean ridge systems (Dick et al., 1984; Dick, 1989; Seyler et al., 2001). Abyssal peridotites from fast-spreading ridges (spreading

rate $\geq 10 \text{ cm yr}^{-1}$) are more scarce, and the only samples from these systems come from the Hess Deep (Bodinier & Godard, 2003).

The majority of abyssal peridotite samples show a coarse-grained texture, with grain diameters ranging from 0.1 to 1 cm, and varying degrees of plastic deformation (Dick, 1989). Serpentinization is usually very high, varying from 20 % to 100 % replacement of olivine and pyroxene. This pervasive alteration is a major difficulty in the reconstruction of primary bulk compositions of abyssal peridotites. This reconstruction requires firstly the modal and chemical analyses of at least one of the primary phases, and secondly, the use of modal and chemical correlations between the analyzed phase and the rest of the phases (Dick et al., 1984; Baker & Beckett, 1999). The particular method to accomplish this, however, is still a matter of debate (e.g. Niu, 1997; Niu et al., 1997; Baker & Beckett, 1999; Walter, 1999). For example, the approach followed by Niu et al. (1997) resulted in a clear positive correlation between bulk FeO^* (total Fe as FeO) and bulk MgO of their data set, which led them to postulate that abyssal peridotites have experienced substantial olivine addition during their evolution, and therefore that they are not simple residues. Niu (1997) and Niu et al. (1997) interpreted abyssal peridotites as residues into which cumulus olivine was later added by partial crystallization of MORB. In contrast, Baker and Beckett (1999) based their reconstruction of the bulk composition of abyssal peridotites on the positive correlation between $\text{mg}^{\# \text{ol}}$ [$(\text{Mg}/\text{Mg}+\text{Fe}^*)$ in olivine] and modal olivine, and found no statistically significant correlation between FeO^* and MgO. They also pointed out that their TiO_2 - Na_2O trends suggest no refertilization of the abyssal peridotites during their ascent to the surface. Baker and Beckett (1999) concluded that the correlation found by Niu et al. (1997) is an artifact of their calculation scheme, and therefore, that there is no evidence for significant olivine addition.

A number of databases containing modal analysis of abyssal peridotites, mostly from recalculations, can be found in the literature (see e.g. Dick et al., 1984; Niu, 1997; Baker & Beckett, 1999; Bodinier & Godard, 2003, and references therein). They yield typical modal abundances of 65 - 84 vol% for olivine, 14 - 26 vol% for orthopyroxene, and 1 - 11 vol% for clinopyroxene. Plagioclase is usually absent, and spinel content is generally less than 0.6 vol%. The mean values from these data bases are more constrained, giving modal volume fractions of 73.6 - 75 vol% for olivine, 20.7 - 21 vol% for orthopyroxene, 3.5 - 4.9 vol% for clinopyroxene, and 0.5 - 0.68 vol% for spinel. When converted to garnet facies with mineral compositions for a xenolith with mg# for olivine matching that of average abyssal bulk and olivine compositions, the mean values change to 78.6 vol% for olivine, 12.5 vol% for orthopyroxene, 4.4 vol% for clinopyroxene, and 4.5 vol% for garnet (Boyd, 1989), reflecting the consumption of orthopyroxene and spinel to give more olivine and garnet. This transition in the simplified system MgO-Al₂O₃-SiO₂ (MAS) can in essence be written as (e.g. Klemme & O'Neill, 2000)

In accordance with the discussion above, the range of modal compositions observed in abyssal peridotites can be explained in terms of different degrees of partial melting in the source region (Dick et al., 1984; Baker & Beckett, 1999; Walter, 1999, 2003). Of particular interest for this thesis is that simple melting models at MORs can be used to calculate the variation of both melt and solid phase composition (and therefore their thermophysical properties) as a function of the degree of melting experienced by the original peridotite. This, in turn, provides a means of estimating the depth-dependent composition (i.e. the composition changes with depth because the extent of melting changes with depth) of the oceanic lithosphere away from the MOR. The composition of the melt and its effect on density estimations will be treated in Chapters 3 and 4.

Therefore, only a brief discussion on the methodology to calculate the composition of the oceanic lithosphere will be given here.

Niu (1997) presented the first quantitative melting model applied to abyssal peridotites. He adopted a simple forward approach that includes four basic steps: (a) estimation of bulk compositions of the residues, (b) calculation of the residual mineral modes by a simple norm-mode conversion, (c) examination of the systematics of residual modes as a function of the extent of melting and melting conditions, and (d) comparison of the model predictions with actual abyssal peridotites. In his model, Niu (1997) assumed that a single polybaric melting reaction was appropriate to describe the evolution of the residue along the melting path, and that the mineral modes calculated from abyssal peridotites were representative of the modes at the conditions of melting. These assumptions were criticized by Walter (1999), who showed that a single polybaric melting reaction could not describe accurately the complex variation of melting reactions in a polybaric process, nor could the modes from abyssal peridotites be used to calculate high-pressure and -temperature melt reactions. As a result of Niu's assumptions, his model seems to overestimate/underestimate the amount of orthopyroxene/clinopyroxene that dissolves into the melt (Walter, 1999). However, Niu's model correctly predicts that: (a) the relation between residual mineral modes and the extent of melting follows a quasi-linear trend, and (b) a simple CIPW norm scheme (named for its inventors Cross, Iddings, Pirsson, & Washington, 1903) can be used to transform model residue compositions into normative mineral modes (see Fig. 5 in Niu (1997)). The latter is a consequence of the fact that the end-member normative mineral components have compositions similar to the mineral compositions in abyssal peridotites. The norm-mode conversion is necessary to allow a direct comparison between experimentally predicted changes in mineral modes and those from natural residues from the mantle (this is because samples of natural residues invariably have re-equilibrated at temperatures and pressures different from those during melt extraction; Walter, 2003). In doing

so, however, the rich variety of melting reactions that actually occur over the pressure range 1.0 - 2.0 GPa are “homogenized”, leaving model’s predictions subject to somewhat unquantifiable uncertainties (e.g. Walter, 1999, 2003). In order to perform the norm-mode conversion, Niu (1997) presented a series of empirical relations that allow the calculation of olivine, orthopyroxene, and clinopyroxene in the residual peridotite from the CIPW normative minerals. Therefore, residual modes as a function of extent of melting can be calculated using the linear relationships presented by Niu (1997), corrected by the overestimation of orthopyroxene and the underestimation of clinopyroxene in the way indicated by Walter (1999). This approach has the advantage of being simple to implement in a numerical code. It should be noted that this approach is only valid for a spinel-bearing peridotite, and it needs to be modified when applied to a peridotite within the garnet stability field. When this is the case, I use the experimental results of Leshner and Baker (1997), corrected for the different parent source adopted in this thesis. The preferred final model used in this thesis for both spinel and garnet lherzolites is shown in Fig. 2.1. Several estimations from different melting models are included for comparison.

2.2.2 Primitive upper mantle

The composition of the original, fertile peridotite can be petrologically approximated from at least two different, but complementary, lines of evidence: (a) if it is assumed that melt extraction from a common upper mantle protolith is the main cause of chemical variability, the identification of trends in major-element composition of xenolith suites should give a good estimate for the major-element composition of the fertile upper mantle; (b) partial melting experiments based on the proposition that the resultant melts from partially melted peridotites must reproduce the major MORB characteristics. Extensive work has been made in these two fields over the past fifty years. Results

from both approaches point toward a preferred “pyrolitic” (Ringwood, 1962a, 1962b) composition, with mg# 88 - 89 as the main source of MORB (see e.g. Hirose & Kushiro, 1993; McDonough & Sun, 1995; Green & Falloon, 1998; Kushiro, 2001; Walter, 2003, and references therein). Not surprisingly, the sublithospheric continental mantle has been shown to have identical characteristics (e.g. Griffin et al., 1999b; Poudjom-Djomani et al., 2001; Walter, 2003). Table 2.1 lists the major-element composition of the primitive upper mantle from different sources.

In addition, any petrological model of the upper mantle needs to be consistent with two additional sources of information, namely the seismic profile across the mantle and cosmochemical observations (McDonough & Sun, 1995). In this context, the pyrolite model has also been successful in predicting not only the observed velocities in the upper mantle but also the depths of seismic discontinuities in the transition zone (e.g. Murakami & Yoshioka, 2001; Bina, 2003, see also Chapter 3 and 4). It is also in basic agreement with the hypothetical composition obtained from mass balance calculations assuming average solar system element ratios for the whole Earth (Palme & O'Neill, 2003). The coexisting mineral proportions and phase transformations of pyrolite at high temperatures and pressures were estimated by Irifune and Isshiki (1998) (Fig. 2.2). This study shows that the olivine modal abundance ($\sim 60\%$) remains almost constant down to depths of ~ 400 km, changing slightly at the $\alpha - \beta$ (wadsleyite or “modified spinel”) phase change (Fig. 2.2). The remaining, non-olivine, components are orthopyroxene, clinopyroxene, and garnet, and these undergo more gradual high-pressure transitions as the pyroxenes dissolve into the garnet. The first gradual change occurs with the transformation of the orthopyroxene into Ca-poor clinopyroxene, which is completed at about 10 GPa (~ 300 km) (Takahashi & Ito, 1987; Irifune & Isshiki, 1998; Fei & Berkta, 1999). At pressures larger than about 8 GPa, the solubility of pyroxenes in garnet increases significantly, forming the “garnet-majorite” solid solution eventually transforming to silicate perovskite. Above 15 GPa, clinopyroxene dissolves into majorite

completely (Irifune & Isshiki, 1998).

This thesis deals explicitly with the properties of the mantle down to depths of ~ 300 km, and therefore the composition of the sublithospheric material in the upper mantle will be modelled by different volume fractions of its three main constituents: olivine, pyroxenes, and garnet (or spinel at pressures of $\lesssim 2$ GPa). Because these volumetric proportions change within this depth interval, an average composition chosen at a depth corresponding to 7 GPa is assumed throughout for the sublithospheric mantle. In detail, this assumption will slightly underestimate the pyroxene content above this depth and overestimate it below it. However, it will be shown in Chapters 4 and 5 that these effects are relatively unimportant in all estimations of composition-dependent physical properties such as whole rock density and seismic velocities. This is mainly due to the fact that the olivine and garnet contents, which are the phases that can greatly affect the estimations, remain almost constant within this depth interval. Fig. 2.2 shows the volumetric proportions of mineral phases estimated by Irifune and Isshiki (1998) together with those used throughout this thesis. Since it is assumed that the sublithospheric mantle participates actively in the homogenizing process of convection, its composition will be held constant throughout all calculations, unless indicated otherwise.

2.2.3 Continental lithosphere

In contrast to what happens with oceanic lithosphere, which is eventually recycled into the mantle, most of the continental lithospheric mantle acts like a long-term reservoir of heterogeneities, and in some cases it seems to serve as a “life-raft” in preserving the continental crust. Lithospheric mantle samples beneath continents are often of the same age as the overlying crust, as indicated by Re-Os systematics (Pearson et al., 2002), particularly in Archean domains, suggesting a long-term relation between the lithospheric mantle and the crust. This was clearly shown by Griffin et al. (1999c)

for the Siberian Craton, where distinct mantle domains coincide with mapped crustal terranes, indicating that during the assemblage of the craton, each terrane carried its own lithospheric root. These studies indicate that crust formation and the evolution of the subcontinental lithospheric mantle are linked processes, suggesting that detailed analysis of crustal volumes can provide relevant information on the formation of the underlying lithospheric mantle and *vice versa* (Poudjom-Djomani et al., 2001). This is particularly useful when applied to basaltic melt extraction episodes. Re-Os ages show that cratonic xenoliths experienced the major depletion in Archean times, while oceanic and pericratonic lithospheric mantles apparently underwent major depletion episodes during Phanerozoic and Proterozoic times (Griffin et al., 1999b; Pearson et al., 2002). It is now generally accepted that there is marked secular evolution in composition (i.e. depletion) in the subcontinental lithospheric mantle, from depleted Archean domains to more fertile Phanerozoic domains (Hawkesworth et al., 1999; Gaul et al., 2000; Zheng et al., 2001; O'Reilly et al., 2001).

Boyd (1989) and Pearson et al. (1994) were among the first to recognize some fundamental compositional distinctions between Archean and Phanerozoic lithospheric mantles. These differences are commonly illustrated in a plot of modal olivine (or olivine/orthopyroxene ratio) against the mg# of olivine (Fig. 2.3A). In Phanerozoic lherzolites, increasing depletion is accompanied by an increase in olivine content, whole rock Mg/Si, and mg#, corresponding to the “oceanic trend” of Boyd (1989). In contrast, Archean lherzolites or harzburgites are characterized by higher mg# at comparable olivine contents (Fig. 2.3A). A similar distinction is exhibited in a CaO - Al₂O₃ plot (Fig. 2.3B), where Archean domains are characterized by low Ca - Al contents, while Phanerozoic domains show a higher content in these elements.

In a seminal paper, Griffin et al. (1999b) showed that a clear correlation exists between all major oxides (except FeO) and the whole-rock Al₂O₃ content in both xeno-

liths and emplaced peridotites of different ages. The Cr_2O_3 content of garnet xenocrysts also correlates well with the Al_2O_3 content of the host rock. This important finding permits to calculate major-element whole-rock compositions for different lithospheric domains only from their Al_2O_3 content, which at the same time allows to convert Al-depth curves (from thermobarometry) to bulk composition versus depth, using the mg# as a cross-check. Alternatively, the mean Cr_2O_3 content of garnet can be used for the same purpose. Griffin et al. (1999b) subdivided the subcontinental lithospheric mantle into three categories, based on their tectonothermal age, which generally correlate with the three continental domains adopted in this thesis: 1) Archons (last major tectonothermal event older than 2.5 Ga), 2) Protons (between 2.5 - 1.0 Ga), and 3) Tectons (younger than 1.0 Ga). Unfortunately, the algorithms used by Griffin et al. (1999b) for Archons are based on regressions through a large xenolith database, which is highly dominated by xenoliths from the Kaapvaal craton, and therefore they might have a strong data bias (W. Griffin, pers. commun.). As a consequence, the orthopyroxene/olivine ratio obtained in this way tends to reproduce the elevated ratios observed in the Kaapvaal craton (a consequence of the high SiO_2 concentration in these samples, Boyd, 1989; Griffin et al., 1999b). However, as more data are gathered in other Archon terranes, it is apparent that this high orthopyroxene/olivine ratio is mainly limited to a specific part of the Kaapvaal craton (the Western Terrane), and not a representative feature of Archons worldwide (Carlson et al., 2005, W. Griffin, pers. commun.). More recent studies in the Siberian (Boyd et al., 1997, W. Griffin, pers. commun.), Slave (Griffin et al., 1999a; Kopylova & Russell, 2000), and North Atlantic (Bernstein et al., 1998) cratons, show that this effect is much less obvious in these areas. Hence, particular care should be taken when modelling the bulk composition of particular Archean domains, especially because a lower orthopyroxene/olivine ratio implies also a necessary increment in garnet to make up for the lost CaO and Al_2O_3 , since in the most depleted compositions, all of these elements reside in the orthopyroxene.

Another highly debated issue about the continental lithospheric mantle is the meaning of the so-called “high-T sheared peridotites”, which have been generally assumed to represent the LAB (e.g. Boyd, 1987; Griffin et al., 1999b). This view has been challenged by several authors based on seismic, petrological, and geochemical evidence (see discussion in Carlson et al., 2005). As a consequence, it is now believed that high-T sheared peridotites form in the lower cratonic lithosphere, where a zone of melt accumulation/metasomatism occurs, below which a thin, less depleted, (but still more depleted than the primitive upper mantle) layer might exist. The evidence for this latter layer extending to depths $\gtrsim 350$ km comes basically from detailed global seismic tomography studies (e.g. Ritsema & van Heijst, 2000; Ritsema et al., 2004, W. Griffin, pers. commun.) which clearly show a seismic keel down to 250 - 350 km depth under some cratons (Fig. 2.4). On the other hand, seismic studies might be sampling only thermal anomalies at these depths, and not real compositional heterogeneities (e.g. King, 2005). This issue will be discussed and clarified in Chapter 5, where I present synthetic and real models of Archean domains.

In what follows, a brief characterization of the three continental lithospheric domains is given in terms of their major-element composition.

2.2.3.1 Archean lithosphere

Archean lithospheric mantle is probably the most well studied lithospheric domain, after the oceanic domain. One of the most conspicuous features of Archean cratons is the clear correlation between these terranes and fast seismic anomalies in the upper 250 - 350 km depth range, as indicated by global seismic models (e.g. Ritsema & van Heijst, 2000; Ritsema et al., 2004). This is illustrated in Fig. 2.4, which shows shear wave anomalies at two depths, for the intervals 100 - 200 km and 200 - 300 km. Shown in this figure are typical Archean areas from where xenolith suites have been studied. Velocity anomalies

greater than ± 2 % are saturated in the color scale. It is clear that the first-order distinction in seismic velocity between oceanic and continental domains extends well below a depth of 200 km. In particular, fast velocity anomalies extend to depths greater than 300 km in many of the Archean domains, although some exceptions exist (e.g. Southern Yilgarn, Southern Slave, Northern Amazonian).

As previously mentioned, most of the compositional features that were previously thought to be representative of all Archean domains are starting to be changed in favour of a more local view. Distinct compositional and structural mantle stratigraphies have been described in different Archean terranes (Boyd, 1989; Boyd et al., 1997; Griffin et al., 1999a; Kopylova & Russell, 2000; Zheng et al., 2001), indicating that generalizations among different Archean cratons might be misleading. There are, however, some important features in terms of composition that are consistent and always present in Archean domains. Foremost among these is the occurrence of significant amounts of depleted (Fe-poor) harzburgites and lherzolites with high mg# and strongly subcalcic garnets (low Ca/Al). Clinopyroxene is subordinate, even in lherzolites, reaching maximum values of ~ 3 vol% (Zheng et al., 2001). Olivine ranges from Fo₉₂ to Fo₉₄ and comprises modal fractions of ~ 70 % in a typical Archean lithosphere (e.g. Siberia, Kaapvaal, Slave) (Gaul et al., 2000). Orthopyroxene composition is mainly enstatite, which typically reaches modal fractions between 20 - 32 %. The low Mg/Si ratio, reflecting the high abundance of orthopyroxene, is also commonly cited as a particular feature of some cratons (e.g. O'Reilly et al., 2001; Zheng et al., 2001), although not necessarily representative of Archean domains worldwide.

In this context, Walter (2003) pointed out that the high orthopyroxene content reported in xenoliths from some areas of the Kaapvaal, Slave, and Siberian cratons is not likely the result of melt extraction only, but also of varying degrees of metasomatism. However, samples from the Tanzanian, Greenland, Canadian, and some areas of

the Siberian and Slave cratons can be readily interpreted as residues after 30 to more than 50 % melt extraction. This observation led Walter (2003) to differentiate Archean cratonic lithosphere into two main types: (a) Low-SiO₂ cratonic lithosphere, which has compositional features that can be explained by melt extraction processes only, and (b) high-SiO₂ cratonic lithosphere, which is modelled by melt extraction followed by varying degrees of secondary addition of orthopyroxene. Both mantle types are characterized by high degrees of partial melting, which consumes the fayalite-rich components of olivine and most of the clinopyroxene during basalt extraction. The Fe-rich olivine end-member fayalite (Fe₂SiO₄) has a density $\rho_{Fa} \simeq 4380 \text{ kg m}^{-3}$ and a solidus temperature $T_{solidus} \simeq 1200 \text{ }^{\circ}\text{C}$ at room conditions, while forsterite (Mg₂SiO₄) has a density $\rho_{Fo} \simeq 3220 \text{ kg m}^{-3}$ and a $T_{solidus} \simeq 1900 \text{ }^{\circ}\text{C}$ at the same conditions (Bass, 1995; Fei & Berkta, 1999). Therefore, as a consequence of this continuous Fe removal by melt extraction, the solidus of the residual mineral assemblage would have to rise, while the mean density would decrease. Also, since the solubility of water is much higher in the melt than in mantle minerals, aqueous fluids might have effectively been removed from the Archean lithospheric mantle, leaving a “dry” rheologically strong residue (Afonso & Ranalli, 2004). The combination of relatively low density, low Fe content, “dry” rheology, and low geothermal gradients, makes the Archean lithosphere stable and resistant to mechanisms such as convective thinning, delamination, and reworking (Afonso & Ranalli, 2004).

Another side effect of melt extraction is the removal of the highly incompatible radioactive elements potassium (K), thorium (Th), and uranium (U) from the lithospheric mantle. The total content of these heat producing elements (HPE) determine the relative mantle contribution to the surface heat flow (SHF) in Archean cratons and the temperature distribution with depth in the lithosphere. It can be expected that highly depleted Archean xenoliths would have the lowest concentrations of HPE. Interestingly, in a recent compilation of HPE measurements in cratonic, off-craton, and massif peridotites, Rudnick et al. (1998) found an inverse correlation. These authors interpreted

this “anomalous” behaviour as being a consequence of several processes such as post-extrusion chemical alteration, analytical detection limits, and sampling bias. Rudnick et al. (1998) presented several arguments that allowed them to conclude that the average HPE content from analyzed cratonic samples cannot be representative of the heat production of Archean mantle roots. This indicates that melt extraction processes are masked in the HPE content of xenoliths, and therefore the former cannot be estimated or accounted for by means of element mass balance methods.

2.2.3.2 Proterozoic lithosphere

There are not many xenolith suites from the Proterozoic that can be used to derive the main characteristics of this domain. Most of the work in Proterozoic terranes include few xenolith suites and garnet concentrates from Northern Siberia, Namibia, the Colorado Plateau, South Australia, and Northern Botswana (Griffin et al., 1999b, W. L. Griffin, pers. commun.). In terms of melt depletion, thermal thickness, surface heat flow (SHF), and seismic signatures, Proterozoic terranes are usually considered to represent an intermediate case between Archean and Phanerozoic domains (e.g. Griffin et al., 1999b; Hawkesworth et al., 1999; O'Reilly et al., 2001; Poudjom-Djomani et al., 2001). All indicators of depletion (e.g. Al, Ca, mg#, etc.) measured in Proterozoic samples are consistent with this view (see e.g. Table 2 of Poudjom-Djomani et al. (2001)). However, the range of variations in their lithospheric features covers practically all values from one extreme to the other, making difficult to establish meaningful generalizations. The geochemical LAB in these domains varies from ~ 130 km depth in the Colorado Plateau to $\gtrsim 170$ km depth in Northern Botswana and South Australia (W. L. Griffin, pers. commun.). The seismological and thermally inferred LAB usually lies between these two values as well (Artemieva & Mooney, 2001, 2002, see also Fig. 2.4). Modal mineral estimations range between 67 - 71 vol% for olivine, 15 - 17 vol% for orthopyroxene, 6 -

8 vol% for clinopyroxene, and 7 - 8 vol% for garnet. The olivine composition generally ranges between Fo_{90.4} and Fo_{90.8} (Griffin et al., 1999b).

2.2.3.3 Phanerozoic lithosphere

Samples of Phanerozoic subcontinental mantle include xenoliths suites from alkalic basalts, and orogenic or Alpine lherzolites that have been tectonically emplaced, typically at convergent margins. Xenoliths commonly range from a few to tens of centimetres in diameter and exhibit a wide range of mineralogy and chemistry, but are always dominated by spinel peridotites with more rare garnet peridotites.

Phanerozoic garnet peridotites are quite uniform worldwide. They show the lowest degree of melt depletion, with high Ca and Al, reaching values close to that of the asthenosphere (O'Reilly et al., 2001). The Phanerozoic spinel peridotites are more variable, and commonly are more depleted than the garnet peridotites (Griffin et al., 1999b). This contrast in composition between the two facies suggests a generalized layering, with “frozen asthenosphere” material underlying an upper subcontinental lithospheric mantle exhibiting a more refractory composition (W. Griffin, pers. commun.).

Although the random nature of sampling complicates the detailed spatial reconstruction of the lithospheric mantle beneath a given xenolith suite, geotherms calculated with thermobarometry indicate equilibration temperatures ranging from 800 to 1200 °C, and relatively shallow LAB in comparison with Archean or Proterozoic domains (Poudjom-Djomani et al., 2001). This agrees well with independent estimations of lithospheric thickness based on surface heat flow (e.g. Artemieva & Mooney, 2001) and seismic (Ritsma et al., 2004) modelling. Re-enrichment processes through a number of metasomatic episodes are commonly evidenced in mantle-derived xenoliths, although the extent to which these processes alter the physical properties of the mantle is still unclear (Gaul

et al., 2000). Modal clinopyroxene and garnet reach their highest average values among continental domains, close to 20 % and 10 %, respectively, although relative abundances can change from one place to another. The Fo content (well correlated with the mg# of the rock) in olivine typically ranges between Fo₉₀ and Fo_{91.5}, particularly at shallow lithospheric levels (Gaul et al., 2000; O'Reilly et al., 2001). The correlation between modal phases and mg# is more scattered than for abyssal peridotites, although similar trends associated with melt extraction are apparent from xenolith data (see Fig. 2.3; Walter, 2003).

In general, the major-element composition of Phanerozoic xenoliths is consistent with that of a fertile upper mantle residue after 0 - 30 % melt extraction. The relatively less depleted, hotter, and fluid-rich Phanerozoic lithospheric mantle is more likely to be affected by tectonic processes, and it might not contribute significantly to the total strength of the lithosphere (Afonso & Ranalli, 2004).

Table 2.1: Primitive upper mantle (PUM) compositions

	MS95	BS94	HK93	N97	TM85(CI)
SiO ₂	45.00	45.50	44.48	45.50	49.90
TiO ₂	0.20	0.11	0.16	0.16	0.16
Al ₂ O ₃	4.45	3.98	3.59	4.20	3.65
Cr ₂ O ₃	0.38	0.68	0.31	0.45	0.44
FeO	8.05	7.18	8.10	7.70	8.00
MnO	0.14	0.13	0.12	0.13	0.13
MgO	37.80	38.30	39.22	38.33	35.15
CaO	3.55	3.57	3.44	3.40	2.90
NiO	0.25	0.23	0.25	0.26	0.25
Na ₂ O	0.36	0.31	0.30	0.30	0.34
K ₂ O	0.03		0.02		0.02
<i>mg#</i>	89.3	90.48	89.62	89.87	88.7

MS95 McDonough & Sun (1995)

BS94 Baker & Stolper (1994)

HK93 Hirose & Kushiro (1993)

N97 Niu (1997)

TM85(CI) CI carbonaceous model of Taylor & McLennan (1985)

Figure 2.1: Residual modes of spinel and garnet lherzolite as a function of melt extraction. Continuous lines are the trends adopted in this study. Olivine = Ol, orthopyroxene = Opx, clinopyroxene = Cpx, spinel = Sp, garnet = Grt. A) Residual modes of spinel lherzolite constituent minerals in weight %. Calculations from Walter (1999) are included for comparison; black circles = Ol, black squares = Opx, black triangles = Cpx. B) Residual modes of spinel lherzolite constituent minerals in volume %. Experimental data and associated uncertainty at 1 GPa from Baker & Stolper (1994); black circles = Ol, black squares = Opx, black triangles = Cpx, black diamonds = Sp. C) Residual modes of garnet lherzolite constituent minerals in volume %. Experimental data and associated uncertainty at 3.6 GPa from Lesher & Baker (1997), corrected for the slightly different primitive composition adopted in this thesis.

Figure 2.2: Equilibrium mineral proportions for a model mantle composition (pyrolite) as a function of depth (pressure). Mineral proportions are in volume %. Opx, Cpx, and Grt as in Fig. (2.1); α - ol = orthorhombic olivine, β - ol = wadsleyite. Black diamonds indicate the experimental results of Irifune & Isshiki (1998); white circles are the average mantle mineral proportions adopted in this thesis for the first 300 km. The grey horizontal band indicates the maximum depth (pressure) of the models constructed in this study. (Figure based on Fig. 1 of Irifune & Isshiki (1998)).

Figure 2.3: A) Plot of $mg\#$ versus modal proportion of olivine for mantle-derived xenoliths from lithospheric domains of different ages (Figure modified from Griffin et al. (1999b)). B) Plot of CaO - Al_2O_3 calculated from garnet xenocryst suites and xenolith averages from different lithospheric domains (Figure modified from O'Reilly et al. (2001)).

Figure 2.4: S-wave tomographic slices from model S20RTS (Ritsema & van Heijst, 2000) at depths of 100 - 200 km (A) and 200 - 300 km (B). Velocities are referenced to PREM. The scale is $\pm 7\%$, but it saturates after $\pm 2\%$. White stars indicate typical Archean locations where xenolith suites have been studied. (Figure modified from King (2005)).

CHAPTER 3

Thermo-elastic Properties of the Lithospheric and Sublithospheric Mantle Derived From Mineral Physics of Composites

3.1 Introduction

Several methodologies have been proposed to model the physical properties of the lithosphere, all of them making use of regional geophysical observables as constraints to the models. In addition to composition, the main parameters controlling the final outputs of thermal and seismic models are the elastic parameters (i.e. bulk and shear modulus) and the coefficient of thermal expansion (CTE) assumed for the lithospheric mantle. The former control wave velocities, and therefore the interpretations regarding the thermal state and composition of the mantle. The latter also affects wave velocities, but more importantly, it determines the density of the materials, and consequently the calculated elevation, gravity, and geoid fields.

Although there have been numerous attempts to obtain representative values of the CTE for the whole mantle, there are still ambiguities as to which are the appropriate values for the lithospheric mantle. Proposed average values given by different authors range from as low as $1.6 \times 10^{-5} \text{ K}^{-1}$ (Stacey, 1992) to as high as $4.2 \times 10^{-5} \text{ K}^{-1}$ (Doin & Fleitout, 1996), and they are commonly used indistinctly for lithospheres of different composition and thermal state. Similarly, P_n wave velocities for the lithospheric mantle are also assumed to be homogeneous (with typical values of $\sim 8.0 \text{ km s}^{-1}$) over long distances, while they have been shown to be highly variable, ranging from ~ 7.6 to 8.6 km s^{-1} for lithospheres of different ages (e.g. Németh & Hajnal, 1998; Levshin et al., 2001). Moreover, geophysical models usually consider a homogeneous lithospheric mantle, with a composition rich in olivine, mechanically strong, and denser than the underlying asthenosphere. This picture is rather simplistic, and it is in disagreement

with recent data that indicates that lithospheres of different nature (i.e. oceanic vs. continental) and ages have distinct compositional and mechanical properties (cf. Chapter 2, also Griffin et al., 1999c; Hawkesworth et al., 1999; O'Reilly et al., 2001; Poudjom-Djomani et al., 2001; Afonso & Ranalli, 2004, and references therein). Hence, it is of interest to determine representative values of the elastic properties and CTE for different lithospheres that permit a more accurate modelling.

In this chapter, representative values of CTE and elastic parameters for lithospheres of different nature and ages are determined. The first section of the chapter introduces a new model to calculate elastic parameters of rocks. Rigorous comparisons with many different types of rocks and synthetic composites are also presented to explore the accuracy and versatility of the model. Subsequently, the fundamentals of important thermodynamic parameters, and the methods to estimate them as a function of pressure, temperature, and composition, are introduced. In contrast to the majority of previous studies, where values are calculated from inversion techniques or experimental data on olivine only (e.g. Parsons & Sclater, 1977; Stein & Stein, 1992; Doin & Fleitout, 1996), the approach presented here will rest exclusively on the mineral physics of composites. This approach has several advantages over the previous analyses due to: (a) inversion techniques imply an assumed physical model that fully describes the evolution of the system (e.g. plate model, half-space cooling model), which does not exist for continental lithosphere; (b) inversion models give “homogenized” values for the materials, and therefore cannot provide relationships between composition and physical parameters; (c) only mineralogical data give information about the temperature and pressure dependence of the parameters; (d) compositional heterogeneities prevent the use of experimental data on olivine only; and (e) this methodology is the only one that provides an independent approach to test previous estimations.

The elastic properties of mantle rocks, based on the properties of its constituents

only (i.e. minerals), are calculated by means of the shear-lag model (Cox, 1952), which is here improved and expanded for three- and four-phase composites. It is shown that the model gives excellent predictions of the Young's modulus for two-phase composites, and good estimates of wave velocities for three- and four-phase rocks. This model is preferred over other models (Reuss-Voigt-Hill; Hashin-Shtrikman, etc.) because it is the only one that can be used to calculate stress-distribution processes within the material and at the interfaces, providing a promising approach for future rheological considerations. The CTE is calculated using systematics of the pressure-temperature dependence of volume for the main constituents of the uppermost mantle. The usual rule of mixtures is applied to estimate the CTE of the composite, since this method gives the best predictions at temperatures pertaining to the lithosphere. The results and their implications in terms of lithospheric modelling are discussed for lithospheres of different age and nature. I compare the results for oceanic lithosphere with those obtained from inversion techniques, which should coincide if both approaches are valid and representative. Finally, I discuss the major sources of uncertainty in the model and their impact on the final results.

3.2 Elastic properties: a new analytical model

3.2.1 Two-phase composites

The shear-lag model was originally proposed for describing the effect of stress transfer from the matrix to the embedded discontinuous fibres in fibre-reinforced composites (Cox, 1952). Although the original model considers only the load transfer from the matrix to the fibres by means of shear stresses at the fibre-matrix interface, several modifications have been made to account for the stress transfer across the fibre ends (e.g. Nair & Kim, 1992; Hsueh, 1995; Zhao & Ji, 1997; Starink & Syngellakis, 1999, and references therein). The analytical solutions obtained from the governing equations, and

therefore the accuracy of the model, are largely dependent on the imposed boundary conditions at the fibre end. A common approach is to set stress boundary conditions, based on various arbitrary assumptions (e.g. Clyne, 1999; Nair & Kim, 1992). However, as Hsueh (1995) pointed out, this stress is not a predetermined value, and therefore the boundary conditions cannot be chosen unambiguously. Here I adopt a scheme similar to that described in Hsueh (1995), with general boundary conditions based only on well-established mechanical principles. The formulation is, however, modified in order to express the final analytical solutions in a simple closed form and to extend the model from two to three- and four-phase composites.

The unit cell is shown in Fig. 3.1. It is composed of a uniform cylindrical matrix of length $2L$ and radius R , containing a discontinuous cylindrical fibre of radius r_1 and length $2l$. Fibre and matrix are coaxial, and cylindrical coordinates r , θ , and x apply, where r and θ are the polar coordinates of the projection of a point in the polar plane, and x is the distance from the polar plane, taken at the mid-point of the unit cell, to that point. The unit cell is subject to a uniform tensile stress σ_a at its ends, where only the matrix is present. The applied stress is parallel to the fibre axis, and it is assumed that there is no sliding between the matrix and the fibre at the interface $r = r_1$. At this interface, because Young's moduli of the two phases are different, stresses from the matrix are transferred to the fibre by interfacial shear. In the same way, an axial stress $\sigma_f(l)$, which is considered to be independent of r , is also transferred at the ends of the fibre. The assumption of no sliding between matrix and fibres implies that the interfacial strength is high enough to resist dissipative mechanisms such as grain boundary sliding, and therefore anelastic effects are negligible. It will be shown further in this chapter that this is a suitable assumption for calculating P-wave velocities at pressures and temperatures pertaining to the lithosphere, and in most cases, to the sublithospheric mantle as well (see Section 3.6).

The equations describing the stress transfer in and along the unit cell are obtained as follows. Force equilibrium in the system (Fig. 3.1) requires that

$$2 \int_0^{r_1} r \sigma_f(x) dr + 2 \int_{r_1}^R r \sigma_m(x, r) dr = R^2 \sigma_a \quad (3.1)$$

$$\frac{d\sigma_f(x)}{dx} = -\frac{2\tau(r_1, x)}{r_1} \quad (3.2)$$

$$r \frac{\partial \sigma_m(x, r)}{\partial x} + r \frac{\partial \tau(x, r)}{\partial r} = -\tau(x, r) \quad (3.3)$$

$$2\pi r_1 \tau(r_1, x) = 2\pi r \tau(r, x) \quad (3.4)$$

where $\tau(r, x)$ and $\sigma_m(r, x)$ are respectively the shear and axial stress in the matrix, and $\tau(r_1, x)$ is the shear stress at the matrix-fibre interface.

Hooke's law holds each phase, and therefore

$$\sigma_f(x) = E_f \frac{du_f(x)}{dx} \quad (3.5)$$

$$\sigma_m(r, x) = E_m \frac{\partial u_m(r, x)}{\partial x} \quad (3.6)$$

$$\frac{\partial u_m(r, x)}{\partial r} = \frac{1}{G_m} \tau(r, x) = 2\varepsilon_s \quad (3.7)$$

where E_f , E_m , G_m , $u_f(x)$, $u_m(r, x)$, and ε_s are the Young's modulus of the fibre and of the matrix, the shear modulus of the matrix, the axial displacement of the fibre, the displacement of the matrix, and the shear strain in the matrix, respectively. The axial stress in the fibre is independent of r , and thus $u_f(x)$ and $u_m(r, x)$ must be equal at $r = r_1$ (i.e. no interfacial sliding).

Combining Eqs. (3.4) and (3.7) and integrating yields (e.g. Hull and Clyne, 1996)

$$\tau(r_1, x) = \frac{(u_m(R, x) - u_m(r_1, x))G_m}{r_1 \ln(R/r_1)} \quad (3.8)$$

where $u_m(R, x)$ and $u_m(r_1, x)$ are the axial displacements of the matrix at $r = R$ and $r = r_1$, respectively, for a given value of x . Combination of Eqs. (3.4), (3.7), and (3.8) gives

$$\frac{\ln(R/r_1)}{(u_m(R, x) - u_m(r_1, x))} \int_{u_m(r_1, x)}^{u_m(r, x)} du = \int_{r_1}^r \frac{dr}{r} \quad (3.9)$$

from which $u_m(r, x)$ can be calculated. Assuming an isotropic behaviour for the matrix (i.e. $G_m = E_m/2(1 + \nu_m)$, where ν_m is the Poisson's ratio), substitution of $u_m(r, x)$ from Eq. (3.9) into (3.6) yields

$$\sigma_m = E_m \frac{du_m(r_1, x)}{dx} + \left(E_m \frac{du_m(R, x)}{dx} - E_m \frac{du_m(r_1, x)}{dx} \right) \frac{\ln(r/r_1)}{\ln(R/r_1)} \quad (3.10)$$

Recalling that

$$\frac{du_m(r_1, x)}{dx} = \frac{du_f(x)}{dx} \quad (3.11)$$

Eq. (3.5) permits to rewrite Eq. (3.10) as

$$\sigma_m(r, x) = \frac{E_m}{E_f} \sigma_f(x) + \left(E_m \frac{du_m(R, x)}{dx} - \frac{E_m}{E_f} \sigma_f(x) \right) \frac{\ln(r/r_1)}{\ln(R/r_1)} \quad (3.12)$$

Using Eq. (3.1) gives

$$\frac{du_m(R, x)}{dx} = \frac{R^2 \sigma_a + \left\langle \left(r_1^2 - \frac{(R^2 - r_1^2)}{2 \ln(R/r_1)} \right) \frac{E_m}{E_f} - r_1^2 \right\rangle \sigma_f(x)}{E_m \left\langle R^2 - \frac{(R^2 - r_1^2)}{2 \ln(R/r_1)} \right\rangle} \quad (3.13)$$

Finally, differentiating Eq. (3.2) with respect to x , and manipulating Eqs. (3.4), (3.5), (3.6), (3.7), and (3.8) to express $\tau(r_1, x)$ as a function of $\sigma_f(x)$, the following differential equation is obtained

$$\frac{d^2 \sigma_f(x)}{dx^2} = \frac{\sigma_f(x) H S}{E_f R^2} - H \sigma_a \quad (3.14)$$

where

$$H = \frac{R^2}{r_1^2 (1 + v_m) \left\langle R^2 \ln(R/r_1) - \frac{(R^2 - r_1^2)}{2} \right\rangle} \quad (3.15)$$

and

$$S = r_1^2 E_f + (R^2 - r_1^2) E_m \quad (3.16)$$

The general solution of Eq. (3.14) is of the form $\sigma_f(x) = \sigma_{fH}(x) + \sigma_{fP}(x)$, where

$\sigma_{fH}(x)$ is the solution of the homogeneous part and $\sigma_{fP}(x)$ is the solution of the non-homogeneous part (e.g. Kreyszig, 1988). It can be proven that such a solution can be written as

$$\sigma_f(x) = \frac{R^2 E_f \sigma_a}{S} + C_1 \cosh(\beta x) + C_2 \sinh(\beta x) \quad (3.17)$$

where

$$\beta = \sqrt{\frac{SH}{R^2 E_f}} \quad (3.18)$$

Similarly, from Eqs. (3.2) and (3.17)

$$\tau_f(r_1, x) = -\frac{r_1 \beta}{2} [C_2 \cosh(\beta x) + C_1 \sinh(\beta x)] \quad (3.19)$$

The two constants C_1 and C_2 are determined by applying appropriate boundary conditions. Here I follow an approach similar to that proposed by Hsueh (1995), where two fictitious fibres (made of the matrix material), each with length $L - l$ and width $r = r_1$ are added in the region between the fibre and the ends of the unit cell (dashed in Fig. 3.1). This approach is the only one which gives analytical solutions for the stress distribution in the matrix region beyond the limit $x = \pm l$.

The far end of the fictitious fibre (i.e. at $x = \pm L$) and the matrix are acted upon by the uniform stress σ_a . The fictitious fibre transfers this stress to the bonded ends of the real fibre, but because of the distortion of the stress field in the matrix due to the presence of the strong fibre, the magnitudes of $\sigma_f(l)$ and σ_a are neither the same nor a prescribed value, as assumed in some previous work (e.g. Nardone, 1987; Clyne,

1999, Zhao & Ji, 1997; Starink & Syngellakis, 1999). Because of the similar geometry, Eqs. (3.17) and (3.19) can be used to describe the stress transfer through and along the fictitious fibre, $\sigma_{ff}(x)$ and $\tau_{ff}(r_1, x)$, simply by replacing the Young's modulus of the matrix E_m for E_f in Eqs. (3.17) and (3.19). However, since the stress distribution in the fictitious fibre is not symmetric with respect to the mid-point of the fibre (as it is in the real fibre), Eqs. (3.17) and (3.19) can be rewritten for the fictitious fibres as

$$\sigma_{ff}(x) = C_3 \exp(\beta_f x) + C_4 \exp(-\beta_f x) + \sigma_a \quad (3.20)$$

$$\tau_{ff}(r_1, x) = -\frac{r_1 \beta_f}{2} [C_3 \exp(\beta_f x) - C_4 \exp(-\beta_f x)] \quad (3.21)$$

where C_3 and C_4 are two new constants that need to be determined from boundary conditions, and

$$\beta_f = \sqrt{H} \quad (3.22)$$

The most general boundary conditions that can be applied to the unit cell are (Hsueh, 1995)

$$\sigma_{ff}(L) = \sigma_a \quad ; \quad \sigma_f(l) = \sigma_{ff}(l) \quad ; \quad \tau_f(r_1, l) = \tau_{ff}(r_1, l) \quad ; \quad \tau_f(r_1, 0) = 0 \quad (3.23)$$

Solving Eqs. (3.17) – (3.21) with consideration of boundary conditions (3.23) yields the following solutions for the constants C_1, C_2, C_3 , and C_4

$$C_1 = 2 \frac{\frac{\sigma_a(R^2 - r_1^2)(E_m - E_f)}{S}}{\left\langle 2 \cosh(\beta l) - \frac{\beta \{2 \sinh(\beta l) [\exp(\beta_f l) - \exp[\beta_f(2L - l)]]\}}{\beta_f \{\exp(\beta_f l) + \exp[\beta_f(2L - l)]\}} \right\rangle} \quad (3.24)$$

$$C_2 = 0 \quad (3.25)$$

$$C_3 = 2 \frac{\beta A \sinh(\beta l)}{\beta_f \{\exp(\beta_f l) + \exp[\beta_f(2L - l)]\}} \quad (3.26)$$

$$C_4 = -C_3 \exp(2\beta_f L) \quad (3.27)$$

Predicted stresses in the fibre and the matrix using Eqs. (3.17) - (3.21) are given in Fig. 3.2. As found previously (e.g. Nair & Kim, 1992; Hull & Clyne, 1996, Zhao & Ji, 1997), the interfacial shear stress reaches a maximum at the fibre ends and a minimum at the mid-point. The axial stress undergoes a significant amplification from the applied stress at the end of the unit cell, σ_a , to the stress $\sigma_f(r_1, l)$ acting at the fibre ends. This effect was verified by finite element analysis (Nair & Kim, 1992; Hsueh, 2000), and challenges previous assumptions regarding the stress at the fibre ends (e.g. Nardone, 1987, Zhao & Ji, 1997).

The choice of a representative value for R and L in the unit cell is somehow ambiguous, since different combinations of these parameters can give the same volume for the unit cell. Different ways of doing this are proposed in the literature (Clyne, 1999; Taya & Arsenault, 1989; Starink & Syngellakis, 1999). However, it has been noted that basically two end-member geometries (e.g. for long and short fibres) are sufficient to estimate the volume of the unit cell (Hsueh, 2000). Hsueh (2000) presented an ingenious approach of calculating R and L , taking into account these two different geometries, by means of

the parameter p , which is a function of the fibre aspect ratio. It was found that this method gives good estimates of the Young's modulus, similar to those obtained by other common methods (e.g. Eshelby model) (Hsueh, 2000). Here, I follow this approach for calculating representative unit cell dimensions.

Eqs. (3.17) – (3.27) can be used to predict the elastic constants of two-phase composites. The analysis can be done basically in two different ways: (a) by calculating average stresses and strains, or (b) by calculating average displacements. Both schemes give similar results, though the former is somewhat more tedious.

(a) *Average stress and strain*: The fundamental equation describing the modulus of the composite can be written as (e.g. Nair & Kim, 1992)

$$E_c = \frac{(1 - f_f)\overline{\sigma_m} + f_f\overline{\sigma_f}}{\overline{\varepsilon}_{c(a)}} \quad (3.28)$$

where $\overline{\varepsilon}_{c(a)}$ is the average strain of the composite, $\overline{\sigma_m}$ is the average stress in the matrix, $\overline{\sigma_f}$ is the average stress in the fibre, and f_f is the volume fraction of the fibre. The average strain is

$$\overline{\varepsilon}_{c(a)} = f_f \frac{\overline{\sigma_f}}{E_f} + (1 - f_f) \frac{\overline{\sigma_m}}{E_m} \quad (3.29)$$

and the average stresses in both the matrix and fibre can be expressed as

$$\overline{\sigma_m} = \frac{2\pi \left[\left(\int_0^l \int_{r_1}^R r \sigma_m(x, r) + \int_l^L \int_0^{r_1} r \sigma_{ff}(x) + \int_l^L \int_{r_1}^R r \sigma_m(x, r) \right) dr dx \right]}{(L - l)R^2\pi + l\pi(R^2 - r_1^2)} \quad (3.30)$$

$$\overline{\sigma_f} = \frac{2\pi}{\pi r_1^2 l} \int_0^l \int_0^{r_1} r \sigma_f(x) dr dx \quad (3.31)$$

The first integral in Eq. (3.30) represents the total stress acting in a volume equal to $l\pi(R^2 - r_1^2)$; the other two integrals represents the total stress acting in a volume equal to $(L - l)R^2\pi$. The stresses $\sigma_f(x)$ and $\sigma_{ff}(x)$ are given by Eqs. (3.17) and (3.20), respectively. The function $\sigma_m(x, r)$ in Eq. (3.30) describes the variation of the stress in the matrix. However, there is no need to know the explicit form of this function, since it can be eliminated by using the equilibrium condition expressed in Eq. (3.1). The combination of Eqs. (3.1) and (3.30) yields

$$\begin{aligned} \overline{\sigma_m} = & \left\{ 2\pi \left[\int_0^l \left(\frac{R^2 \sigma_a}{2} - \int_0^{r_1} r \sigma_f(x) dr \right) dx + \int_l^L \int_0^{r_1} r \sigma_{ff}(x) dr dx \right. \right. \\ & \left. \left. + \int_l^L \left(\frac{R^2 \sigma_a}{2} - \int_0^{r_1} r \sigma_f(x) dr \right) dx \right] \right\} \\ & \times \frac{1}{(L - l)R^2\pi + l\pi(R^2 - r_1^2)} \quad (3.32) \end{aligned}$$

Finally, combining Eqs. (3.29), (3.31), and (3.32), and substituting into Eq. (3.28), the Young's modulus of the composite can be calculated.

(b) *Average displacements*: The fundamental equation in this approach is the usual relation

$$E_c = \frac{\sigma_a}{\overline{\varepsilon}_{c(b)}} \quad (3.33)$$

where σ_a is the stress applied to the unit cell, and $\overline{\varepsilon}_{c(b)}$ is the average strain of the composite, here expressed as

$$\bar{\varepsilon}_c(b) = \frac{w_o}{L} \quad (3.34)$$

where L is the half length of the unit cell (see Fig. 3.1) and w_o is the average displacement at $x = \pm L$. The value of L as a function of the volume fraction of the fibre is calculated as (Hsueh, 2000)

$$L = l f_f^{2p-1} \quad ; \quad p = \frac{1}{2} - \frac{1}{6} \exp\left(\frac{-l}{5r_1}\right) \quad ; \quad R = r_1 f_f^{-p} \quad (3.35)$$

The average displacement at $x = \pm l$ can be expressed as

$$w_l = \frac{2}{R^2} \left(\int_0^l \int_0^{r_1} r \frac{\sigma_f(x)}{E_f} + \int_0^l \int_{r_1}^R r \frac{\sigma_m(x, r)}{E_m} \right) dr dx \quad (3.36)$$

Similarly, the average displacement at $x = \pm L$ relative to $x = \pm l$ is

$$w_L = \frac{2}{R^2} \left(\int_l^L \int_0^{r_1} r \frac{\sigma_{ff}(x)}{E_m} + \int_l^L \int_{r_1}^R r \frac{\sigma_m(x, r)}{E_m} \right) dr dx = \frac{(L-l)\sigma_a}{E_m} \quad (3.37)$$

Again, the explicit formulation of the stress in the matrix $\sigma_m(x, r)$ is not required, since it can be eliminated by using Eq. (3.1). The total average displacement of the unit cell w_o is the sum of Eqs. (3.36) and (3.37). Therefore, combining Eqs. (3.34), (3.36), (3.37), (3.17), and (3.20), and substituting them into Eq. (3.33), the final expression for the Young's modulus of the composite is obtained as

$$E_c = L \sigma_a \times \left\langle \frac{L \sigma_a}{E_m} + \left(\frac{C_1 \sinh(\beta l)}{\beta} + \frac{l R^2 E_f \sigma_a}{S} \right) \times \left(\frac{1}{E_f} - \frac{1}{E_m} \right) \frac{r_1^2}{R^2} \right\rangle^{-1} \quad (3.38)$$

where S , β , and C_1 are given by Eqs. (3.16), (3.18) and (3.24), respectively.

The values predicted by Eq. (3.38) are compared with extensive experimental data and finite element analysis in Fig. 3.3. Excellent agreement between the published data and the predicted Young's modulus of the composites was obtained in all cases. Also plotted in Fig. 3.3 are predictions based on the equations presented by Ji and Wang (1999) to fit the experimental data on hot-pressed olivine-enstatite composites, those obtained from the equations presented by Taya and Arsenault (1989) and by Starink and Syngellakis (1999), and those from the Reuss-Voigt-Hill (R-V-H) average method (Hill, 1952). Table 3.1 lists the elastic properties of the constituent phases of the composites. The equation used by Taya and Arsenault (1989), also derived from the shear-lag model, neglects the stress intensification at the fibre ends. This equation is always found to underestimate the modulus of the composite, as determined experimentally, by about 15 – 65 %, in particular when the aspect ratio is small (see also Nair & Kim, 1992; Hull & Clyne, 1996). On the other hand, the R-V-H model usually overestimates the modulus of the composite, the associated error being particularly significant when the matrix is relatively soft (i.e. Young's modulus of the order of 2 – 6 GPa), as can be seen in Fig. 3.3C, 3.3E, and 3.3I. Eq. (3.38) always provides good predictions, even when other methods fail to do so. Note that the apparent lesser accuracy of predictions in Fig. 3.3K in comparison with the rest of the figures is a false impression due to the scale used in this figure and the small difference between the Young's moduli of the phases ($E_f/E_m=1.08$). The mean absolute error is 1 %, which is about the same assigned to velocity measurements from which the moduli are derived (S. Ji, pers. commun.). The non-linearity of the experimental results of Ji and Wang (1999) seems to be related to the microstructural evolution of phase connectivity and continuity in the samples, although unquantifiable porosity effects also might affect the results (Ji & Wang, 1999). The modified model of Starink and Syngellakis (1999) gives a better approximation than previous models. However, the accuracy of this model relies strongly on the aspect ratio,

and therefore its validity is based upon a detailed knowledge of the microstructure of the reinforcements. Strikingly, the best predictions for particulate reinforcements, where the aspect ratio should not be greater than ~ 1.5 , are obtained for aspect ratio values of $\gtrsim 2$. This is illustrated in Fig. 3.4, where several experimental data on particulate reinforced Al-SiC composites are plotted together with the predictions from Eq. (3.38), and the above mentioned models. It can be seen that the Starink and Syngellakis model (Starink & Syngellakis, 1999), using the fibre aspect ratio $s = 1.5$, underpredicts the data by about 15 – 25 % (see also Fig. 6 in Starink & Syngellakis, 1999), challenging its applicability as a general method. Eq. (3.38) still gives the best predictions (similar to those by Eshelby model) in all cases.

3.2.2 Three- and four-phase composites

In this section, I derive simple analytical expressions for the elastic properties of three- and four-phase composites, based on an appropriate combination of the modified shear-lag model discussed in the previous section and the method of cells. It will also be shown that the model's versatility allows it to be used for composites having different reinforcements-matrix geometries, as well as for natural polycrystalline/polyminerale rocks. The structure of a composite having two minor phases embedded in a matrix is schematized in Fig. 3.5. A fundamental assumption behind any model for heterogeneous composites is that their heterogeneities can be “homogenized” by choosing a correct *representative volume element* (RVE). In the case of a rock, it can be thought that if there is a major phase and two minor phases, the matrix of the RVE will be the major phase containing single inclusions (or fibres) with equivalent volume fractions. The volume fractions are represented as

$$f_i = \frac{V_i}{V_c} \quad (3.39)$$

where f_i is the volume fraction of the i -phase and V_i and V_c are the volumes of the i -phase and of the composite, respectively. Hence, the following relation holds for a three-phase composite

$$V_{f1} + V_{f2} + V_m = V_c \quad (3.40)$$

The real structure of the rock (Fig. 3.5A) is idealized in Fig. 3.5B as a combination of four RVE, each containing one fibre that represents the sum of the volumes of the crystals of one single phase divided by two. The fibres account for the integrated mechanical interaction of many single crystals. The choice of this particular configuration of four RVE is justified since it is suitable to assume that, on average, the rock will contain grains that interact mechanically as elements in series and in parallel at the same time. Therefore, these two mechanisms must be taken into account when describing the final Young's modulus of the composite.

Referring to Fig. 3.5, the total volume V'_c in RVE 1 is

$$V'_c = \frac{1}{4} (V_{f1} + V_{f2} + V_m) \quad (3.41)$$

and also

$$V'_c = V'_{f1} + V'_{m1} \quad (3.42)$$

where V'_{m1} and V'_{f1} are the new matrix and fibre volumes, respectively. The latter is

$$V'_{f1} = \frac{1}{2}V_{f1} \quad (3.43)$$

Substituting Eq. (3.43) into (3.41) and (3.42) yields

$$V'_{m1} = -\frac{1}{4}(V_{f1} - V_{f2} - V_m) \quad (3.44)$$

from which the volume fraction of the matrix in RVE 1 is obtained

$$f'_{m1} = \frac{V'_{m1}}{1/4V_c} = f_{f2} + f_m - f_{f1} \quad (3.45)$$

In the same way, the volume fraction of the fibre in RVE 1 is

$$f'_{f1} = \frac{1/2V_{f1}}{1/4V_c} = \frac{2V_{f1}}{V_c} = 2f_{f1} \quad (3.46)$$

The new volume fractions for the fibre f'_{f2} and the matrix f'_{m2} in the RVE 2 can be calculated following the same procedure to give

$$f'_{m2} = f_{f1} + f_m - f_{f2} \quad (3.47)$$

$$f'_{f2} = 2f_{f2} \quad (3.48)$$

With these expressions for the volume fractions of the RVE, it is possible to calculate the Young's modulus for each RVE by using Eq. (3.38). Only two moduli are needed,

since the modulus of the RVE 1, E_{c1} , is equal to that of the RVE 4, and the same situation applies for RVE 2 and RVE 3, both of them having modulus E_{c2} .

In order to obtain the Young's modulus of a three-phase composite, the RVE acting in series (i.e. RVE 1 with RVE 3, and RVE 2 with RVE 4) are considered to undergo isostress, while the two RVE acting in parallel (i.e. RVE 1 + 3 with RVE 2 + 4) are assumed to undergo isostrain load conditions. Ravichandran (1994) followed a somewhat similar approach in the unit-cell model for two-phase composites. The Young's modulus E_{CA} resulting from the combination of RVE 1 and 3 is therefore

$$E_{CA} = \frac{E_{c1}E_{c2}}{E_{c1}f_2 + E_{c2}f_1} \quad (3.49)$$

where E_{c1} and E_{c2} are the Young's moduli of the unit cells containing fibres of the phase 1 and 2 (given by Eq. (3.38)), respectively, and f_1 and f_2 are the volume fractions of each RVE, considered to be the same and equal to $1/2$. By means of Eq. (3.49) and the isostrain condition, the final modulus of the three-phase composite E_{CT} can be expressed as

$$E_{CT} = \frac{E_{c1}E_{c2}}{(E_{c1}f_2 + E_{c2}f_1)}(f_1 + f_2) + \frac{E_{c1}E_{c2}}{(E_{c1}f_2 + E_{c2}f_1)}(f_1 + f_2) \quad (3.50)$$

which, since $(f_1 + f_2)$ is now equal to $1/2$, can be rewritten as

$$E_{CT} = \frac{2E_{c1}E_{c2}}{E_{c1} + E_{c2}} \quad (3.51)$$

In order to check the validity of our model for predicting elastic parameters of rocks composed of three phases, I compare the results with experimental data on different

rocks. In doing this, it is important to select only data on three-phase rocks for which the modal composition is known. Also, the change in elastic moduli with temperature and pressure needs to be considered for each mineral before using Eqs. (3.38) and (3.51). Table 3.2 lists modal compositions and Young's moduli used in the calculations. There are, however, three limitations that affect the quality of the comparisons: (a) published elastic moduli are not obtained in uniaxial or triaxial tests, as it would be preferred, but they are estimated from velocity measurements assuming isotropy and homogeneity for both monomineralic aggregates and polyminerale composites; (b) because of the boundary conditions applied to the model, its predictions are expected to give upper bound values; and (c) this kind of data is limited in the literature.

It is assumed, therefore, that the Young's modulus E , shear modulus G , Poisson's ratio v , bulk modulus K , and P-wave velocities V_P can be calculated from elasticity relationships for isotropic and homogeneous materials as given by (cf. Sokolnikoff, 1956)

$$E = \frac{9KG}{3K + G} \quad (3.52)$$

$$v = \frac{3K - 2G}{6K + 2G} \quad (3.53)$$

$$G = \frac{E}{2(1 + v)} \quad (3.54)$$

$$V_P = \sqrt{\frac{K + \frac{4}{3}G}{\rho}} \quad (3.55)$$

The Poisson's ratio of the composite v_c is calculated with the following formula

$$v_c = f_{f1}v_{f1} + f_{f2}v_{f2} + f_mv_m \quad (3.56)$$

where v_{f1} , v_{f2} , and v_m are the Poisson's ratios of the fibre 1, fibre 2, and matrix, respectively. Although Eq. (3.56) is strictly an expression for the longitudinal Poisson's ratio (see e.g. Hull & Clyne, 1996), since the fibre configuration is used as an averaging method, there is no *a priori* obstacle for not using Eq. (3.56). Predictions for V_P from Eq. (3.51) combined with Eq. (3.38) are compared with available data in Fig. 3.6. The model provides a good estimate of the measured values, similar to those predicted by the well-known R-V-H average method. The absolute error is found to be $\lesssim 2\%$ in all cases, which lies well within the best predictions associated with other methods (see e.g. Ji et al., 2003; Afonso et al., 2005).

Another source of experimental data that can be useful for testing the present method is measurements in concrete samples. This material is considered to behave as a three-phase composite, due to the presence of an Interfacial Transition Zone (ITZ) around the inclusions in the cement paste (e.g. Yang, 1998; Li et al., 1999). The geometry of the ITZ might be quite different from that of a fibre composite, and it is still poorly known. However, there is a general agreement that the volume fraction of the ITZ should not be greater than ~ 0.14 . This value is high enough to affect noticeably the properties of the concrete (Meta & Monteiro, 1993; Li et al., 1999). A similar situation is found in composites of alumina platelets in a mullite matrix (APM), where a “soft” silica-rich phase surrounds the matrix particles. Also in this case, the microstructure of the material is not well understood, but it has been shown that the volume fraction of the soft phase should be restricted to $\sim 0.05 - 0.2$ (Ledbetter et al., 2001). Volume fractions larger than the latter value are unrealistic and not supported by microscopic observations.

Considering the above volume fraction values as constraints, an indirect validation of the model can be attempted (Afonso & Ranalli, 2005a, 2005b). Due to the lack of detailed information regarding the precise value of the volume fraction of the “soft” phase in concrete and APM samples, I calculate the theoretical variation of the Young’s modulus in the composite as a function of the “soft” phase volume fraction. In all calculations, the volume fractions of the inclusions are maintained constant, which are predefined values in the experiments, and the matrix and “soft” phase volume fractions are varied proportionally. If the approach is correct, predictions from the model should agree with volumes fractions proposed for these materials.

Fig. 3.7 illustrates the case for an APM composite. The variation of the Young’s modulus of the composite is plotted as a function of the volume fraction of the “soft” phase around the matrix particles. The volume fraction of the alumina phase is maintained constant and equal to 0.2, as in the real sample (Ledbetter et al., 2001). The moduli of the alumina phase, the mullite matrix, and the silica-rich phase are $E_{Al} = 399.6$ GPa, $E_m = 229.1$ GPa, and $E_s = 82.45$ GPa, respectively. The experimental measurement provided by Ledbetter et al. (2001) is also included (222 GPa). Therefore, the projection on the horizontal axis of the intersection of the solid line with the experimental value (black dot in Fig. 3.7), gives the expected volume fraction of the “soft” phase as predicted by the model. The estimated volume fraction (0.13 - 0.14) is within the experimental error and in perfect agreement with the values given by Ledbetter et al. (2001). In this case, there is almost no distinction between the predictions of the R-V-H average method and the present model. This is due to the relatively small E_{Al}/E_m ratio, which makes the Reuss and Voigt bounds to be close to each other and to vary almost linearly.

Fig. 3.8 shows the predictions (solid lines) of the Young’s modulus of the composite as a function of the ITZ volume fraction for the case of concrete samples. The moduli of

the cement paste and the aggregate (sand) are $E_{cem} = 20.76$ GPa, and $E_{ag} = 80$ GPa, respectively. For the ITZ, a typical value of $0.45 E_{cem}$ is assumed (Yang, 1998; Lutz et al., 1997). The numbers on each curve of Fig. 3.8 show the volume fraction of the main phase (i.e. aggregate). Experimental results reported by Yang (1998) are also included (black dots). Again, the projection of the intersection between the measured values and the curves gives the theoretical value for the volume fraction of the ITZ. All predicted values lie in the range of $0.01 - 0.14$, and with the exception of only one point, all of them are restricted to the expected range of $0.04 - 0.14$ (grey area in Fig. 3.8). The variation pattern is also interesting, and some qualitative conclusions can be drawn. The figure shows that a general increase in the theoretical ITZ volume fraction is experienced from low aggregate volume fraction values to moderate values (approximately 0.3). Once the aggregate has reached volume fractions of ~ 0.3 , there is a clear decrease in the ITZ volume fraction, reaching values close to 0 for aggregate volume fractions of 0.5. This indicates that, although the general effect is to harden the composite (i.e. the ratio E_c/E_m always increase), there is a relative elastic softening in the composite for low aggregate volume fractions. In other words, the effect of the third phase is more significant at aggregate volume fractions < 0.3 , making the hardening effect inferior than that expected from the addition of reinforcement. Once a critical value (~ 0.3) has been reached, the effect of the reinforcement is more important than that of the ITZ and a general hardening is expected. In this case, predictions from R-V-H average method are well above the expected values (crosses in Fig. 3.8). Overestimations in ITZ volume fractions are greater for large values of aggregate volume fractions, reaching absolute errors of ~ 300 %.

When modelling four-phase rocks, the elastic properties of ortho- and clinopyroxenes are averaged into a single phase taking into consideration their respective volume fractions. In this way, the elastic modulus of pyroxenes M is represented as

$$M = f_{ortho} M_{ortho} + f_{clino} M_{clino} \quad (3.57)$$

where f_{ortho} and f_{clino} are the respective volume fractions, and M_{ortho} and M_{clino} the respective elastic moduli (e.g. Afonso & Ranalli, 2005a; Afonso et al., 2005). The same scheme for obtaining the elastic moduli of three-phase composites can be expanded to four-phase composites by adding five new RVE acting in series and in parallel. However, this more complex procedure gives no significant improvement in the final estimations of the elastic properties of the composite.

3.3 Thermodynamic parameters

3.3.1 General considerations

Thermodynamics is concerned with relations involving heat, mechanical energy, and other aspects of energy and energy transfer. The most widely used approach is that of classical thermodynamics, which is the study of equilibrium states of matter, in which the properties are assumed uniform in space and time. The common “unit” of study is the *thermodynamic system*: a quantity of matter separated from the surroundings by a flexible boundary through which the system exchanges heat and work, but no mass. It is important then to clearly define where and when the concepts of classical thermodynamics can be applied, especially the one of “system in equilibrium”. A system in a state of equilibrium must be free of currents, such as those generated by mechanical stirring or buoyancy changes by rapid heating. Only when this is true the thermodynamic parameters can be defined by the classical approach. This is obviously an exceptional situation when dealing with lithospheric, and especially sublithospheric processes. Therefore, the question of whether the formal relations from classical thermodynamics can be applied to

our case study is fundamental. For this, I will introduce the concepts of *thermodynamic relaxation time* (TRT) and *process action time* (PAT). The former is the time taken by the material to adjust to a new state through thermal and chemical diffusion, while the latter is the time between the sudden pulses of mass or energy from the surroundings that drive the system out of equilibrium (e.g. magmatic intrusions, sudden changes in temperature; Kundu, 1990). A “quasi-equilibrium”, or “slow” process is one in which the PAT is greater than the TRT; the system reaches equilibrium between each step of the process. If the average PAT is short compared to the TRT, the process can be called “fast,” and is a non-equilibrium process. Therefore, only systems where, from a macroscopic viewpoint, transfers of mass and energy are always in balance, and where sudden perturbations in mass or energy are absent (e.g. lithospheric sections in steady state, isentropic mantle volumes) will be treated in this thesis. With this in mind, the goal is to use different thermodynamic relations to obtain realistic values for the thermodynamic parameters that control the dynamics of the lithospheric-sublithospheric system, namely the CTE, the specific heat, c , and the thermal conductivity, k .

3.3.2 Compressibility of silicate minerals and melts

3.3.2.1 Density of silicate minerals

There are several equations of state (EoS) that have been proposed to extrapolate densities of single silicate minerals to high-pressure and high-temperature (HP-HT) conditions (cf. Anderson, 1995; Poirier, 2000). The most common isothermal equations of state in the literature are the second-order Birch-Murnaghan EoS, the third-order Birch-Murnaghan EoS, the third-order logarithmic EoS, and the Vinet EoS (e.g. Vočadlo et al., 2000; Poirier, 2000). Strictly, the first two are derived from Taylor series expansions of the Helmholtz energy under a Eulerian scheme, the third one uses a finite Hencky

strain scheme, and the latter is derived from interatomic potentials. While the Vinet EoS is more appropriate for very large compressions (e.g. lower mantle conditions), any of the other three are valid at upper mantle conditions, and a discrimination between them is not obvious. Moreover, predictions from the third-order Birch-Murnaghan EoS and the third-order logarithmic EoS are almost identical at pressures < 150 GPa (Fig. 3.9), and both have been used in lithospheric contexts (e.g. Aoki & Takahashi, 2004; Afonso et al., 2005). This makes difficult at first sight to decide which one is more appropriate. I will discuss this further in detail below.

Finite strain isothermal EoS based on Taylor series expansions of the free energy under a Eulerian scheme are commonly used to fit HP experimental data. The Eulerian description is preferred over the Lagrangian alternative because in the former the quantities are expressed as functions of the coordinates of the points in the deformed (strained) state, which are the ones obtained in experiments, and also because of its closer approach to convergence. These equations have been proven to give accurate estimations of mineral compressibility along the 300 K isotherm when appropriate parameters are used (e.g. Jackson & Rigden, 1996; Poirier, 2000). They have been also successful in fitting HP-HT data when a correction for thermal pressure is applied (Poirier, 2000). In this context, there are essentially two different ways to accomplish this (Anderson, 1995; Pavese, 2002):

- (a) By splitting pressure into a static component (only dependent on the strain) and a thermal part (only dependent on temperature).
- (b) By replacing the temperature-independent variables in an isothermal EoS with their temperature-dependent counterparts.

Although many uncertainties still remain upon these theoretical models used to include the temperature effect, the latter (b) has been recently reported, based on meticu-

lous comparisons with numerical simulations, to give better predictions than the former (Pavese, 2002), or negligible differences from experimental measurements (Nishihara et al., 2005). Based on these results, I will adopt the second approach throughout this thesis. In this case, the thermal EoS can be thought of as an extension of the isothermal EoS. The latter is formally represented by a function of the form

$$P = P(\rho, \rho_0, K_0, K'_0, K''_0) \quad (3.58)$$

where ρ_0 , K_0 , K'_0 , and K''_0 are density, bulk modulus, and its first and second derivatives with respect to pressure at $P = 0$, and at a given reference temperature. To explicitly include the temperature effect, these parameters are replaced with $\rho_{0(T, 0)}$, $K_{0(T, 0)}$, $K'_{0(T, 0)}$, and $K''_{0(T, 0)}$, which still give the corresponding quantities at $P = 0$, but at an arbitrary temperature T .

Although both the logarithmic and the third-order Birch-Murnaghan EoS seem to be appropriate in a lithospheric-upper mantle context, the latter will be always used (implying no explicit dependency on $K''_{0(T, 0)}$), corrected by thermal expansivity as indicated above, for computing compressions at upper mantle pressures and temperatures, unless indicated otherwise. There are two main reasons for this: (a) most of the thermodynamic parameters for minerals found in the literature are fitted with this EoS; (b) the logarithmic EoS and the second-order Birch-Murnaghan EoS have been recently shown to be somehow less accurate (see e.g. Cohen et al., 2000; Vočadlo et al., 2000). The third-order Birch-Murnaghan EoS is written as (note that when $K'_{0(T, 0)} = 4$, this EoS reduces to the second-order one)

$$P = \frac{3}{2} K_{0(T,0)} \left[\left(\frac{\rho(T,P)}{\rho(T,0)} \right)^{7/3} - \left(\frac{\rho(T,P)}{\rho(T,0)} \right)^{5/3} \right] \left\{ 1 + \frac{3}{4} (K'_{0(T,0)} - 4) \left[\left(\frac{\rho(T,P)}{\rho(T,0)} \right)^{2/3} - 1 \right] \right\} \quad (3.59)$$

where $\rho_{(T,P)}$, is the pressure-temperature-dependent density, and the other parameters as in Eq. (3.58).

Assuming that $K'_{0(T,0)}$ is independent on pressure and temperature (a common assumption due to the small values of the second derivatives and the uncertainties associated with them (e.g. Jackson & Rigden, 1996; Poirier, 2000), the temperature effect on $K_{0(T,0)}$ and $\rho_{(T,0)}$ can be introduced as

$$K_{0(T,0)} = K_{0(T_r,0)} + \left(\frac{\partial K_{0(T,0)}}{\partial T} \right)_P (T - T_r) \quad (3.60)$$

$$\rho_{(T,0)} = \rho_{(T_r,0)} \exp \left(- \int_{T_r}^T \alpha(T) dT \right) \quad (3.61)$$

where $K_{0(T_r,0)}$, $\rho_{(T_r,0)}$, and $\alpha(T)$ are the isothermal bulk modulus at $T = T_r$ (usually 300 K) and ambient pressure, the density at $T = T_r$, and the coefficient of thermal expansion as a function of T , respectively. The latter is here represented as a polynomial function of temperature (e.g. Fei, 1995)

$$\alpha(T) = a + bT + cT^{-2} \quad (3.62)$$

A final simplification is made by considering the expansion of the exponential series in Eq. (3.61) only to its second order. Consequently, the more familiar form

$$\rho_{(T,0)} = \rho_{(Tr,0)} \left(1 - \int_{Tr}^T \alpha(T) dT \right) \quad (3.63)$$

is obtained.

Thermodynamic parameters for mantle relevant minerals have been well investigated and several compilations can be found in the literature (e.g. Knittle, 1995; Fei, 1995; Anderson & Isaak, 1995; Jackson & Rigden, 1996; Chopelas, 2000; Poirier, 2000; Aoki & Takahashi, 2004; Nishihara et al., 2005, and references therein). All the parameters used in this thesis are listed in Table 3.3

3.3.2.2 Density of silicate melts

The density of silicate melts as a function of pressure, temperature, and composition can be obtained in a way similar to that for solid phases (e.g. Lange & Charmichael, 1987; Cella & Rapolla, 1997). I will follow here the method presented by Lange and Charmichael (1987). In this model, the isothermal compressibility of the silicate melt β_T is linearly dependent on composition

$$\beta_T = \sum X_i \overline{\beta_{i,T}} \quad (3.64)$$

where X_i is the mole fraction of the constituent oxides and $\overline{\beta_{i,T}}$ is the isothermal compressibility of the respective oxides, given by

$$\overline{\beta_{i,T}} = \beta_{reference} + \frac{d\beta_{reference}}{dT}(T - Tr) \quad (3.65)$$

The compressibility is related to the isothermal bulk modulus by

$$K_T = \frac{1}{\beta_{i,T}} \quad (3.66)$$

Experimental values for these parameters and their temperature derivatives are given in Lange and Charnick (1987). I will assume here $K'_{0(T,0)} = 4$ for silicate melts, in agreement with values reported in Lange and Charnick (1987). Therefore, substituting the above parameters in Eq. (3.59), the density of the melt can be estimated. Fig. 3.10 shows the results for a potential temperature $T_p = 1300$ °C. It can be proven that for a wide range of potential temperatures ($1280 < T < 1500$ °C) and compositions, the results are almost identical for depths > 10 km (see e.g. Cella & Rapolla, 1997). On the contrary, the pressure influence on melts densities is the main factor, mainly above ~ 100 km depth, due to their high compressibility. At these depths, the influence of partial melting in decreasing the average density of the rock is a key factor. However, below ~ 100 km depth, melts reach densities of $\sim 3060 - 3070$ kg m $^{-3}$, and the effect of small percentages of partial melting does not affect significantly the average density.

3.3.3 Coefficient of thermal expansion

The volumetric coefficient of thermal expansion (CTE) is one of the most important thermodynamic parameters in modelling the dynamics of the Earth's interior. It controls the density of the materials, and therefore fundamental processes such as isostasy, magma migration, slab subduction, plume structure, and mantle convection (e.g. Hansen et al., 1993; Ketchum et al., 1995; Suzuki et al., 1998; Schubert et al., 2001; Schmeling et al., 2003). Despite the significance of the CTE in geophysical modelling, there is no consensus regarding the appropriate values for lithospheric mantle materials for both oceanic and continental lithospheres. Currently used values (varying from 1.6 –

$2.0 \times 10^{-5} \text{ K}^{-1}$ (Stacey, 1992; Jing et al., 2002), to $4.2 \times 10^{-5} \text{ K}^{-1}$ (Doin & Fleitout, 1996)) are generally based only on experimental data on olivine crystals and/or on inversion techniques, and lateral heterogeneities are not taken into account.

A number of models have been proposed for the CTE of composites, among which the Turner, Kerner, Eshelby, and Garmong models are the most popular (cf. Hahn, 1991). However, besides the fact that they are used only for two-phase composites, these models account for the elastic interactions between phases, and none of them gives good estimates of the CTE when the phases are free to flow in a ductile manner. When this is the case, the simple rule of mixtures provides the best predictions (e.g. Hahn, 1991; Skirl et al., 1998)

$$\alpha_c = \sum_{i=1}^{i=n} \alpha_i f_i \quad (3.67)$$

where α_c is the CTE of the composite, α_i and f_i are the CTE and the volume fraction of the i -phase, respectively, and n is the number of phases present in the composite. In the upper mantle, the fastest changes in temperature capable of generating elastic thermal stresses are associated with advection of material (e.g. slab subduction, plume uprise). However, these processes have lower rates than those at which thermoelastic stresses can be relaxed by rock creep. Therefore, Eq. (3.67) is expected to give the best approximations of the CTE of the composite.

The effect of temperature and pressure on the thermal expansivity of the phases must be taken into account before using them in Eq. (3.67). The thermal dependence of the CTE is given by Eq. (3.62). The density at a given temperature $\rho(T)$ can therefore be calculated from Eq. (3.63). The effect of pressure on the CTE is usually described by the Anderson-Grüneisen parameter δ_T (Chopelas, 2000; Afonso et al., 2005)

$$\alpha(P, T) = \alpha(T) \left(\frac{\rho(P, T)}{\rho(T)} \right)^{-\delta_T \frac{\rho(T)}{\rho(P, T)}} \quad (3.68)$$

For pressure ranges within the first 300 km of depth it can be assumed that the term $\rho(T)/\rho(P, T)$ in the exponent is equal to unity without introducing significant errors. A typical average $\delta_T = 5.5$, consistent with theoretical and experimental estimations (see Table 3.3; e.g. Reynard & Price, 1990; Anderson, 1992; Chopelas, 2000), is assumed. The term within brackets in Eq. (3.68) represents the relative change in density with pressure (i.e. compression) along an isotherm and is calculated using an isothermal EoS (Afonso et al., 2005).

The final distribution with depth of the CTE is the result of the combined effects of temperature and pressure. In the case of silicates, an increase in temperature produces an increase in the value of the CTE. This is shown in Fig. 3.11 for the case of olivine, orthopyroxene, and garnet. Although the temperature derivative of the CTE is slightly different for these minerals (olivine shows the largest variation), all of them obey this general rule. Also plotted in this figure is the pressure effect (dashed lines) on the CTE, calculated with Eqs. (3.68), and assuming a continental Phanerozoic type geotherm (Fig. 3.12). It can be seen that the result of increasing pressure is a reduction in the value of CTE for the three minerals. The pressure effect is particularly important in pyroxenes (see Table 3.3).

3.3.4 Specific heat

Specific heats at constant pressure and at constant volume are defined as (see e.g. Kundu, 1990)

$$c_p = \left(\frac{\partial H}{\partial T} \right)_p \quad (3.69)$$

$$c_v = \left(\frac{\partial E}{\partial T} \right)_v \quad (3.70)$$

where E and H are the internal energy and enthalpy, respectively. Specific heats do not vary significantly with pressure, and the variation with temperature is only important at temperatures below the Debye temperature, Θ_D , of the mineral. Since common values of Θ_D for typical mantle minerals range between 700 - 900 °C (Poirier, 2000), it is usually assumed that they can be taken as constants for mantle modelling purposes. Typical values of c_p and c_v are given in Table 3.3.

3.3.5 Thermal conductivity

The thermal conductivity, k , is a tensor of rank two that varies with pressure and temperature. However, it is almost isotropic in most rocks, and the pressure effect can be ignored within the lithosphere without introducing significant errors (Clauser & Huenges, 1995; Hofmeister, 1999). The variation of k with temperature and pressure for mantle minerals is relatively well known at temperatures < 1000 °C (Clauser & Huenges, 1995). Above these temperatures a theoretical model is needed. Hofmeister (1999) reviewed experimental and theoretical estimations of k for different silicates, and presented a model based on phonon lifetimes to estimate values of k in the mantle. Predictions from her model give average values for the upper mantle in the range 3.0 - 3.5 W m⁻¹ K⁻¹, which agree well with independent average estimations from studies of the variation in seafloor depth (Schubert et al., 2001). McKenzie et al. (2005) have recently applied Hofmeister's model to study the thermal structure of both oceanic

and continental lithosphere. These authors pointed out that the main effect of the temperature dependence of k is to reduce the temperatures in the middle parts of the lithosphere with respect to models with constant k . This is an obvious consequence of having high conductivity values at the top and small values at the bottom of the lithospheric mantle, which translates into a greater spacing between isotherms in the upper part and a smaller spacing towards the bottom (McKenzie et al., 2005). In thick continental roots, however, the thermal conductivity should increase at depths > 150 km due to the combined effects of low temperatures and high pressures (e.g. Jaupart & Mareschal, 1999). Unless indicated otherwise, in this thesis I will follow Hofmeister's model to calculate values of k at different depths. The approach will be discussed in detail in Chapter 4. For the crust, however, average constant values will be used, taking the appropriate values for the modelled lithologies from Clauser and Huenges (1995).

3.4 1-D Modelling results for CTE and V_P

The temperature and pressure effects on mineral properties have been discussed in previous sections. However, in order to give accurate values of CTE and P-wave velocity for the different lithospheric domains, representative pressure and temperature gradients for each domain need to be chosen. The thermal effect is incorporated by solving the steady-state, 1-D heat conduction equation with radiogenic heat production for a three-layer lithospheric model (i.e. upper crust, lower crust, lithospheric mantle), with type rock parameters and analytical solutions taken from Afonso and Ranalli (2004). As a first attempt, three major lithospheric domains will be considered: 1) Archean, 2) Phanerozoic continental, and 3) oceanic lithosphere. Typical average modal compositions for the three domains are listed in Table 3.4. The resultant geotherms are shown in Fig. 3.12. The lithospheric thermal thickness is defined for each domain as the depth at which the respective geotherm reaches the 1300 °C mantle adiabat. For comparison,

xenolith data from the Siberian, South African, and Tanzanian cratons (Rudnick et al., 1998), are also included. The pressure effect is only important in thick plates, and in the case of the CTE it is simply included by assuming an appropriate average density $\bar{\rho}$ for each domain, and using the formula $P_l = \bar{\rho} g z$. This is justified for typical lithospheric thicknesses, where the ratio $\rho_{(P,T)}/\rho_{(T)}$ is always lower than ~ 1.07 . Consequently, the lithostatic pressure can be easily estimated and used in Eq. (3.59) to obtain $\rho_{(P,T)}/\rho_{(T)}$. The mantle densities obtained in this simple manner are only first-order accurate. Since we are considering general end-member domains, detailed crustal structures are not necessary. We take $\bar{\rho}$ in the first 30 km in continental lithosphere to be constant and equal to 2780 kg m^{-3} . In oceanic lithosphere, a constant value of $\bar{\rho} = 2900 \text{ kg m}^{-3}$ is assumed for the first 8 km. Note that if the crustal thickness is modified, parameters will change in response to the pressure variation associated with the change in density. However, pressure effects at Moho levels are relatively unimportant and do not affect significantly the value of the parameters.

Predicted values of CTE and P-wave velocity are calculated for the three lithospheric domains. In the case of oceanic lithosphere, two different cases were considered: a “young” lithospheric section of age $\lesssim 20 \text{ Ma}$, and an “old” section of age $\sim 100 \text{ Ma}$. Temperature and pressure effects are calculated using the values in Table 3.3. Results are shown in Figs. 3.13 and 3.14 as function of temperature and pressure (i.e. depth). The depth displayed in these figures can be converted to temperature, according to the geotherms in Fig. 3.12.

3.4.1 Archean lithosphere

Archean lithosphere shows the simplest pattern in both CTE and seismic velocities. Cold geotherms in these regions preclude a significant increase in the CTE, and are associated with thick lithospheres, which increase the relative importance of the pressure effect on

minerals. This is illustrated in Fig. 3.13A, where at pressures $\gtrsim 1.5$ GPa, the pressure effect prevails over the temperature effect, making the CTE decrease systematically down to depths of ~ 200 km. The relatively high content in orthopyroxene (see Table 3.4) in Archean lithospheres favours this situation because of the strong pressure effect in this mineral (see Fig. 3.11).

For modelling purposes, the opposite effects of temperature and pressure allow to choose an average value for the whole lithosphere, since the variation with depth is relatively unimportant. Values between 3.04 and $3.11 \times 10^{-5} \text{ K}^{-1}$ are acceptable. However, changing the geotherm in particular cases can alter these figures. Nevertheless, variations of more than $\pm 0.06 \times 10^{-5} \text{ K}^{-1}$ are unlikely to occur (see Section 3.6.2).

Predicted seismic velocities V_P as a function of temperature and pressure (i.e. depth) are shown in Fig. 3.14A. Values between 30 - 40 km of depth are in good agreement with estimates of P_n for cratonic areas (e.g. Németh & Hajnal, 1998; Levshin et al., 2001; Grand et al., 2002). Archean lithosphere exhibits a relatively simple pattern of V_P variation. A constant depth-derivative $\partial V_P / \partial z \sim 1.2 \times 10^{-3} \text{ s}^{-1}$ is estimated, which yields velocities of $\sim 8.4 \text{ km s}^{-1}$ at 200 km of depth, in agreement with estimates from seismic studies (e.g. Balling, 1995; Németh & Hajnal, 1998).

3.4.2 Phanerozoic continental lithosphere

Predictions of CTE and P-wave velocities for Phanerozoic continental lithosphere are shown in Figs. 3.13B and 3.14B, respectively. Here, the simple patterns revealed for Archean lithosphere disappear. In the case of the CTE, an increase with depth is evident, due to the relatively “hot” geotherm. Since the lithospheric thermal thickness is ~ 110 km, pressure effects are moderate and temperature dependence dominates the variation of the CTE. The results indicate a variation from $\sim 3.3 \times 10^{-5}$ to $3.5 \times 10^{-5} \text{ K}^{-1}$

at pressures equivalent to 30 and 100 km, respectively. However, larger variations should be expected with slight changes in the geotherms and/or Moho depths. Neglecting temperature and pressure dependence in the CTE can lead to errors of $\sim 20\%$ in subsidence (e.g. Ketcham et al., 1995) and lithospheric thickness estimations.

The predicted variation of the CTE with depth suggests that this parameter can be approximated in numerical models by a simple polynomial expression of the form $\alpha(z) = \alpha_1 + \alpha_2 z - \alpha_3 z^{-2}$, where α_1 , α_2 , and α_3 are constants of the order of 10^{-5} , 10^{-8} , and 10^{-4} , respectively, whose precise values need to be determined for each particular case. Using the geotherm representative of Phanerozoic lithosphere (see Fig. 7), I find $\alpha(z) = 3.3 \times 10^{-5} + 2 \times 10^{-8} z - 5 \times 10^{-4} z^{-2}$, where z is in km. This expression introduces errors $< 1\%$ in the value of the CTE in a depth range of 25 to 100 km with respect to model predictions. Although a polynomial expression can be useful for modelling purposes, the methodology presented in this thesis should be used to calculate the pertaining parameters as a function of temperature and pressure whenever possible, since uncertainties in geotherms can result in $\sim 3\%$ error on CTE estimations.

The P-wave velocity variation with depth in Phanerozoic lithosphere shows a more intricate pattern. A small decrease is expected in the range 25 - 40 km, followed by an almost constant value of $\sim 8.08 \text{ km s}^{-1}$ between 40 and 60 km, and a systematic increase with a depth-derivative $\partial V_p / \partial z \sim 1.12 \times 10^{-3} \text{ s}^{-1}$ from 60 km downwards. These velocities are in good agreement with the typical Pn values of about $8.0 - 8.1 \text{ km s}^{-1}$ measured in Phanerozoic areas, although the depth-derivative seems to be slightly low. However, the maximum variability is still small (between ~ 8.08 and 8.13 km s^{-1} , Fig. 3.14B) and a near constant P-wave velocity in the depth range 40 - 100 km is expected in areas with a thermal thickness $\sim 100 \text{ km}$.

3.4.3 Oceanic lithosphere: ≤ 20 Ma and ~ 100 Ma

Oceanic lithosphere exhibits a variation pattern for the CTE similar to that of Phanerozoic continental lithosphere. However, the amplitude of the variation is larger, due to the higher content in olivine and steeper geotherms. In young plates (age $\lesssim 20$ Ma), values of the CTE range non-linearly from 3.25 to $3.82 \times 10^{-5} \text{ K}^{-1}$ at pressures equivalent to depths of 10 and 50 km, respectively (Fig. 3.13C). The latter value is the highest CTE found in this chapter. Again, the non-linear variation pattern precludes the use of a single average value. Using the type geotherm in Fig. 3.12, a good approximation in a depth range of 8 to 50 km can be obtained with the polynomial formula $\alpha(z) = 3.5 \times 10^{-5} + 7.2 \times 10^{-8} z - 2.78 \times 10^{-4} z^{-2}$, with z in km. When old lithospheres (~ 100 Ma) are considered, and taking into account the spinel-garnet phase transformation, values for the CTE are slightly smaller than in young oceanic lithospheres. Predicted values lie in the range of 3.0 to $3.7 \times 10^{-5} \text{ K}^{-1}$ at pressures equivalent to depths of 10 and 80 km, respectively, using a type geotherm (Fig. 3.13D). In this case, the best-fitting function can be expressed as $\alpha(z) = 3.11 \times 10^{-5} + 7.9 \times 10^{-8} z - 1.5 \times 10^{-4} z^{-2}$.

Independent estimations of average CTE in oceanic lithosphere have been obtained from inversion techniques. Parsons and Sclater (1977) reported best-fitting values of $3.28 \pm 1.19 \times 10^{-5}$ and $3.1 \pm 1.11 \times 10^{-5} \text{ K}^{-1}$ for the North Pacific and North Atlantic, respectively. Stein and Stein (1992) found a slightly smaller value of $3.1 \pm 0.8 \times 10^{-5} \text{ K}^{-1}$ for the same regions. Doin and Fleitout (1996) obtained values ranging from 3.34 to $4.2 \times 10^{-5} \text{ K}^{-1}$, with a preferred CTE of $3.85 \times 10^{-5} \text{ K}^{-1}$. Predictions from our model are in very good agreement with the majority of these values. Indeed, our mean CTE for old oceanic lithosphere is $\sim 3.45 \times 10^{-5} \text{ K}^{-1}$. However, the estimations given here indicate that the values used by Doin and Fleitout (1996) are too large to be used as average values in lithospheric models.

The P-wave velocity variation with depth is plotted in Figs. 3.14C and 3.14D. In the case of young oceanic lithosphere the velocity decreases linearly from ~ 8.16 to 7.73 km s^{-1} in the first 60 km. These values are consistent with *in-situ* measurements in young oceanic lithospheres (e.g. Canales et al., 1998), although the rapid variation of the geotherms with distance from the ridge in these regions makes velocities vary considerably (see Section 3.6.2). Since the base of the lithosphere is at around 60 km depth, the spinel-garnet transition does not take place within the region shown in Fig. 3.14C. In old lithospheres, a reduction in P-wave velocity with depth is also observed. However, the pattern is affected by the spinel-garnet phase transformation at $\sim 2 \text{ GPa}$. At this pressure, the velocity jumps from 8.11 to 8.18 km s^{-1} . Although there is experimental evidence that indicates a narrow transitional zone (e.g. Robinson & Wood, 1998), the depth at which the phase transformation occurs is still unclear (e.g. Robinson & Wood, 1998; Klemme & O'Neill, 2000; Presnall et al., 2002). Furthermore, the thickness of the transition zone was recently shown to be greatly dependent on the Cr content (Klemme, 2004), which is not well constrained for the oceanic lithospheric mantle. Consequently, results for this transitional zone are subject to unquantifiable uncertainties.

3.5 V_P anomalies, geoid anomalies, and elevation

Recent numerical algorithms integrate thermal regime and regional observables such as gravity, geoid and elevation in modelling the lithospheric structure (e.g. Zeyen et al., 2002; Fernàndez et al., 2004a, 2004b). The density of the lithospheric mantle and its temperature dependence through the CTE are key parameters linking the equations that describe the lithosphere. The variations of CTE values with composition/age of the lithospheric mantle can have noticeable effects on the calculated elevation and geoid height, and hence on the lithospheric thickness obtained from these integrated lithospheric models. On the other hand, the effect on the gravity anomalies will be almost

negligible due to the $1/r^2$ dependence of the gravity field, where r is the distance to the density anomaly. These effects can be quantified in a simple manner by calculating variations in elevation, geoid height, and V_P anomalies relative to a reference model with a typical constant value of $3.5 \times 10^{-5} \text{ K}^{-1}$ for the CTE.

In an Archean lithosphere whose mantle extends from a depth of 40 km down to 180 - 220 km, differences of $\Delta E \sim 270 - 348 \text{ m}$ and $\Delta N \sim 6 \text{ m}$ relative to the standard model are obtained for topographic elevation and geoid height, respectively. In Phanerozoic lithosphere, variations are much less evident, yielding $\Delta E \lesssim 30 \text{ m}$ and $\Delta N \sim 0.24 \text{ m}$. For the oceanic domain (water-unloaded), differences of $\Delta E \sim -38 \text{ m}$ and $\Delta N \sim -0.15 \text{ m}$ are obtained for the case of a young lithosphere ($\lesssim 20 \text{ Ma}$), and $\Delta E \sim 22 \text{ m}$ and $\Delta N \sim 0.2 \text{ m}$ for an old lithosphere ($\sim 100 \text{ Ma}$). These differences are related to variations in the average lithospheric mantle density as a consequence of the P, T dependence of the CTE. Estimated average density anomalies for the lithospheric mantle are 6.2 kg m^{-3} for Archean lithosphere; 1.0 kg m^{-3} for Phanerozoic lithosphere; -2.9 kg m^{-3} for young oceanic lithosphere; and 0.9 kg m^{-3} for old oceanic lithosphere.

Similarly, variations in the travel time of P-waves can be estimated by comparing the obtained V_P values (Fig. 3.14) with those predicted by the PREM model (Dziewonski & Anderson, 1981). For an Archean lithosphere in the depth range between 40 and 220 km, the average calculated P-wave velocities from our model are about 3 % higher than those from the PREM model. Such significant residuals are in agreement with global V_P tomography studies, which show deviations of up to + 3 % in cratonic regions (e.g. Zhou, 1996). Shear wave tomography also displays deviations of up to + 6 % beneath ancient continental lithosphere (e.g. Ritsema & van Heijst, 2000; Villaseñor et al., 2001), which result in V_P anomalies of $\sim 4\%$ if we consider that $d \ln V_S / d \ln V_P \sim 1.5$ for the first 220 km (Bolton & Masters, 2001). The P-wave velocities obtained from our model are higher than those proposed by O'Reilly et al. (2001) for Archean lithospheres at

100 km depth (8.18 km s^{-1}), inferred from the same mineralogical composition used in this chapter, but applying a different model for aggregates. However, this value is rather low if we consider that the PREM model proposes a velocity of 8.07 km s^{-1} at this depth, which results in an increase of only $+ 1.3 \%$. Actually, deep seismic profiling data show P_n values of $8.25 - 8.35 \text{ km s}^{-1}$ beneath the Baltic Shield and the East European Platform (e.g. Kozlovskaya et al., 2002; Grand et al., 2002) and P-wave velocities of up to $8.5 - 8.7 \text{ km s}^{-1}$ in the range of $125 - 200 \text{ km}$ depth beneath the Fennoscandian Shield (Ansorge & Mueller, 1995), although these estimations are likely affected by anisotropy or dunitic/eclogitic compositions (E. Kozlovskaya, pers. commun.). Differences between the predictions of the present model and the PREM model are drastically reduced to $\pm 0.3 \%$ for Phanerozoic and oceanic lithospheres.

3.6 Discussion

In this section, I evaluate possible error margins affecting the results as a consequence of seismic attenuation and uncertainties in experimental data and temperature.

3.6.1 Attenuation effects

The methodology for calculating the elastic properties of composites introduced in Section 3.2 relies on the assumption that both the fibre ends and the interface along the fibre length are perfectly bonded to the matrix, and therefore the system is considered an elastic medium. Models that include debonding and “weak” interfaces have been developed based on the shear lag model, as well as on other models (e.g. Yoda et al., 1978; Starink & Syngellakis, 1999; Li et al., 1999). They indicate that the average properties of the composite are noticeably dependent on both the physical properties of the interface and the magnitude and frequency of the applied stress. However, when the properties of

the interface are not markedly different from those of the phases, and when the magnitude and frequency of the applied stress are relatively small and high, respectively, the effect of debonding is unimportant (Hull & Clyne, 1996; Starink & Syngellakis, 1999). Applied to seismic wave propagation, the assumption of no sliding between phases implies that anelastic effects such as grain boundary sliding are neglected. In the present context, the model is requested to be valid at relevant seismic frequencies ($0.01 < f < 1$ Hz) and at pressure and temperature ranges adequate for the lithospheric mantle, specifically between $\sim 0.5 - 6$ GPa, and $200 - 1300$ °C, respectively. In this section, I show that physical attenuation (represented in terms of the specific quality factor Q) due to anelastic effects is not a significant factor when calculating P-wave velocities in the lithospheric mantle.

Many studies on the attenuation of seismic waves due to anelasticity have been carried out in the last 30 years (e.g. Kanamori & Anderson, 1977; Minster & Anderson, 1981; Karato, 1993; Gribb & Cooper, 1998; Jackson et al., 2002; Faul et al., 2004, and references therein). In summary, the most relevant conclusions concerning the lithospheric mantle are: (a) at seismic frequencies $0.01 < f < 10$ Hz and temperatures < 1000 °C, mantle assemblages are essentially elastic; (b) losses in shear are much more important than in compression (i.e. $Q_K \gg Q_G$); (c) Q is weakly dependent on frequency in the wide range $0.001 < f < 1$ Hz; and (d) under the reasonable assumption of $Q_K^{-1} \sim 0$, then $Q_P = 9/4 Q_S$. All of the above results indicate that our calculations of P-wave velocities ought to be correct up to temperatures of ~ 1000 °C, which encloses much of the thermal lithosphere, and that between 1000 and 1300 °C they are much less affected by anelasticity than S-wave velocities. When Q is considered to be slightly frequency-dependent, the phase velocity of P-waves is related to Q_P as (Minster & Anderson, 1981; Karato, 1993)

$$V_P(T_o, T) = V_{P_o}(T) \left[1 - \left(\frac{1}{2} \right) \cot \left(\frac{\pi \alpha}{2} \right) Q_P^{-1}(T_o, T) \right] \quad (3.71)$$

where V_{P_o} is the unrelaxed high frequency wave velocity at a given temperature, T_o the oscillation period, and α a constant with values between 0.2 - 0.3. In the range $1000 < T < 1300$ °C, the Q_s^{-1} for olivine can be adequately represented by

$$Q_s^{-1} = A [T_o d^{-1} \exp(-E/RT)]^\alpha \quad (3.72)$$

where d is the grain size, $A = 750 \text{ s}^{-\alpha} \mu\text{m}^\alpha$, $\alpha = 0.26$, $E = 424 \text{ kJ mol}^{-1}$, and R the universal gas constant (e.g. Jackson et al., 2002). Substituting Eq. (3.72) into Eq. (3.71) using the relation in (d), I finally obtain for P-waves

$$V_P(T_o, T) = V_{P_o}(T) \left\{ \left[1 - \left(\frac{2}{9} \right) \cot \left(\frac{\pi \alpha}{2} \right) A [T_o d^{-1} \exp(-E/RT)]^\alpha \right] \right\} \quad (3.73)$$

Eq. (3.73) can be used to estimate anelastic effects on P-waves in the temperature range $1000 < T < 1300$ °C. Fig. 3.15 shows the absolute error in velocity calculations for various representative values of oscillation periods T_o (1 - 100 s). It is clear that for common values of attenuation and seismic frequencies the majority of the data lies well below the value of 0.6 %. Only for extreme values of Q_p and frequencies of ~ 100 and ~ 0.001 Hz, respectively, Eq. (3.73) predicts maximum absolute errors of ~ 1 % for P-wave velocities calculated without considering anelasticity. Furthermore, these figures are considered to be upper limits due to the influence of pressure on Q_p , which tends to reduce physical attenuation (e.g. Jackson et al., 2002).

Therefore, it is concluded that anelastic effects are not an important factor controlling the quality of the results for P-wave velocities in the lithospheric mantle as predicted by the present model. It should be emphasized, however, that this conclusion applies only to the uppermost mantle (i.e. lithospheric and shallow sublithospheric mantle), and it should not be generalized to the whole upper mantle. Seismic attenuation is a strong non-linear function of temperature, and can be a significant factor at sublithospheric temperatures (Karato, 1993).

3.6.2 Uncertainties in experimental mineral data and temperature

Any attempt to estimate the bulk properties of a multiphase aggregate as a function of the individual properties of its constituents is subject to significant, and often unquantifiable, uncertainties (e.g. Everett & Arsenault, 1991; Hull & Clyne, 1996). The most important factors controlling the estimations of CTE and P-wave velocities for the lithospheric mantle can be grouped in two different categories: *intrinsic* (i.e. associated with the model and its assumptions) and *extrinsic* (i.e. related to the input data). Intrinsic effects are mainly due to the averaging technique used in estimating both elastic parameters and CTE. Since it is virtually impossible to obtain analytical solutions that include all possible interactions, heterogeneities, and spatial distribution of each phase and of the aggregate, many simplifications have to be made. However, applying well established physical concepts and suitable combinations of them, the bulk properties of the composite can be approximately evaluated and compared to experimental data to test the validity of the model (cf. Everett & Arsenault, 1991; Hull & Clyne, 1996; see also Ji et al., 2003 for a discussion on errors). Extrinsic factors are more important in the present context for two major reasons: (a) they control the behaviour of the phases due to temperature and pressure changes, and therefore the final properties of the aggregate; and (b) there is no control on them, and consequently they cannot be modelled

accurately. Foremost among these factors are the uncertainties in experimental mineral data and in the chosen geotherm.

Laboratory measurements of elasticity and volumetric CTE of mantle relevant minerals have been actively investigated and detailed compilations of elastic moduli, CTE, and their pressure and temperature derivatives are available in the literature (e.g. Anderson, 1988; Fei, 1995; Bass, 1995; Knittle, 1995; Chopelas, 2000; Schutt & Leshner, 2006). Although experimental errors in single crystals are thought to be negligible, and the isotropic moduli for the same mineral are reasonably consistent among different sources, their temperature and pressure first and second derivatives still exhibit some discrepancies among different authors (e.g. Bass, 1995; Fujisawa, 1998; Zha et al., 1998). Similarly, values of CTE and its derivatives in the literature vary as much as ~ 40 and 10% , respectively, for the same mineral (e.g. Saxena & Shen, 1992; Fei, 1995). This scatter in data is difficult to evaluate objectively, since discrepancies are different for different minerals, and possible combinations are unassessable. However, considering the spectrum of values given for these parameters, a sensitivity analysis indicates that calculations of CTE and P-wave velocities may be affected by experimental uncertainties as much as ± 8 and $\pm 0.8\%$, respectively. Refined estimations of elastic parameters for relevant mantle mineral series of complex composition (e.g. pyroxenes and garnet) at lithospheric conditions (e.g. by computational simulations) are still necessary to reduce uncertainties on theoretical estimations.

Uncertainties in the thermal field of a particular region also affect the final results due to the temperature dependence of mineral properties. Usually, errors associated with stable Archean lithosphere are less important than in Phanerozoic terranes, where surface heat flow can vary between < 50 to $> 90 \text{ mW m}^{-2}$ (Artemieva & Mooney, 2001) and the steady-state condition not always applies. Hence, for an assumed discrepancy of $\sim 100^\circ\text{C}$ in geotherms in deep portions of Archean lithosphere, variations of CTE and

P-wave velocities as predicted by our model are unlikely to be more than ± 2 and ± 0.4 %, respectively. In Phanerozoic regions, the range of possible geotherms and associated uncertainties are more important, leading to a greater uncertainty in calculated CTE and P-wave velocities.

As an example of the variability on the results due to changes in geotherms, Fig. 3.16 shows the variation of CTE and P-wave velocity of an average Phanerozoic peridotite (Table 3.4; Poudjom-Djomani et al., 2001) for a range of realistic geotherms. The spectrum covered by the two mantle geotherms with gradients ~ 17 and 10 $^{\circ}\text{C km}^{-1}$ should not be directly correlated with uncertainties in a particular geotherm; it only indicates realistic bounds for possible Phanerozoic geotherms. It can be seen that in the case of seismic velocities, the variation due to the combined effect of temperature and pressure makes the iso-velocity lines to be almost parallel to the geotherms (Fig. 3.16A). This implies that P-wave velocities should not vary considerably with depth in Phanerozoic lithosphere for a given geotherm, consequently reducing the variability associated with uncertainties in the thermal field. Assuming a rather high uncertainty of $\sim \pm 15$ % for a given geotherm, estimation of P-wave velocities should be within the error margins of ± 0.6 %. In the case of the CTE, iso-CTE lines have a smaller dT/dP value than iso-velocity lines, indicating that the pressure effect is slightly less important (Fig. 3.16B). Since uncertainties in lithostatic pressure are smaller than in temperature for a given geotherm, this change in the slope of iso-CTE lines assigns a somewhat wider error margin to CTE estimations in comparison with P-wave velocities. Assuming the same previous uncertainty for the geotherm, CTE values can be affected by $\sim \pm 3$ %, which translates into a possible CTE variations of $\pm 0.1 \times 10^{-5} \text{ K}^{-1}$.

Following the same procedure, errors for old oceanic lithosphere (> 100 Ma) are found to be in the range of ± 0.5 and ± 2 % for P-wave velocity and CTE, respectively. In the case of young oceanic lithosphere (< 20 Ma), uncertainties in the thermal field are

the greatest due to hydrothermal circulation in the oceanic crust, and therefore results for P-wave velocities and CTE are expected to be subjected to errors $> \pm 1.5$ and ± 3 %, respectively.

An additional extrinsic source of error results from the average composition chosen to represent a particular lithospheric mantle. I have used average compositional estimations from xenoliths data thought to be representative of the lithospheric domains (Table 3.4), which may not be accurate for all cases. However, a formal error analysis is not possible in this case due to the scarcity of detailed information.

The uncertainties discussed above have significant implications on tomography studies. They suggest that errors associated with experimental data and thermal fields can result in velocity anomalies that are comparable to those obtained in seismic tomography (e.g. Zhou, 1996; Vasco et al., 2003). Therefore, even excluding errors induced by the uncertainties on velocity measurements, tomography studies cannot be used to resolve unambiguously compositional heterogeneities in lithospheric domains with P-wave anomalies $\lesssim 1.5$ % (i.e. S-wave anomalies $\lesssim 3\%$, assuming $d\ln V_S/d\ln V_P \sim 1.5$; Bolton & Masters, 2001). Similar results were recently obtained by Artemieva et al. (2004) using global correlation coefficients for attenuation, shear velocity, and thermal structure in the continental upper mantle. It is desirable therefore to integrate the modelling of geoid and gravity anomalies, absolute elevation, and thermal structure with seismic and xenolith information to better constrain possible major compositional variations in the lithospheric mantle. This is the purpose of the next two Chapters.

Table 3.1: Elastic properties of constituent phases of two-phase composites

Composite	Matrix	Fibre	E_m [GPa]	E_f [GPa]	ν_m	ν_f
Al-SiC	Aluminium	SiC	70	450	0.34	0.22
WC-Co	Cobalt	WC	207	700	0.31	0.19
Dental comp.	Resin	Silica	4	77.2	0.35	0.25
Epoxy-Silica	Epoxy	Silica	2.1	94	0.4	0.25
Glass-tungsten	Glass	Tungsten	81	355	0.2	0.24
Polymer-glass	Polymer	Glass	1.69	70.3	0.44	0.21
FEM			1	20	0.3	0.3
KCl-NaCl	KCl	NaCl	24	36.5	0.25	0.25
Fo-En	Forsterite	Enstatite	186.8	206.5	0.21	0.22

See Fig. 3.3 for references

Table 3.2: Modal compositions (vol%) and Young's moduli for the tested rocks

Rock	Composition	E(GPa) ^a
<i>Peridotite</i> ^b S1-S3-S32 (at 0.6 GPa)	Ol (73 %)	197.2
	Opx (21 %)	187.2
	Cpx (6 %)	167
<i>Harzburgite</i> ^b BD1675 (at 1 GPa)	Ol (60 %)	201.2
	Opx (24 %)	190
	Serp (16 %)	43.2 ^c
<i>Charnockite</i> ^b A2 (at 0.4 GPa)	Fsp (64 %)	96.9
	Qz (30 %)	95.6
	Opx (6 %)	186
<i>Eclogite</i> ^b XG 98-15 (at 0.6 GPa)	Cpx (50 %)	167
	Grt (42 %)	243
	Mica (8 %)	90

^a Calculated from data in Bass (1995)

^b From database in Ji et al. (2002)

^c Calculated from a rock sample with 98% chrysotile and lizardite (Christensen, 1979)

Table 3.3: Thermodynamic parameters of relevant minerals (symbols defined in the text)

	a [10 ⁻⁵ K ⁻¹]	b [10 ⁻⁸]	c	d ^a	$K_{0(T,r,0)}$ [GPa]	$\rho_{(T,r,0)}$ [kg m ⁻³]	$\left(\frac{\partial K_0(T,0)}{\partial T}\right)_P$ [MPa K ⁻¹]	$K'_{(T,0)}$	δ_T
Ol Fo ₉₀	2.37	1.26	1.207x10 ⁻³	-0.465	129.43	3350	-20.0	4.2	5.5
Ol Fo ₉₁	2.37	1.26	1.207x10 ⁻³	-0.465	129.43	3335	-20.0	4.2	5.5
Ol Fo ₉₂	2.26	1.3	1.33x10 ⁻³	-0.427	129.43	3326	-20.0	3.8	5.5
Ol Fo ₉₃	2.26	1.3	1.33x10 ⁻³	-0.427	129.43	3310	-20.0	3.8	5.5
Opx En ₉₀	2.947	0.2694	-0.5588		107.8	3305	-20.0	5	5.5
Opx En ₉₁	2.947	0.2694	-0.5588		107.8	3296	-20.0	5	5.5
Opx En ₉₂	2.947	0.2694	-0.5588		107.8	3288	-20.0	5	5.5
Opx En ₉₃	2.947	0.2694	-0.5588		107.8	3280	-20.0	5	5.5
Cpx (Diopside)	3.33	0.269	-0.559		114	3345	-20.0	4.5	5.5
Spinel	2.94	0.975	-0.365		207	3760-3900 ^b	-20.0	5	5.5
Grt (pyrope-rich)	2.311	0.5956	-0.4538		169.4	3720-3766 ^c	-20.0	4	5.5

	K_s [GPa]	G [GPa]	$\frac{\partial K_s}{\partial P}$	$\frac{\partial K_s}{\partial T}$ [MPa K ⁻¹]	$\frac{\partial G}{\partial P}$	$\frac{\partial G}{\partial T}$ [MPa K ⁻¹]	c_p [J kg ⁻¹ K ⁻¹] ^g	c_v [J kg ⁻¹ K ⁻¹] ^g
Ol Fo ₉₀	129.5	77.6	4.56	-18	1.71	-13.6	838	838
Ol Fo ₉₁	129.5	77.6	4.56	-18	1.71	-13.6	838	838
Ol Fo ₉₂	129.4	79.1	5.13	-16.9	1.79	-13.8	838	838
Ol Fo ₉₃	129.4	79.1	5.13	-16.9	1.79	-13.8	838	838
Opx En ₉₀	107.8	75.7	9.6	-26.8	2.06	-11.9	780	780
Opx En ₉₁	107.8	75.7	9.6	-26.8	2.06	-11.9	780	780
Opx En ₉₂	107.8	75.7	9.6	-26.8	2.06	-11.9	780	780
Opx En ₉₃	107.8	75.7	9.6	-26.8	2.06	-11.9	780	780
Cpx (Diopside)	114	64.9	4.6 ^d	-24 ^e	2 ^e	-11 ^e	780	780
Spinel	196.7	108.3	5	-15.7	1.7 ^f	-9.4	760	760
Grt (pyrope-rich)	171.2	92.6	4.93	-19.5	1.56	-10.2	760	760

^a This parameter is used only for olivine, whose CTE is calculated with $\alpha(T) = a + bT + cT^{-1} + dT^{-2}$ (Suzuki et al., 1998).

^b The density of spinel varies considerably with Cr and Fe contents. The density is changed accordingly in each particular case.

^c Same as with spinel.

^d Assumed to be equal to $\frac{\partial K_0}{\partial P}$, from Knittle (1995).

^e Assumed values (Knittle, 1995).

^f From other spinel structured oxides (Knittle, 1995).

^g Average values taken from Schubert et al. (2001).

Table 3.4: Modal compositions (vol%) of Archean, Phanerozoic continental, and oceanic lithospheres

Lithosphere	Olivine	Orthopyroxene	Clinopyroxene	Garnet	Spinel
Archean	62 (Fo ₉₂₋₉₃)	30	3	5	
Phanerozoic	60 (Fo ₉₀)	17	15	8	
Oceanic (< 2 GPa)	73.5	21	5		0.5
Oceanic (> 2 GPa)	74	19.4	5	1.6	

Estimates are based on several works cited in Chapter two.

Figure 3.1: Schematic drawing of the unit cell and coordinate axes used for analyzing the stress transfer between the matrix and the short fibre (shaded). Dashed cylindrical volumes represent the imaginary fibres added to analyze the stress transfer at the fibre ends

Figure 3.2: Normalized axial and shear stresses predicted by Eqs. (3.17) - (3.27) for $E_f / E_m = 10$, and $V_f = 0.15$ as a function of the normalized axial distance from fibre midpoint. σ_f and τ_f are the axial and shear stresses in the real fibre and at its interface, respectively. σ_{ff} and τ_{ff} are the axial and shear stresses in the matrix region (i.e. fictitious fibre).

Figure 3.3: Experimentally determined Young's moduli of various two-phase composites (E_c) compared to predicted values using Eq. (3.38) (solid line). V_f is the volume fraction of the fibre. Also included are predictions from equations presented by Taya & Arsenault (1989) (dashed-dotted line), R-V-H (dashed line), Starink & Syngellakis (1999) (dotted line), and Ji & Wang (1999) (dashed-dotted-dotted line). Experimental data (black dots) compiled from different sources cited in Afonso and Ranalli (2005a) and Afonso et al. (2005). Elastic properties of constituent phases are listed in Table 3.1.

Figure 3.4: Comparison of predicted and experimentally determined Young's moduli of particulate reinforced Al-SiC composites, using various models. Eq. (3.38) with $s = 1.5$ (thick solid line) gives the best predictions, almost identical to those by Eshelby model, not included in the figure for clarity.

Figure 3.5: Scheme of a “real” three-phase composite (A) and of the mechanical equivalent (B) used to calculate Young’s modulus of a three-phase composite.

Figure 3.6: Comparison of predicted and measured P-wave velocities as a function of the volume fractions of different minerals. In all cases, the volume fraction of the matrix is maintained constant while the volume fraction of the phases are changed continuously (see Table 3.2). Solid lines are the predictions of the model using Eqs. (3.38), (3.51), and (3.56). Dashed lines are R-V-H averages. Black dots represent experimental data. Ae is the absolute error %, calculated as $\frac{|V_{\text{predicted}} - V_{\text{measured}}|}{V_{\text{measured}}} \times 100$. In all the cases, the three main constituents comprise $> 98\%$ of the sample.

Figure 3.7: Variation of Young's modulus of a composite of alumina platelets in a mullite matrix as a function of the "soft" surrounding phase volume fraction. The solid line represents predictions from Eqs. (3.38) and (3.51). Dashed line represents predictions by the R-V-H method. The black dot is the intersection between the experimental measurement and theoretical estimation.

Figure 3.8: Comparison of predicted and measured Young's moduli in concrete samples as a function of the ITZ volume fraction. Solid lines are predictions from Eqs. (3.38) and (3.51). Dotted lines are predictions by the R-V-H method. Black dots represent the intersection between measured values and theoretical predictions by the present model. The projection on the horizontal axis gives the expected volume fraction for the ITZ. The projection of the crosses on the horizontal axis gives the predictions of the R-V-H method.

Figure 3.9: P/K_0 as function of ρ/ρ_0 for the Eulerian Birch-Murnaghan and logarithmic EoS (assuming $K'_0 = 4$). For relatively small compressions ($\rho/\rho_0 < 1.5$) both EoS predict identical results for the range $3.5 < K'_0 < 5$.

Figure 3.10: Melt density versus depth for a pyrolitic mantle with a potential temperature $T_p = 1300$ °C.

Figure 3.11: Variation of the CTE with temperature and pressure for olivine, orthopyroxene, and garnet. Solid lines indicate only the temperature dependence of CTE. Dashed lines include the pressure effect calculated from Eq. (3.68) assuming a continental Phanerozoic type geotherm (Fig. 3.12). Parameters used in calculations are listed in Table 3.3.

Figure 3.12: Type geotherms for the three lithospheric domains considered in this chapter (modified from Afonso & Ranalli (2004)).

Figure 3.13: Variation of the CTE with depth for Archean, Phanerozoic continental, and oceanic lithospheric domains. Solid lines: predictions from the model; dashed-dotted lines: polynomial approximations given in Section 3.4; dashed lines: type geotherms. Temperature refers only to the geotherms. Note the different scale for the CTE used in the Archean (A).

Figure 3.14: Variation of the P-wave velocity with depth for Archean, Phanerozoic continental, and oceanic lithospheric domains. Solid lines: predictions from the model; dashed lines: type geotherms. Note the different horizontal scale used in the Archean (A).

Figure 3.15: Absolute errors (Ae) in P-wave velocity calculations as a function of period T_o in the temperature range $1200 < T < 1300$ °C. The error is a measure of the departure of P-wave velocities from elastic behaviour due to anelasticity effects (seismic attenuation) above temperatures of ~ 1000 °C. For representative values of T_o (1 - 100 s), the absolute error is always well below 0.6 %, which represent maximum deviations of $+0.05 \text{ km s}^{-1}$.

Figure 3.16: P-wave velocity and CTE as functions of temperature and pressure for a peridotite with $\text{Fo}_{90} = 60\%$, $\text{Opx} = 17\%$, $\text{Cpx} = 15\%$, and $\text{Grt} = 8\%$ (Phanerozoic, Table 3.4). Solid lines are predictions from the model; numbers on lines indicate P-wave velocities in km s^{-1} (A) and CTE values in 10^{-5} K^{-1} (B). Thin dashed lines denote unrealistic values for extreme cold/hot geotherms. Thick dashed lines represent possible end members of Phanerozoic mantle geotherms (almost linear due to the low radiogenic heat production). Uncertainties of $\pm 15\%$ in any given geotherm within the shaded areas result in variations of $\leq \pm 0.05 \text{ km s}^{-1}$ ($\leq \pm 0.6\%$) and $\sim 0.1 \times 10^{-5} \text{ K}^{-1}$ ($\pm 3\%$) in P-wave velocities and CTE, respectively.

CHAPTER 4

Combined Geophysical - Petrological Modelling of the Lithosphere: LitMod

4.1 Introduction

This chapter is devoted to present the new finite-element code LitMod and the concepts behind it, which will be used throughout the rest of this thesis. This new code permits to perform an integrated geophysical - petrological modelling of 2-D lithospheric/sublithospheric cross-sections from the surface down to depths of ~ 300 km. The code solves simultaneously the heat transfer, thermodynamical, geopotential, isostasy, and rheological equations for a particular lithospheric structure with any given composition, and yields density, thermal and seismological structure, surface heat flow (SHF), rheological strength, gravity anomalies, elevation, and geoid height. The approach used in LitMod integrates mineral physics, geochemical, petrological, and geophysical data. Compressibility, partial melting, and compositional heterogeneities are also included. Elevation is estimated self-consistently with a new approach that permits us to distinguish between lithospheric and sublithospheric buoyancy contributions, assuming that individual columns are locally compensated within the upper mantle. In this way, real transects and/or purely synthetic models can be modelled (Chapter 5). Predictions of geophysical observables are used in both cases to control the reliability of the proposed model. In particular, when modelling real transects, a forward approach (i.e. trial-and-error) is used in which differences between predictions and observed values are minimized in each run. The final result is a lithospheric model that simultaneously fit all available observables. This approach reduces the uncertainties associated with the modelling of each of these observables alone, or with the combinations of pairs commonly used in the literature. It also allows us to distinguish, and have a better control on, density variations at different depths, since these observables are differentially sensitive to shallow/deep density anomalies.

4.2 Methodology and previous code

LitMod is based on the previous finite-element code CAGES, originally developed by Zeyen and Fernández (1994). This code is a collection of FORTRAN77 subroutines, which has been tested and applied to many lithospheric transects (e.g. Zeyen & Fernández, 1994; Zeyen et al., 2002; Fernández et al., 2004a, 2004b; Zeyen et al., 2005), demonstrating its reliability. The approach used by CAGES to calculate the thermal structure, SHF, and gravity/geoid anomalies is kept in LitMod with slight modifications. However, the methods to estimate the elevation, seismic velocities, density structure, total strength, and temperature-pressure-composition-dependent parameters such as the coefficient of thermal expansion, α , and thermal conductivity, k , are all new or significantly modified.

LitMod divides the lithospheric section into triangular elements that make up the different bodies used in the model, and calculates heat flow, temperature, density, seismic velocities, and lithostatic pressure at each node of the mesh. The mesh is automatically adjusted to fit the geometry of the different bodies. Each body (commonly including only one type of lithology) in the model is characterized by its own set of thermophysical parameters: thermal conductivity tensor, volumetric heat production rate, friction coefficient, density, etc. Although LitMod allows anisotropy in the thermal conductivity tensor, it will be usually considered isotropic (i.e. scalar), unless indicated otherwise. The volumetric heat production rate is assumed here to be a constant for each body, since it is mainly a function of lithology (e.g. Kukkonen & Lahtinen, 2001). The relative effects of temperature and pressure on density are taken into account either through the coefficient of thermal expansion or by solving the full set of EoS for each material (see Section 3.3, Chapter 3). The crust is usually modelled with different bodies that account for the assumed different lithologies (e.g. granitic upper crust, granulitic lower crust, etc.). Since temperature and pressure variations within these bodies do not affect

their densities considerably, constant density values are usually assigned. The latter is not true for sediments (more compressible) and for the lithospheric mantle, where an explicit dependence on temperature and pressure is always assumed (see Section 4.4.1).

A preliminary version of LitMod is available from the author upon request.

4.3 Heat transfer equation

In accordance with the discussion in Section 3.3.1 of Chapter 3, the following algorithm assumes steady-state conditions and neglects advective processes. Under these conditions, the 2-D temperature distribution in the lithosphere is described by the conductive heat transfer equation (Carslaw & Jaeger, 1959)

$$\nabla \cdot (-k \nabla T) - A(x, y) = 0 \quad (4.1)$$

where T is temperature [$^{\circ}\text{C}$ or K], k the thermal conductivity [$\text{W m}^{-1} \text{K}^{-1}$], A the volumetric heat production rate [W m^{-3}], and x, y , Cartesian spatial coordinates. The steady-state assumption applies to all the modelled transects, and it will be discussed in more detail in the next section for each particular case.

For the temperature dependence of k in the mantle, Hofmeister's model (Hofmeister, 1999) is assumed. The numerical implementation follows the relations

$$k_{(T)} = \frac{b}{1 + cT} \quad ; \quad T < 550 \text{ }^{\circ}\text{C} \quad (4.2a)$$

$$k_{(T)} = \frac{b}{1.5 + dT} \quad ; \quad T > 550 \text{ }^{\circ}\text{C} \quad (4.2b)$$

where $b = 5.3$, $c = 1.5 \times 10^{-3}$, and $d = 5.5 \times 10^{-4}$. These relations differ from the original model of Hofmeister (1999) by less than one standard deviation of the experiments, and are almost identical to the expression adopted by McKenzie et al. (2005). Fig. 4.1 shows a comparison between the different models. It can be seen that values predicted by Eq. (4.2b) are slightly overestimated with respect to the other two models. This is done here to simulate the higher conductivities of pyroxenes and the radiative contribution (Hofmeister, 1999), although the uncertainties on these effects are still quite large. For thick lithospheres (> 180 km), where the pressure effect start to offset the temperature dependence, Eq. (4.2b) is sometimes replaced by the expression given by Jaupart and Mareschal (1999) for thick cratonic lithospheres, which accounts for both lattice conduction and radiation and takes the following form

$$k_{(T)} = \frac{1.0}{0.174 + 0.000265 T} + 0.368 \times 10^{-9} T^3 \quad (4.2c)$$

The behaviour of Eq. (4.2c) with temperature is also plotted in Fig. 4.1.

Equation (4.1) is solved with the finite-element technique using the Galerkin's ponderation method (e.g. Zienkiewicz, 1977), subject to the following boundary conditions:

- (a) Fixed temperature at the surface of the model.
- (b) No heat flow across the sides of the model.
- (c) Fixed temperature at the bottom of the model.

Generally, the choice of the surface temperature, T_o , is straightforward. Changes of the order of 20°C in T_o do not affect the results significantly. Here, I assume a value of 0°C when the whole section is underwater, and 10°C when all of it is above sea

level or when it contains both underwater and subaerial sections (e.g. passive margins). The second boundary condition is widely used in thermal modelling and it requires no further explanation. The third boundary condition, however, is not always obvious and needs some discussion.

Clearly, the value for the assumed basal temperature of the model will depend on its thickness. Since the goal is not only the modelling of the lithosphere, but also of the sublithospheric domain, typical pyroxene thermobarometry on peridotite xenoliths is not very useful. Instead, estimations from high-pressure and high-temperature experiments on mineral phase equilibria (cf. Fei & Berkta, 1999) need to be used. At the same time, the present model cannot be expected to be reliable at depths (pressures) greater than ~ 300 km (10 GPa), since the orthopyroxene gradual transformation to Ca-poor clinopyroxene is completed at about 10 GPa (Takahashi & Ito, 1987; Irifune & Isshiki, 1998; Fei & Berkta, 1999), changing the assumed four-phase composition for the sublithospheric domain (see Section 2.2.2 in Chapter 2). The study by Ito and Katsura (1989) is of particular interest here, since it gives a temperature estimation at 350 km, based on phase equilibria of olivine-wadsleyite / wadsleyite-ringwoodite (spinel) in the system Mg_2SiO_4 - Fe_2SiO_4 . Their results have been widely used in the literature as a pressure calibration point for multi-anvil apparatus, and they have been also qualitatively confirmed by several more recent quenching experiments (Fei & Berkta, 1999) and ultrasonic interferometry/x-ray diffraction experiments in wadsleyite samples (Li et al., 2001). Ito and Katsura (1989) give an estimation of 1400 °C at 350 km and of 1600 ± 100 °C at 655 km. Although these authors do not provide the uncertainties associated with the former value, we can attempt to give a probable range based on the factors that affect the estimation, foremost among which are the extrapolation method used by Ito and Katsura (1989), and the dependence of the system on the Mg/(Mg+Fe) ratio (mg#). The first of these assigns a minimum uncertainty of ± 100 °C to the estimation at 350 km, since it is obtained from the value at 655 km by assuming constant adiabatic

gradient and heat capacity, and average volumes and enthalpies of transformation (Ito & Katsura, 1989). The second factor is known to have a strong effect on the transformation temperature and pressure (e.g. the end member Fe_2SiO_4 does not change to wadsleyite at all). However, there is strong evidence that the $\text{mg}\#$ for the upper mantle is relatively constant and close to 0.89 (e.g. Ito & Katsura, 1989; McDonough & Sun, 1995; Fei & Bertka, 1999; Griffin et al., 1999b; Poudjom-Djomani et al., 2001; Kushiro, 2001). Therefore, following the results of Fei and Bertka (1999), a variation of ± 0.1 in the $\text{mg}\#$ should translate in an uncertainty $< \pm 100$ °C. From the above, the propagation of the uncertainty in the estimation of temperature at 350 km should be of the order of ± 120 °C.

In summary, a basal temperature value of $\sim 1400 \pm 100$ °C for models with a maximum depth of 300 km seems to be a reasonable option. This is also consistent with estimation of potential temperatures at MORs (e.g. McKenzie & Bickle, 1988; Langmuir et al., 1992; Asimow et al., 2001; Kushiro, 2001). It is worthy of note that whatever value is chosen, it must be consistent with other lines of evidence (e.g. seismic velocities, geopotential field, elevation, etc).

Once the basal temperature is chosen, an adiabatic gradient is simulated for the sublithospheric mantle by controlling the value of its thermal conductivity. In the simplest case, an infinitely high k can be chosen to force an isothermal sublithospheric domain. However, in most cases I will choose a value for k that gives a typical average gradient of $0.3 - 0.4$ °C km^{-1} . To avoid unrealistic peaks on the geotherm at the base of the lithosphere, a “buffer body” is applied between the lithospheric and sublithospheric domains with the composition of the latter. This body plays the role of forcing a continuous variation of temperature between the two domains. The physical meaning of it is that in a fluid with strongly temperature-dependent viscosity, convection is limited to a region of low viscosity (Zaranek & Parmentier, 2004). Below the rigid stagnant upper

part (i.e. lithosphere) there is a rheologically active thermal boundary layer where heat is transferred by both conduction and convection (i.e the subrheological boundary layer of Reese et al., 1999), where the geotherm becomes strongly curved. The region beneath this layer convects and is essentially adiabatic (e.g. Schubert et al., 2001). A typical thickness for this rheological boundary layer is $\lesssim 50$ km (see Chapter 6 and references therein).

4.4 Elevation

Local isostasy has been proven to be a suitable approximation in regions where short-wavelength, elastically supported features such as buried and/or topographic loads are not present (Turcotte & Schubert, 1982; Watts, 2001). Indeed, calculations always show a good long-wavelength correlation between the calculated and observed elevation in modelled real transects, which are also controlled by the fitting of the other observables (see next chapter). LitMod assumes therefore that isostatic equilibrium is reached by means of local isostasy, with the compensation level being at the base of the model.

In order to estimate the absolute elevation one needs to perform a calibration with respect to a reference column. I take this reference column at a mid-oceanic ridge (MOR), where average elevations, petrogenetic processes, and lithospheric structures are well known. The final formulae that LitMod solves to obtain the absolute elevation are similar to those in Lachenbruch and Morgan (1990), where the elevation above (E_a) and below (E_b) the sea level are given respectively by

$$E_a = \int_{L_{top}}^{L_{bottom}} \frac{\rho_b - \rho_l(z)}{\rho_b} dz - \Pi \quad (4.3)$$

$$E_b = E_a \frac{\rho_b}{\rho_b - \rho_w} \quad (4.4)$$

where L_{top} is taken at the top of the column, L_{bottom} is taken at the bottom of the column (i.e. at the model's maximum depth Z_{MAX}), ρ_b (assumed constant) is the density of the mantle at Z_{MAX} , $\rho_l(z)$ is the depth-dependent density, ρ_w is the density of seawater (constant), and Π is a system parameter. Although Eqs. (4.3) and (4.4) are formally identical to those in Lachenbruch and Morgan (1990), the meaning of some parameters are completely different and should not be confused. Eqs. (4.3) and (4.4) can be solved for any model if we know the form of the function $\rho_l(z)$ for every column, and the value of Π . In the following I will explain how to obtain these two input parameters.

4.4.1 Depth-dependent density

The depth-dependent density for each column is calculated following the approach presented in Chapter 3. First, a certain structure is defined, and the respective mineral compositions and thermodynamic parameters of the different materials are assigned. Once the temperature field is obtained, the code solves for the density at each node as follows:

- 1) For crustal bodies the density is calculated with the following formula

$$\rho_{(T,P)} = \rho_o - \rho_o \alpha (T - T_o) + \rho_o \beta (P - P_o) \quad (4.5)$$

where α and β are the coefficient of thermal expansion and compressibility, respectively.

- 2) For the different mantle domains the code solves the full set of EoS for each

material, as described in Chapter 3, in an iterative manner. The pressures at each node are calculated for every column from the surface to the bottom. In each iteration a new node is added and the updated overburden pressure is recalculated with the usual lithostatic equation

$$P = \overline{\rho_l(z)} g z \quad (4.6)$$

This pressure is then used to fit the EoS and to obtain the P-T-dependent density. This new density is then used in the next iteration to update the overburden pressure for the next node. This approach has been compared with one that uses an extra loop within each node, which iterates pressure and density until the difference between the pressures (and densities) obtained in the i -th and $(i-1)$ -th iterations is smaller than a threshold value (set at 0.1 MPa). No significant improvement in the final values of pressure and densities was achieved with this extra loop.

4.4.2 The parameter Π

In order to calculate the Π parameter, the average density, lithospheric structure, and the elevation of a reference column is required. Referring to Fig. 4.2, the mean density of the water-unloaded ridge column is

$$\rho_{ridge} = \frac{(Z_{comp} - Z_{crust}) \times \rho_{MR} + (Z_{crust} \times \rho_{crust})}{Z_{comp}} \quad (4.7)$$

Therefore, from Eqs. (4.3), (4.4), and Fig. 4.2 one can write

$$\Pi = Z_{MAX} - \frac{(\rho_{ridge} \times Z_{comp}) + (E_{ridge} \times \rho_w)}{\rho_b} \quad (4.8)$$

Eq. (4.8) shows that the Π parameter is the depth (from sea level) of a fictitious column of height H_f that has a density ρ_b as its mean density (Fig. 4.2). Π will change every time we modify the compensation depth, and hence, the mean density ρ_b . Because the latter also changes with depth, the overall effect of changing Π in the final elevation calculation is nil (i.e. Z_{MAX} and ρ_b counterbalance each other). This permits to choose different compensation depths for the same model and still obtain the same elevation, provided the new ρ_b and Π for that particular compensation depth are recalculated.

4.4.3 The ridge model

It is clear from the above discussion that the two most important inputs for calculating the elevation of our model are ρ_b (the basal density) and ρ_{MR} (the average density of the MOR, including crust and mantle). Both values can be obtained by modelling the density distribution with depth under a MOR, applying the concepts presented in Chapter 3. The choice of a reference column at a MOR is supported by the detailed knowledge of this particular tectonic setting (e.g. Phipps Morgan et al., 1992; Buck et al., 1998; Cann et al., 1999; German et al., 2004). These studies cover a wide spectrum of disciplines, from satellite bathymetric estimations to complex thermodynamic computational simulations. As a consequence, the MOR system is one of the best known tectonic environments, and probably also the best understood. Although the model presented in this section relies mostly on well-known data which represent an uncontroversial consensus within the scientific community (e.g. the existence of partial melting), it needs to be recognized that other necessary information may reflect only the actual state of knowledge (e.g. distribution of partial melting with depth).

There are six main factors that need to be taken explicitly into account when calculating the final density distribution with depth in a MOR column, namely (a) composition of the source (Primitive Upper Mantle), (b) solid phase compressibility, (c) melt compressibility, (d) total amount of partial melting (F), (e) depth-distribution of melt ($F(z)$), and (f) chemical variation of both solid and melt phases vs. degree of partial melting. The first factor was already discussed in detail in Chapter 2. Therefore, following the arguments presented there, it will be assumed that the major-element composition of the MORB source (i.e. sublithospheric mantle) can be approximated by the Primitive Upper Mantle (PUM) composition of McDonough and Sun (1995), which gives preferred modal compositions identical to the ones reported in Irifune and Isshiki (1998): Ol/Opx/Cpx/Gnt of 59/12/16/13. It will be shown that this modal composition predicts seismic velocities and densities that are in good agreement with those given by seismological models such as PREM (Dziewonski & Anderson, 1981) and *ak135* (Kennett et al., 1995). The second and third factors have been discussed in Chapter 3, and the same approach is used here to calculate P-T-dependent densities as a function of composition. The last three factors are closely related to each other, and therefore they can be estimated in a coherent manner by assuming a particular ridge model. In this respect, there are basically two classic end-member models that have been proposed to describe the flow regimes, melt extraction, and melt production at MORs: *passive models* and *active models*.

A *passive model* is one in which the flow beneath the MOR is driven by plate spreading alone, without internal buoyancy contributions. It is based on the classical solution of a corner flow, with off-axis streamlines that turn at depth (Fig. 4.3A). In this model, the base of the melting regime is represented by the mantle solidus, while the lateral boundaries of the melting regime are defined by where the mantle flows horizontally and no longer melts (the cooling of the plate results in a freezing front which is defined by the solidus of the material). Consequently, the melting zone has a general triangular shape,

with one of the apices coinciding with the ridge axis. The actual shape of the melting zone might vary slightly depending on the vertical flow velocity. However, as Langmuir et al. (1992) pointed out, different shapes lead to the same chemical characteristics for the lithosphere. During an increment of spreading, points on and/or outside the lateral boundaries move horizontally without experiencing any further melting. A point inside the triangular melting regime always has a vertical velocity component (greater close to the axis), and therefore it moves up and experiences an additional melting increment. The actual melting contours depend on various factors such as the chosen solidus, the melting function, $F(z)$, and the average mantle temperature below the solidus (i.e. “hot” mantle intersects the solidus at greater pressures than “cold” mantle). At steady-state, the residue of melting is represented by the column that emerges outside the melting regime (Fig. 4.3A), known as the *residual mantle column* (Langmuir et al., 1992). This column carries the information about the melting process, and therefore it can be used to estimate the *mean extent of melting*, $\bar{F}$, defined as the total amount of melt produced (F), divided by the total amount of mantle that has melted in one episode of spreading (Langmuir et al., 1992). In other words, $\bar{F}$ is the final volume fraction of melt after one spreading episode with respect to the original volume of mantle that produced the melt. This model results in a total volume of melt proportional to $\bar{F}^2$ (see next section).

In an *active model* buoyancy forces arising from melt retention and residue depletion play an important role in driving the flow and perturbing the simple corner flow (Fig. 4.3B). In the simplest and most extreme case, there is an enhanced upwelling beneath the axis and a downward component off-axis, and therefore all the unclosed streamlines that cross the solidus are continued until a uniform depth before turning aside (Forsyth, 1992). The mantle volume undergoing decompression melting is now restricted to a narrow rectangular area, giving a total volume of melt that is proportional to $\bar{F}$ (rather than to $\bar{F}^2$ as in passive flow models) (Forsyth, 1992). In the limit case showed in Fig. 4.3B, all the mantle melts to its maximum amount ($F_{max} = \bar{F}$) at the shallowest

pressure P_f (i.e. the pressure at which melting stops). Even when F and $F(z)$ are identical to those of the passive model, $\overline{F}$ is doubled. Since the oceanic crustal thickness is proportional to $\overline{F}$ (or F ; see below), thicker crusts are generally associated with active contributions beneath the MOR (Langmuir et al., 1992).

Although an active component may be present in some ridge segments (e.g. Niu et al., 2001), and certainly in others (e.g. Iceland, Azores; White, 1999), the general agreement is that a typical MOR is mainly a passive feature underlain by a mantle of quasi-constant potential temperature (McKenzie & Bickle, 1988; Langmuir et al., 1992; Buck et al. 1998; Schubert et al., 2001). This model has been successfully applied to explain all the major features of a MOR system, from the thickness of the oceanic crust (e.g. Klein & Langmuir, 1987) to the compositional and viscosity structure of the oceanic lithosphere (Phipps Morgan, 1997). Thus, I will seek accurate estimations for the last three factors cited above following this model. It will be shown that for the present purposes, both models give similar results.

4.4.3.1 Total amount of partial melting

Partial melting experiments on natural mantle peridotites have provided important constraints on the total amount of partial melting that can be produced at certain P-T conditions. It is now generally accepted that mantle peridotites with $88 < \text{mg\#} < 91$ can produce MORBs by 15 - 25 % partial melting (Kushiro, 2001). Recent computational simulations in the CaO-MgO-Al₂O₃-SiO₂-NaO₂ system (Presnall et al., 2002) and in the CaO-MgO-Al₂O₃-SiO₂-NaO₂-FeO-Fe₂O₃-TiO₂-Cr₂O₃ system (Asimow et al., 2001) have confirmed this estimation. It is recognized, however, that the amount of partial melting can vary significantly from one segment of a ridge to another (e.g. Niu et al., 2001). Nevertheless, there exists a correlation between F and the thickness of oceanic crust, h_c , at the ridge that can be used to constraint the total amount of partial

melting for a “standard” oceanic crust $\sim 6 - 7$ km thick. Klein and Langmuir (1987) were among the first to define a formalism for the relationship between h_c and F . Defining the pressure of intersection of the solidus as P_o and the pressure at which melting stops as P_f , then the total amount of melt F present within a unit column is

$$F = \int_{P_o}^{P_f} F(P) \, dP \quad (4.9)$$

Since now the depth distribution of melt is defined in terms of units of pressure rather than in units of length (i.e. depth), the mean fraction of melting $\overline{F}$ becomes

$$\overline{F} = \frac{\int_{P_o}^{P_f} F(P) \, dP}{(P_o - P_f)} \quad (4.10)$$

In general, the function $F(P)$ will be a complex function of P (depth). However, it can always be approximated with an average constant slope, $\gamma = (dF/dP)_s$, sometimes called *the productivity function* (e.g. Asimow et al., 1999). Accordingly, the amount of melt present at any pressure is given by $F(P) = \gamma (P_o - P)$, and Eq. (4.9) becomes

$$F = \int_{P_o}^{P_f} \gamma(P_o - P) \, dP \quad (4.11)$$

or, using Eq.(4.10)

$$F = \overline{F}(P_o - P_f) \quad (4.12)$$

Note that in Eq. (4.11) the productivity function γ has units of P^{-1} (i.e. melt produced per unit of pressure release). Thus, F is given in units of P (e.g. GPa). Assuming that the total amount of melt produced in each increment of spreading is segregated to form the oceanic crust, then Eqs. (4.9) and (4.11) give the crustal thickness h_c (strictly, the weight of a melt column of height h_c ; Klein & Langmuir, 1987; Langmuir et al., 1992) as

$$\rho_c g h_c = \bar{F}(P_o - P_f) \quad (4.13)$$

Taking pressure in GPa, densities in kg m^{-3} , and $\bar{F}$ in %, a good approximation of h_c in km is

$$h_c = \bar{F}(P_o - P_f) \frac{10^4}{\rho_c g} \quad (4.14)$$

For example, for typical values of (Asimow et al., 1999, 2001) $\bar{F} \sim 7.2$ %, $P_o \sim 2.75$ GPa, $P_f \sim 0.2$ GPa, and $\rho_c = 2880 \text{ kg m}^{-3}$, Eq. (4.14) gives $h_c \sim 6.5$ km.

Hence, values of $\bar{F} >$ than about 10 % ($F > 25$ %) are considered to be inconsistent with the normal amount of crust produced, except of course at sites of active upwellings, where the crust can reach anomalous thicknesses of the order of 25 - 30 km (White, 1999).

4.4.3.2 Depth distribution of melt

The distribution of melt in the melting regime as a function of depth is of primary importance in calculating the final average density of a MOR column, due to the high compressibility of melts (Chapter 3). For example, 22 % partial melting at 10 km would

reduce the density of mantle material by ~ 3.4 % (including chemical depletion of the solid phase), while the same amount of partial melting at 80 km would only reduce the density by ~ 1.8 %. Fortunately, both theoretical and experimental considerations indicate that the actual amount of melt retained within a MOR column (i.e. porosity) is small, making its effect on density changes less important (see below; Spiegelman & Kelemen, 2003). Since the form of the melt productivity function γ affects both the porosity and the composition of the solid residue, I will first discuss the depth distribution of this factor.

Several authors have estimated γ resulting from adiabatic decompression of an ascending mantle volume (see Langmuir et al., 1992; Asimow et al., 1999, for a review). Usually a constant value is chosen, ranging between 10 - 20 % per GPa of pressure release. This range implies that if an ascending mantle volume intersects the solidus at 2 GPa, then the maximum extent of melting that the parcel experiences would be 20 % if the lower bound of γ is assumed, or 40 % if the upper bound is used. Therefore, from the discussion in the previous section we can expect that a more representative value for normal MORs would lie closer to the lower bound. Indeed, Klein and Langmuir (1987) and Langmuir et al. (1992), for example, have shown that 12 % GPa⁻¹ seems to be a proper mean value for γ . In contrast, more recent simulations have shown that the productivity is far from constant along the melting regime, but instead it has at least two or three well defined paths with nearly constant γ (Asimow et al., 1999, 2001). Asimow et al. (1999) used thermodynamic computational simulations to model a natural peridotite system. These authors highlight that the productivity for reversible adiabatic depressurization melting is not constant, but rather increases as melting proceeds. At pressures $\gtrsim 1.0$ - 1.5 GPa, F is unlikely to exceed 5 % in both batch and fractional melting regimes. Once the pressure decreases below this value, the productivity increases drastically until the clinopyroxene is totally consumed. This implies that more melt will tend to be present at shallow levels, therefore reducing the average density value more than in the case of

a constant γ . Also, it has strong implications for the final compositional structure of the oceanic lithosphere, and consequently for its relative buoyancy with respect to the underlying mantle. This will be further discussed in the next chapter.

Fig. 4.4 shows a summary of the results presented by Asimow et al. (1999) and Asimow et al. (2001) for both batch and fractional melting models. The widely used linear model is also included in this figure (e.g. Langmuir et al., 1992; Turcotte & Phipps Morgan, 1992). There are two important differences between the non-linear and linear model. First, at comparable P_o , the linear model gives significantly higher $\bar{F}$ than the non-linear case. Since the crustal thickness is proportional to the product of $\bar{F}$ and $(P_o - P_f)$, the linear case predicts much thicker crusts. Second, because of the low productivity in the early stages of melting, as given by the non-linear model, there is a “tail” of low F that tend to decrease $\bar{F}$ even more. These observations show that any given crustal thickness is generated by a melting path with much lower P_o according to the linear model than according to the non-linear model. For example, a $\sim 6 - 7$ km thick crust is obtained by the linear model with a $P_o \sim 2.0$ GPa, but requires a $P_o \sim 2.75$ GPa in the non-linear case. The preferred curve for the non-linear model used in this thesis is shown in Fig. 4.4. It is a representative mean of several batch and fractional models within the “normal” range of $2.0 < P_o < 3.5$ GPa (Langmuir et al., 1992; Asimow et al., 1999, 2001). Numerically, it is represented by two linear functions (F1 and F2 in Fig. 4.4) intercepting at 1.25 GPa. This curve has $P_f = 0.2$ GPa and $P_o = 2.75$ GPa (i.e. ~ 88 km depth), produces an $\bar{F}$ of around 7.2, and according to Eq. (4.14), a crustal thickness of ~ 6.5 km. It is important to note here that, although the form of γ might vary from one work to another, the product of $(P_o - P_f)$ and $\bar{F}$ should be comparable in all cases.

The above melting model can be used as a proxy for modelling the actual melt distribution with depth (i.e. porosity). Although the actual amount and depth distribution of

retained melt beneath a MOR are still under debate, trace-element and U-series disequilibrium modelling indicate maximum retained melt fractions of 2-6 % (e.g. Spiegelman & Kelemen, 2003, and references therein). Therefore, based on these studies and on the above discussion, a maximum retained melt fraction of 4 % is assumed here at the top of the mantle column, which varies linearly with depth until it reaches a value of 2 % at the point where γ experiences a drastic slope change (at 1.25 GPa). Below this point the melt fraction decreases linearly again until the bottom of the melting regime, where it becomes zero.

4.4.3.3 Chemical variation of both solid and melt phases due to partial melting

The final chemical composition of a solid-liquid system is determined basically by three parameters: the initial concentration of the element or component in the system C_o , the bulk distribution coefficient D , and the fraction of liquid F . Applying a simple mass balance for fractional melting, the three parameters are related to each other by an expression of the form (Langmuir et al., 1992)

$$C_L/C_o = (1/D)(1 - F)^{\frac{1}{D}-1} \quad (4.15)$$

where C_L is the concentration of the component in the liquid. Eq. (4.15) forms the basis for most chemical modelling of MORB. However, it was shown in Chapter 3 that the density of a silicate melt at depths > 10 km changes only slightly with composition and potential temperature. Therefore, it will be assumed that the curve shown in Fig. 3.10 is still relevant in this case, and I will focus mainly on the composition of the residual mantle column. The main effect of progressive melting on the final density of a peridotitic rock is the preferential incorporation of Fe into the melt (Chapter 2). Since

olivine and pyroxenes in mantle assemblages have similar $mg\#$, the variation of this ratio with melt extraction in olivine can be used to approximate the effect in the whole mantle assemblage. This can be done in a straightforward manner using a combination of the regressions between modal olivine vs extent of melting, together with that between $mg\#$ vs modal olivine. The former was already discussed in Chapter 2 (Fig. 2.1), and the latter is taken from Baker and Beckett (1999). This approach is preferred over the method used by Phipps Morgan (1997), based on theoretical equations, since the latter always overestimates the effect of melt extraction on the $mg\#$ observed in real samples. Once the average $mg\#$ for olivine is obtained for any given melt fraction, it is used to calculate the densities of the other phases (assuming they have the same $mg\#$) using linear interpolations between the densities given in Table 3.3 for the mineral phases with integer $mg\#$. This correlation method is schematically shown in Fig. 4.5.

The final model for the MOR column obtained with the aforementioned considerations is shown in Fig. 4.6. Density estimations and seismic velocities from spherically symmetric seismological models PREM (Dziewonski & Anderson, 1981) and *ak135* (Kennett et al., 1995) are also included for comparison. Also in this figure are the velocity profiles from seismological models in the oceanic environment PA5 (Gaherty et al., 1999) and ATLTP (Zhao & Helmberger, 1993). As expected, deviations from seismological models become important at depths < 120 km, since the local lithospheric thickness at the MOR is virtually zero, and therefore not comparable to the average lithospheric thickness on a global scale. Also, partial melting effects reduce both the average density and seismic velocities at the MOR, increasing the differences with seismological models. At depths > 120 km, all models agree relatively well. The strong discrepancy with PREM at depths around 220 km is a fictitious effect due to PREM's assumptions on the depth distribution of anisotropy (below 220 km the upper mantle is assumed to be isotropic, while above this depth an average anisotropy of $\sim 3\%$ is included, Dziewonski & Anderson, 1981).

The average mantle density of the MOR column (ρ_{MR}), needed for the isostatic model, can be obtained by integrating the density with respect to depth, and dividing by the total thickness. This calculation gives average densities $\rho_{MR} = 3369.4 \pm 5 \text{ kg m}^{-3}$. This is very close to the value obtained by performing a simple isostatic balance ($\rho_{MR} = 3368 \text{ kg m}^{-3}$) down to 300 km (taken as compensation depth), requiring a ridge elevation of 2.6 km below sea level and a crustal thickness of 7 km. Since the approach to calculate average densities of other mantle columns is the same as the one used to obtain ρ_{MR} , it is clear that the method used in LitMod to calculate elevations is robust and self-consistent.

4.4.4 Deviations from local isostasy

Although the local isostatic approach is justified in most cases, deviations from this assumption might be present in some modelled sections. Intrusions of short wavelength and/or anomalously dense bodies significantly affect the calculated elevation, which is particularly sensitive to lateral density heterogeneities under the local isostasy assumption. Trying to compensate a departure from the observed elevation, for example by reducing the lithospheric thickness under the intrusions, leads to an unrealistic short-wavelength thinning that is not supported by the other observables. When this is the case, the flexural response of the lithosphere will be estimated by solving the governing differential equation for the cylindrical flexure of a thin plate (e.g. Turcotte & Schubert, 1982)

$$q(x) = D \frac{d^4 w(x)}{dx^4} + N \frac{d^2 w(x)}{dx^2} + q_d(x) \quad (4.16)$$

where

$$D = \frac{E T_e^3}{12(1 - \nu^2)} \quad (4.17)$$

is the flexural rigidity, $q_d(x) \approx g w(x) (\rho_m - \rho_{infill})$ the restoring force, w the deflection, N the horizontal force per unit length acting on the direction of the x axis, $q(x)$ the vertical load, E the Young's modulus, ν the Poisson's ratio, T_e the elastic thickness of the thin plate, and g the acceleration of gravity. It can be verified that the horizontal force in Eq. (4.16) can be neglected in our calculations, since the amplification of the deflection by horizontal stresses is of the second order compared with the vertical loads (see Appendix A).

4.5 Gravity anomalies

Topography and density inhomogeneities within the Earth generate variations in the surface gravity. Measured values of gravity on the surface need to be corrected before being compared with the theoretical value given by the International Gravity Formula (e.g. Heiskanen & Moritz, 1967). Any discrepancy between measured and expected values of gravity is called a *gravity anomaly*. There are five basic corrections that need to be applied in order to reduce the measured value to the reference level: *Bouguer*, *free-air*, *terrain*, *tidal*, and *Eötvös* (only for measurements in a moving vehicle). The combination of the last four gives the *Free-air anomaly*, while the combination of all of the above gives the *Bouguer anomaly*. The former correlates strongly with topography at short wavelengths and it is generally used in marine surveys. The latter removes all topographic effects, including the attraction of interposed rocks, and therefore it is more suitable for studying deep density anomalies, for instance those associated with changes in Moho depth (see e.g. Zeyen & Fernández, 1994).

The code LitMod calculates free-air and Bouguer gravity anomalies in two dimen-

sions using the algorithm for polyhedral bodies of Talwani et al. (1959). This algorithm accounts for continuous density variations both laterally and vertically, and is applied to each element of the mesh for which the density has been already calculated in a previous step. The gravity influence of all the elements is then added and calculated either at the top of the model or at the sea level, depending on if the elevation is above or below sea level, respectively. In order to avoid border effects, the models are extended horizontally 1000 km beyond the profile limits. Due to the $1/r^2$ dependency of the gravity field, where r is the distance to the density anomaly, gravity anomalies basically provide information on the density distribution at crustal and shallow subcrustal depths.

4.6 Geoid height

The equipotential surface of gravity that best fits the free ocean surface, excluding tidal and wind effects, is called *the geoid*. Differences between this surface and that given by the International Reference Ellipsoid are called *geoid anomalies* or *geoid heights*. While gravity anomalies are more affected by shallow (crustal) structures, the geoid height provides information on deeper features and on the topography of the lithospheric-sublithospheric boundary. This is mainly due to the fact that the geoid anomaly is the height difference between two equipotential surfaces, and therefore it is a function of $1/r$ instead of $1/r^2$, where r is the distance to the density anomaly.

The calculation of the geoid height is done by converting two adjacent triangular elements of the mesh into rectangular prisms throughout the model, solving the integral of the their gravity potential, and substituting the result into Brun's formula ($\Delta N = \Delta U / g_0$, where ΔN is the geoid anomaly, ΔU the potential anomaly, and g_0 the normal gravity acceleration, given by the International Gravity Formula). One finally obtains (Zeyen et al., 2005)

$$\Delta N = \frac{G \cdot \rho}{g_o} \int_{x_1}^{x_2} \int_{y_1}^{y_2} \int_{z_1}^{z_2} \frac{1}{R} dz dy dx \quad (4.18)$$

or

$$\begin{aligned} \Delta N = & \frac{G \cdot \rho}{g_o} [xy \ln(z + R) + xz \ln(y + R) + yz \ln(x + R)] \Big|_{x_1-x_0}^{x_2-x_0} \Big|_{y_1-y_0}^{y_2-y_0} \Big|_{z_1-z_0}^{z_2-z_0} \\ & - \frac{G \cdot \rho}{g_o} \left[\frac{1}{2} (x^2 f_{(x,y)} + y^2 f_{(y,x)} + z^2 f_{(z,x)}) \right] \Big|_{x_1-x_0}^{x_2-x_0} \Big|_{y_1-y_0}^{y_2-y_0} \Big|_{z_1-z_0}^{z_2-z_0} \end{aligned} \quad (4.19)$$

where

$$f_{(a,b)} = \arcsin \left(\frac{a^2 + b^2 + bR}{\sqrt{a^2 + b^2}(b + R)} \right) \quad (4.20)$$

$$R = \sqrt{x^2 + y^2 + z^2} \quad (4.21)$$

G is the universal gravitational constant ($6.67 \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$), x_1 and x_2 the x -coordinates of the prism boundaries, y_1 and y_2 the y -coordinates of the prism boundaries, z_1 and z_2 the z -coordinates of the prism boundaries, x_0, y_0, z_0 the coordinates of the calculation point, and ρ the density of the prism. Here the x - z plane represents the relevant 2-D vertical cross section. The length in the direction of the y -axis (i.e. section thickness) is taken for all the models to be large enough to simulate two-dimensional anomalies. The contribution of all prisms to the geoid anomaly is the sum

$$\Delta N_T = \sum_1^n \Delta N \quad (4.22)$$

where ΔN is the geoidal response of each prism, and n is the total number of prisms. In some cases, the 1-D geoid formulation given by Turcotte and Schubert (1982) will also be used for comparison. It reads as

$$\Delta N = -\frac{2\pi G}{g_o} \int_0^h z \Delta \rho(z) dz \quad (4.23)$$

where h is the maximum depth of the model.

Throughout the process, the model is assumed to be in isostatic equilibrium to avoid border effects in the geoid calculations. This condition is implicitly fulfilled if the model fits elevation data. From Eqs. (4.18) and (4.23) it can be seen that the geoid anomaly is directly proportional to the *density moment* ($z\Delta\rho$), and therefore it will be particularly susceptible to deep density anomalies. The calculated geoid anomaly with Eq. (4.22) tends to that predicted by Eq. (4.23) when the bodies are extended enough or the lateral density changes are smooth (e.g. oceanic lithosphere).

Geoid height data for this thesis are obtained from the EGM96 model of Lemoine et al. (1998), unless indicated otherwise. This model, extended to spherical harmonic degree 360, was successfully used to compute geoid undulations accurate to better than one metre, using the WGS84 (World Geodetic System 1984) as the reference system. It should be noted that at a regional scale, differences between EGM96 and the more recent GGM02, derived from the Gravity Recovery And Climate Experiment (GRACE), are negligible (Tapley et al., 2005).

Since all masses within the Earth contribute to all harmonic degrees of the observed geoid, a high-pass filter has to be applied in order to compare the predictions from LitMod with the real geoidal response of a section ~ 300 km thick. The equivalent wavelength λ for each harmonic degree, or in other words, the Earth's circumference

divided by the harmonic degree number, is (Bowin, 2000)

$$\lambda = \frac{2\pi R}{n} \quad (4.24)$$

Therefore, low harmonic degrees represent long wavelengths, while high harmonic degrees are associated with shorter wavelengths. Following the general procedure of Bowin (2000), the limiting depth at which a point mass can exist to create the observed geoid anomaly at the Earth's surface can be written as

$$z_{max} = \frac{g_o \Delta N}{\Delta g} \quad (4.25)$$

where g_o is again the normal gravity, ΔN is the geoid anomaly, and Δg is the resulting gravity anomaly. Also, the spectral relation between the spherical harmonic degree n of the geoid and the resulting gravity anomaly is (e.g. Heiskanen & Moritz, 1967)

$$\Delta g_n = \Delta N_n \frac{g_o(n-1)}{R} \quad (4.26)$$

Combining Eqs. (4.24), (4.25), and (4.26), the expression for the maximum possible depth of a causative point mass anomaly is obtained as

$$z_n = \frac{R\lambda}{(2\pi R - \lambda)} \quad (4.27)$$

Thus, subtracting harmonic degrees less than 10-15 from the complete ($n = 360$) geoid removes wavelengths up to 4003 and 2668 km, respectively, yielding a residual geoid that

should exhibit effects of density anomalies at depths < 700 and < 450 km, respectively. It must be emphasized that these estimations represent *maximum possible depths* for a causative mass anomaly, and that the actual mass anomaly is much more likely to be placed at shallower depths (Bowin, 2000).

A series of experiments were conducted to decide to which harmonic degree the data should be filtered to avoid deep perturbations. As an example, Fig. 4.7 compares the complete geoid with those filtered up to degree 10 and 15 for the eastern hemisphere (i.e. only degrees higher than 10 and 15, respectively). It is seen that even when the amplitude of the geoid height changes between the 10 – *th* and 15 – *th* residual geoids, the maximums and minimums seem to remain in the same position. However, the 10 – *th* filtered geoid reproduces surface features such as MORs, fracture zones, and continental margins more accurately, which are thought to be consequences of density anomalies not deeper than ~ 350 km (e.g. deepest roots of Archean lithosphere). At these wavelengths, a transect across a mature passive margin from an oceanic basin to a stable continental domain, typically shows differences of $\sim 12 \pm 4$ m in the geoid, with absolute values around 5 ± 3 m and -6 ± 2 m in continental and old oceanic domains, respectively.

To further distinguish between these two cases of filtering I have conducted another set of experiments in which I plotted more detailed maps of topography together with those for 10 – *th* and 15 – *th* geoid residuals for Australia. Fig. 4.8 shows the results. It is clear from this figure that most of the main tectonic features (e.g. MORs, basins, cratons, platforms, submarine plateaus) are well described by both the 10 – *th* and 15 – *th* residual geoids, although the former locates the MOR in a better position and with better amplitude. The Great Australian Bight Basin is also better depicted by the 10 – *th* residual geoid. These results are consistent with the observation that for greater than harmonic degree 10, the Earth's geoid values show very little change with the addition of higher degree contributions (Bowin, 2000).

In summary, removing harmonic degrees < 10 from the EGM96 model leaves a residual geoid that correlates well the main surface tectonic features of the Earth. It seems appropriate, therefore, to use this residual geoid when modelling lithospheric sections with LitMod. In this thesis, the 10 – *th* residual geoid will be generally used as a reference, unless indicated otherwise.

4.7 Transition zones between different bodies

Representative compositions, densities, and thermoelastic parameters for different bodies may change significantly between different mantle domains. These spatially sudden variations generate “jumps” on model predictions, that sometimes are not supported by available evidence. LitMod permits to assign transition zones (TZ) of any size, between different mantle domains, and recalculates appropriate values of all relevant properties within these TZ. The method used in LitMod assumes that the TZ properties can be envisaged as based on a suitable combination of the end-member properties of the two adjacent mantle domains (e.g. oceanic and continental). In this way, two smoothing functions describing how the properties change along the TZ are applied to the zone located between the prescribed limits x_1 and x_2 , representing either the width or thickness of the respective TZ. The final property, $P(i)$, at the particular node i , is obtained from

$$P(i) = P_1(i) \times F_1(i) + P_2(i) \times F_2(i) \quad (4.28)$$

where P_1 and P_2 are the relevant properties at both extremes of the TZ, and F_1 and F_2 are the two smoothing functions. In LitMod, two different types of smoothing functions are possible: linear and non-linear. The linear set is simply defined as

$$F_1(i) = \left[\frac{(x_2 - x(i))}{(x_2 - x_1)} \right] \quad (4.29a)$$

$$F_2(i) = \left[\frac{(x(i) - x_1)}{(x_2 - x_1)} \right] \quad (4.29b)$$

and the non-linear set as

$$F_1(i) = \left[\frac{x_1 (x_2 - x(i))}{(x_2 - x_1) x(i)} \right]^\Phi \quad (4.30a)$$

$$F_2(i) = \left[\frac{x_2 (x_1 - x(i))}{(x_1 - x_2) x(i)} \right]^\Phi \quad (4.30b)$$

where x is the spatial coordinate (vertical or horizontal), Φ is a decay constant, and the variable i represents the particular node. Unless indicated otherwise, the decay constant is always assumed to be equal to unity. The two smoothing functions are constrained by the following boundary conditions: $F_1 = 1$ at x_1 ; $F_2 = 1$ at x_2 ; $F_1 = 0$ at x_2 ; $F_2 = 0$ at x_1 , for any value of i . Although Eqs. (4.29a - 4.29b) and (4.30a-4.30b) are not the only functions that can be used, there is no a priori reason for choosing more complicated functions. Fig. 4.9 displays the form of these two functions vs. distance in a TZ.

4.8 Rheological equations and strength envelopes

It is commonly accepted that, to the first order, the mechanical behaviour of the lithosphere can be modelled using experimental constraints on rock rheology (Ranalli, 1995; Kohlstedt et al., 1995; Afonso & Ranalli, 2004). Kohlstedt et al. (1995) subdivided the mechanical lithosphere into three domains with distinctive mechanical behaviour:

brittle, semi-brittle (ductile) flow, and high-temperature “plastic” flow. In this thesis I will adopt a different terminology, changing “plastic” to “creep”, in accordance with the continuum mechanics terminology that restricts the term “plastic” to a very specific type of rheology, and using “ductile” as a general term describing a permanent, solid-state deformation in which there is no loss of cohesion neither at a grain-size scale nor at macroscopic scale, with no genetic implications.

Except for a few expanding clays, the brittle regime for most rocks can be adequately described by the Coulomb frictional law, which in the case of pre-existing faults of favourable orientation and negligible cohesion can be written as (e.g. Ranalli, 1995)

$$(\sigma_1 - \sigma_3)_B = (R - 1)\rho gz(1 - \lambda) \quad (4.31a)$$

$$(\sigma_1 - \sigma_3)_B = \frac{(R - 1)}{R}\rho gz(1 - \lambda) \quad (4.31b)$$

$$(\sigma_1 - \sigma_3)_B = \frac{2(R - 1)}{(R + 1)}\rho gz(1 - \lambda) \quad (4.31c)$$

for thrust, normal, and transcurrent faulting, respectively, where $\sigma_1 - \sigma_3$ is the maximum stress difference, ρ is the average density of rocks above the depth z , and λ is the pore fluid factor (ratio of pore fluid pressure to lithostatic pressure). The parameter R is known as the *stress ratio*, and is given by

$$R = [\sqrt{(1 + \mu^2)} - \mu]^{-2} \quad (4.32)$$

where μ is the coefficient of friction.

The most uncertain parameter is the pore fluid pressure, although it has been shown that it is often near-hydrostatic down to depths of ~ 12 km (Zoback & Townend, 2001). In the absence of detailed information regarding specific regions, I take a typical (“hydrostatic”) value $\lambda = 0.38$.

In the semi-brittle (ductile) field the material no longer behaves entirely in a brittle manner, but deforms by a combination of processes such as microfaulting and dislocation glide and climb (Kohlstedt et al., 1995). The onset of this field has been suggested to start at the point where the brittle stress reaches one fifth of the creep stress, while the end of it is marked by the point where the creep stress equals the effective confining pressure (Kohlstedt et al., 1995). The latter can be approximated to the first order as

$$P_{eff} = \rho g z (1 - \lambda) \quad (4.33)$$

where ρ , z and λ are as in Eqs. (4.31). This criterion is sometimes referred to as the “Goetze criterion”. Although, there is no formal constitutive equation for this field, the transitions between the brittle and the ductile semi-brittle (BDT) fields, and between the ductile semi-brittle and the creep field (SBC) have been qualitatively confirmed by laboratory experiments (cf. Kohlstedt et al., 1995; Ranalli, 1995).

For the creep field, a power-law dislocation creep is assumed, which results in a creep strength given by (Ranalli, 1995; Afonso & Ranalli, 2004)

$$(\sigma_1 - \sigma_3)_C = \left(\frac{\dot{\epsilon}}{A} \right)^{1/n} \exp \left(\frac{H}{nRT} \right) \quad (4.34)$$

$$H = E + PV \quad (4.35)$$

where $\dot{\epsilon}$ is the steady-state strain rate, T temperature in degrees Kelvin, P pressure, R the universal gas constant ($8.3144 \text{ J mol}^{-1} \text{ K}^{-1}$), H the creep activation enthalpy, E the activation energy, V the activation volume, and n and A material creep parameters. The creep parameters for various relevant materials are listed in Table 4.1. When modelling the lithosphere, the pressure dependence of creep can be neglected in Eq. (4.35) without introducing significant errors, since the activation volume of olivine is around $5 \times 10^{-6} \text{ m}^3 \text{ mol}^{-1}$ for diffusion creep, and $10 - 25 \times 10^{-6} \text{ m}^3 \text{ mol}^{-1}$ for dislocation creep, while its activation energy ranges between $250 - 540 \text{ kJ mol}^{-1}$ (Karato & Wu, 1993). For example, for dry olivine under dislocation creep, the activation enthalpy is increased by $\sim 11 \%$ at pressures $\sim 6 \text{ GPa}$, which translates in an absolute change of $\sim 2 \text{ MPa}$, as given by Eq. (4.34), at 1500 K .

The total strength of a given lithospheric section is the sum of the depth-integrated strength on each field (Afonso & Ranalli, 2004)

$$TS = \int_0^{z_{BDT}} (\sigma_1 - \sigma_3)_B dz + \int_{z_{BDT}}^{z_{SBD}} (\sigma_1 - \sigma_3)_{SB} dz + \int_{z_{SBD}}^{z_H} (\sigma_1 - \sigma_3)_C dz \quad (4.36)$$

where z_{BDT} is the depth to the BDT transition, z_{SBD} the depth to the SBC transition, and z_H the base of the mechanical lithosphere, here defined as the depth where the strength reaches a value of 5 MPa .

LitMod solves Eqs. (4.31 - 4.36) at each node for any given strain rate. Since the creep field is strain-rate dependent, so is the semi-brittle field. Keeping the remaining variables constant, lower strain rates translate into smaller creep strengths, and therefore thinner semi-brittle fields. For higher strain rates, the opposite applies (i.e. thicker semi-brittle field). In lieu of a more appropriate constitutive relation for the semi-brittle field, the code performs a simple linear extrapolation between the BDT and the SBC

transitions (Kohlstedt et al., 1995).

When dealing with the mechanical (rheological) behaviour of the lithosphere in Chapter 6, processes such as translithospheric shear deformation and non-homogeneous strain rates will be shown to be dominant. This makes the application of simple strength envelopes inadequate for describing lithospheric strength (strength envelopes are strictly limited to pure shear deformation with depth-independent strain rates; e.g. Fernández & Ranalli, 1997). Therefore, although LitMod calculates strength envelopes for any two-dimensional lithospheric model, this thesis does not use rheological profiles as a mean to estimate lithospheric strength.

Table 4.1: Creep parameters for lithospheric rocks [Eq. (4.33)]

Lithology	A [MPa $^{-n}$ s $^{-1}$]	n	E [kJ mol $^{-1}$]	V [m 3 mol $^{-1}$] ^a
Quartzite (wet)	3.2×10^{-4}	2.3	154	
Felsic granulite	8.0×10^{-3}	3.1	243	
Mafic granulite	1.4×10^4	4.2	445	
Maryland diabase (dry)	8.0	4.7	485	
“Undried” diabase (wet)	2.0×10^{-4}	3.4	260	
Peridotite (dry)	2.5×10^4	3.5	532	15-25
Peridotite (wet)	2.0×10^3	4.0	471	10-20

(Modified from Afonso & Ranalli, 2004)

^a Activation volume for olivine under dislocation creep (Karato and Wu, 1993)

Figure 4.1: Variation of thermal conductivity with temperature. White circles and black squares are laboratory measurements (Hofmeister, 1999; and references therein). The vertical dotted line indicates the limit between Eqs. (4.2a) and (4.2b)

Figure 4.2: Isostatic balance used to calculate the absolute elevation of different columns with respect to a reference column at a MOR. E_{ridge} = ridge elevation (negative), Z_{crust} = crustal thickness, Z_{MAX} = model's maximum depth, ρ_w = density of seawater, ρ_{crust} = density of oceanic crust, ρ_{MR} = depth-averaged density of mantle below the MOR, ρ_{ridge} = depth-averaged density of the MOR (crust + mantle), ρ_b = density of the mantle at $z = Z_{MAX}$. Refer to text for the meaning of parameters H_f and Π .

Figure 4.3: Schematic illustration of two end-member flow regimes and melt extraction models at MORs: A) Passive model, B) Active model. The mantle melting zone (i.e. melt regime) is shaded. The flow is indicated by the solid arrows. F is the melt fraction, $\bar{F}$ is the mean extent of melting, F_{max} is the maximum amount of melting, and RCM is the residual mantle column. The extent of melting with depth is shown in vol %. Note that although the columns beneath the MOR are similar in both models, the resultant RMC are markedly different. (Figure modified from Langmuir et al., 1992)

Figure 4.4: Degree of partial melting with depth for different melting models. The two dotted and two dash-dotted curves are isentropic melting models for fractional melting and batch melting at two different P_o , respectively (from Asimow et al. 1999; 2001). The dashed line is the (nearly) linear model of Turcotte & Phipps Morgan (1992). The solid line is the preferred model used in the calculations of Section 4.4.3.2. F1 and F2 are two linear functions used in the numerical implementation of the average non-linear model. Pressure in these functions is in GPa. Other relevant parameters are listed in the right upper corner.

Figure 4.5: A) Correlation between $mg\#$ in olivine and modal olivine (as volume fraction) in abyssal peridotites. Data from Baker & Beckett (1999). B) Modal olivine as a function of melt extraction (From Fig. 2.1B). A mantle parcel that has experienced 20 % melt extraction at a MOR contains ~ 68.3 modal olivine with a $mg\# \sim 90$.

Figure 4.6: A) Modelled density distribution of the reference column at a MOR. Contours are in kg m^{-3} . The arrows indicate density values from seismological models at those depths: Black arrows are from PREM (Dziewonski & Anderson, 1981). Blue arrows are from *ak135* (Kennett et al., 1995). B) Melt fraction distribution with depth used to estimate the final density of column A. C) Modelled P-wave velocity beneath a MOR. Values from seismological models PREM, *ak135*, PA5 (Gaherty et al., 1999), and ATLTP (Zhao & Helmberger, 1993) are shown for comparison.

Figure 4.7a: Topography of the eastern hemisphere.

Figure 4.7b: Geoidal height of the eastern hemisphere from EGM96 with respect to the reference ellipsoid WG584 (after Lemoine et al., 1998).

Figure 4.7c: Residual geoid of the eastern hemisphere after subtracting harmonic degrees less than 10.

Figure 4.8: Topography and residual geoids of Australia. A) Topography; B) Residual geoid after subtracting harmonic degrees less than 10; C) Residual geoid after subtracting harmonic degrees less than 15.

Figure 4.9: Linear and non-linear smoothing functions (F_1 , F_2) used to model the thermophysical parameters in mantle transition zones. The limits of the transition zone are indicated by x_1 and x_2 .

CHAPTER 5

LitMod Applications: Synthetic Models and Real Cases

5.1 Introduction

In this chapter the finite-element code LitMod is applied to a series of synthetic and real 2-D lithospheric models to test its reliability and to provide constraints on the thermal and compositional structures of both oceanic and continental lithosphere. The term “*synthetic*” is used whenever referring to generated models that are unconstrained by actual geophysical and/or petrological information. These models provide an excellent opportunity to explore different idealized scenarios, and hence, to gain knowledge about processes that would be difficult to assess otherwise. In contrast, “*real*” models are lithospheric profiles modelled along real transects where pertinent geophysical/petrological information has been gathered by different methods and used to constraint the lithospheric model. These models are characterized by having detailed crustal structures, obtained from seismic surveys alone or from combinations of gravity and seismic studies.

5.2 Synthetic models

This section presents the results of a series of synthetic models carried out for both oceanic and continental lithosphere. Although there still is some debate as to which model better describes the thermal structure of the oceanic lithosphere, its evolution is relatively simple and well understood (see below). This makes oceanic lithosphere an ideal natural scenario in which LitMod can be tested.

5.2.1 Oceanic lithosphere

There are two fundamental models of oceanic lithosphere for explaining its thermal structure, heat-flow, and depth of the seafloor dependence with age: the *half – space cooling model* (hereafter HSM) and the *plate model* (hereafter PM) (cf. e.g. Schubert et al., 2001). Both models give similar heat flow and bathymetry estimations for oceanic lithospheres younger than ~ 60 Ma, but differ significantly for older plates. Based on a rigorous inversion of a global database, Stein and Stein (1992) proposed a modified PM that apparently fits the “average” trend of heat flow and ocean floor depth in a better way than either previous PMs, such as the one proposed by Parsons and Sclater (1977), or the HSM.

Fig. 5.1 shows a comparison of these models together with a reliable data-set of measurements for both heat flow and seafloor depth. The data show that the HSM systematically overpredicts the depth of the seafloor and underpredicts the heat flow of oceanic lithosphere older than ~ 90 Ma. On the other hand, it is clear that the modified PM of Stein and Stein (1992) (GDH1) gives values that lie on the high-end of the depth data, leaving numerous points out. The GDH1 steady-state depth for old lithospheres is ~ 5600 m, and the one-standard deviation envelope about their mean value reaches 6000 m only marginally (at 150 Ma, Fig. 5.1A). This is one of the characteristic features of the GDH1 model, together with the prediction of a high basal temperature (1450°C) and a relatively thin plate thickness (95 km). Since the GDH1 has been the most commonly cited plate model in the past 15 years, but never rigorously tested against geophysical observables other than depth and heat flow, it is important to discuss its possible biased nature. McKenzie et al. (2005) recently criticized the GDH1 model arguing that its high basal temperature implies a potential temperature $T_p \sim 1408^\circ\text{C}$, which will create a crust 16 km thick by decompression melting. This argument relies basically on the T_p -crustal thickness model of McKenzie and Bickle (1988). However, more recent and

realistic models (e.g. Asimow et al., 2001) have shown that normal ocean crust (7 ± 1 km) can be generated by fractional melting within the range $1300\text{ }^{\circ}\text{C} < T_p < 1400\text{ }^{\circ}\text{C}$, and therefore McKenzie et al.'s (2005) argument becomes less relevant. On the other hand, a basal temperature of $\sim 1450\text{ }^{\circ}\text{C}$ at 95 km seems to be too high according to the discussion in Chapters 3 and 4. Maybe more importantly, the seafloor depth database used by Stein and Stein (1992) includes estimations from the North Pacific, which have been clearly shown to be strongly affected by hot spot swells at 120 and 160 Ma (Renkin & Sclater, 1988), which makes them unrepresentative of a normal trend. This effect is clearly visible in the one standard deviation envelope of Stein and Stein (1992) (Fig. 5.1A). Moreover, the whole North Pacific bathymetry seems to be influenced by a positive global dynamic topography signal (Steinberger et al., 2001), which would produce a general positive anomaly on the whole plate (see Fig. 4c of Stein and Stein, 1992; the same figure also reveals a similar situation at 120 Ma in the Northwestern Atlantic database). The inclusion of this data makes it difficult to assess to which degree the GDH1 model is biased by these positive depth anomalies. It is obvious, however, that the thin/hot plate that GDH1 predicts is compatible with a high-bathymetry biased database. The thermal structure predicted by the GDH1 model can in principle be tested by analyzing the resulting seismic structure, and then comparing it with seismic surveys in oceanic lithosphere. To my knowledge, this has never been carried out. Since the modelling technique presented in this thesis to obtain representative thermophysical parameters is based on different principles (mineral physics rather than inversion methods as in the GDH1), it can be used to provide independent evidence to discriminate between different proposed models of oceanic lithosphere.

The objective of this section is to obtain insights into the evolution of the oceanic lithosphere in terms of its thermal, density, and seismological structure, and compare the results with available models for the evolution of oceanic lithosphere (e.g. Parsons & Sclater, 1977; Stein & Stein, 1992; Doin & Fleitout, 1996; McKenzie et al., 2005).

In order to accomplish this, three different models are presented: (a) a synthetic profile along a transect perpendicular to a mid-oceanic ridge (hereafter OLSM1), (b) an idealized lithospheric profile (base = 1300 °C isotherm) that thickens gradually from 50 to 125 km (hereafter OLSM2), and (c) a “hot” plate model that simulates the temperature distribution of GDH1, which is used to estimate the seismic structure of such a plate (hereafter OLHPM). Also of particular interest here are: (i) the effects of different depletion models (Section 4.4.3.2, Chapter 4), (ii) the evolution of the average density of the oceanic plate with respect to the underlying mantle, and (iii) the predictions of heat flow and ocean-floor depth in sections younger than 60 Ma. The first two topics are closely related, and they provide detailed information on the generation, evolution, and magnitude of the so-called gravitational instability of the oceanic lithosphere (e.g. Schubert et al., 2001). The third topic has relevance to the recent controversy regarding the relative importance of convective cooling by hydrothermal circulation in young oceanic crust (Hofmeister & Criss, 2005a, 2005b; Von Herzen et al., 2005).

5.2.1.1 OLSM1

The modelled transect presented in this section has been constructed using real geophysical observables as constraints to the final model (free-air anomalies, geoid height, and elevation), along a 1560 km-long transect perpendicular to the Mid-Atlantic ridge (Fig. 5.2). However, since no information regarding the crustal structure is available, the transect cannot be considered a real section. For this reason, an average crustal thickness of 7 km was chosen for the whole profile. Datasets used in this transect include: Sandwell and Smith (1997) for free-air gravity anomalies; EGM-96 model (Lemoine et al., 1998), filtered to degree 10 (see Chapter 4), for geoid heights; ETOPO 2 (Etopo2, 2001), with a resolution of 2'x 2', for elevation. The transect runs from oceanic crust ~ 90 Ma to 0 Ma at the ridge (Mueller et al., 1997). This particular transect was chosen

for the following main reasons: (a) the sedimentary cover is very thin ($\lesssim 100$ m) (e.g. Divins, D.L., www.ngdc.noaa.gov/mgg/sedthick/sedthick.html); (b) effects of local hot-spot swells are minimum (although the Bermuda swell may cause a local increase in bathymetry of $\sim 200 - 300$ m in the oldest part of the transect, Shahnas & Pysklywec, 2004)); (c) large scale dynamic topography is minimum (Steinberger et al., 2001); (d) the average half-spreading rate is small ($\sim 1.7 \text{ cm a}^{-1}$); and (e) lateral variability of geophysical observables in the oldest parts is small. All of the above suggest that external effects in this profile should be negligible and will not affect the model's results. Fig. 5.3 compares the real observables (no SHF data is available) with those predicted by the best fitting model obtained in this work. In what follows, the resultant thermal, density, and seismic structure will be discussed in detail.

The final thermal structure corresponding to the model that best fits the observables is shown in Fig. 5.4. For comparison, predicted 200, 600, 1000, and 1300 °C isotherms by the HSM and by the PMs of Stein and Stein (1992) (GDH1) and McKenzie et al. (2005) (hereafter MJP) are indicated for the respective crustal age at 90, 65, and 35 Ma. Note that in all figures the origin of the horizontal scale is at the left (western) side of the transect, and thus the MOR axis (0 Ma age) is located at $x = 1560$ km. Some observations can be derived from Fig. 5.4. Firstly, there is a significant discrepancy between predictions from the GDH1 model and any of the other models, including the one presented here. The maximum temperature difference reaches approximately 400 °C in the middle of the plate, and remains almost constant at all shown ages (e.g. about 20 % for the location of the 1300 °C isotherm). This high temperature signature should be recognizable in seismic surveys, since it is enough to cause a $\sim 4 - 6$ % decrease in the P-wave structure with respect to the other models, assuming no changes in composition (e.g. Godey et al., 2004; see also below). Secondly, because a temperature-dependent k is used here, the model shows lower temperatures in the upper and middle parts of the oceanic plate and higher temperatures near the base relative to models with constant k ,

namely GDH1 and HSM (see also McKenzie et al., 2005). The decrease in temperature in the upper parts of the plate produces an extra load due to thermal contraction that increases the subsidence of the ocean floor. This effect is counteracted to some degree by the smaller spacing of the isotherms towards the bottom of the plate. The net effect of introducing the temperature dependence of k is an increase of 300 - 400 m in the subsidence with respect to the same model with constant $k = 3.3 \text{ W m}^{-1} \text{ K}^{-1}$.

The relatively good agreement between the isotherms predicted in this thesis and those predicted by MJP at ~ 90 Ma is evident. This is not surprising, since both models use a similar temperature dependence for the thermal conductivity (Chapter 4), and it is to be expected that at older ages, where any transient effect is negligible, the agreement will be better. To show that this is actually the case, a model with the same thermal thickness (1300 °C isotherm at ~ 104 km below the ridge crest) as the asymptotic thickness of MJP was constructed. The results are plotted in Fig. 5.5, together with the resulting depth and heat flow. The isotherms distribution with depth is identical in both cases for old plates. Predicted values of heat flow by the two models agree well, while the ocean floor depth in MJP model is slightly greater. The thermal structure of the plate, on the other hand, begins to change at ages $\lesssim 150$ Ma, reflecting the transient effect on the 1-D heat transfer equation of McKenzie et al. (2005).

The variation of the isotherms is reflected in the seafloor depth estimation. The MJP model predicts a continuous increase of the seafloor depth (Fig. 5.5B), even at ages > 85 Ma, which is clearly inconsistent with seafloor depth data (see Fig. 5.1A). This overestimation by the MJP model makes it an unsatisfactory model for describing the evolution of normal oceanic lithosphere. When compared with OLSM1, the internal temperature distribution given by MJP for plates younger than 150 Ma is hotter in the middle parts of the plate, but colder towards its base. Although the basal 1300 °C isotherm is almost the same at any age, the locations of the 1000 and 600 °C isotherms

vary considerably. Because the final elevation is only a function of the depth-integrated instantaneous thermal distribution, the separate effects of colder middle and hotter basal parts on seafloor subsidence approximately cancel each other, giving a final elevation that is almost the same in both models.

It is interesting to note here that the thermal structure of OLSM1 at $x = 1400$ km (roughly 10 Ma), is similar to the one for a ~ 25 Ma old plate in the MJP model (Fig. 5.5A). Both models predict almost identical elevations (around 4000 m) in this case. Yet, although heat flow values from OLSM1 ($\sim 80 \text{ mW m}^{-2}$) fall into the expected range given by measurements in plates of similar age (see Fig. 5.1B), they are significantly smaller than those predicted either by the GDH1 or the MJP plate model (110 - 120 mW m^{-2}). Since the OLSM1 model do not consider hydrothermal circulation, but still fits all the observables, the question of whether convective cooling of oceanic lithosphere is a factual process or an artificial requisite of a given model is raised. The discrepancy between predicted heat flow values by analytical models such as HSM, GDH1, or MJP, and observed values in oceanic lithosphere younger than 60 Ma, has classically been attributed to convective cooling by hydrothermal circulation (e.g. Stein & Stein, 1992; Fisher & Becker, 2000; Von Herzen et al., 2005). Hofmeister and Criss (2005a) recently reviewed and analyzed heat flow data for the oceanic lithosphere. Based on theoretical and experimental evidence, they concluded that the discrepancy between observed and predicted values cannot be attributed to hydrothermal circulation, but rather to the mathematical singularity imposed by analytical models at the ridge axis, where the heat flow becomes infinite. Although there is no doubt that hydrothermal activity on ridge flanks is important on a scale of tens of kilometers (e.g. Fisher & Becker, 2000; Fisher et al., 2003), attributed discrepancies in lithospheres of ~ 50 Ma age imply active convective cooling at distances of the order of 800 - 1000 km away from the ridge. It is not clear how hydrothermal circulation can effectively and systematically affect such an extensive area (Fisher & Becker, 2000; Hofmeister & Criss, 2005a, 2005b; Von Herzen et

al., 2005). Although it is not possible at the moment to make an unambiguous statement on the validity of the concept of convective cooling by hydrothermal circulation, OLSM1 shows that within the range of uncertainties, no convective cooling is necessary to fit the observables at plate ages < 50 Ma. Indeed, predicted heat flow values by OLSM1 for plates younger than 20 Ma ($80 - 90 \text{ mW m}^{-2}$) and at the ridge axis ($\sim 160 \text{ mW m}^{-2}$) agree well with values from measurement databases (Fig. 5.1B).

The density distributions predicted by OLSM1 for both linear and non-linear depletion models are shown in Figs. 5.6 and 5.7, respectively. The first noticeable feature is the relatively abrupt jump in density at the spinel-garnet transition, indicated by the dotted yellow line. Since this phase change is an exothermic reaction (i.e. positive Claperyon slope, Klemme & O'Neill, 2000), it is slowly shifted towards deeper levels the closer it is to the MOR, where it reaches ~ 80 km depth. It is also evident from these figures that the density inversion within the lithosphere due to conductive cooling is, as expected, more pronounced for the non-linear model than for the linear depletion model. This is more visible toward the older sections of OLSM1, where mantle density reaches values of $\gtrsim 3370 \text{ kg m}^{-3}$ right beneath the spinel-garnet transition. Within the garnet stability field (i.e. garnet lherzolite), the linear case shows a thicker core of material with densities $> 3360 \text{ kg m}^{-3}$ than in the non-linear case. This is a consequence of the different pressures (i.e. depths) at which melt depletion starts (see Fig. 4.4). In the linear case, depletion starts at a pressure of 2.0 GPa (~ 65 km depth), while in the non-linear case it begins at 2.75 GPa (~ 90 km depth). Undepleted (more dense) mantle make up therefore the lower 40 km of the plate in the linear case. However, density never reaches values of $\gtrsim 3370 \text{ kg m}^{-3}$, as in the non-linear case.

Also clear from these figures is that within the spinel stability field (i.e. spinel lherzolite), different depletion models do not affect the density structure significantly, although its mean value is slightly larger in the non-linear case. This result is in agreement with

a recent comprehensive study of laboratory data (Schutt & Lesher, 2006). The effect of different depletion models is also negligible when the plate has a thermal thickness < 80 km, equivalent to a plate ~ 35 Ma old in the MJP model, or ~ 65 Ma old in the GDH1 model.

At 1500 km from the ridge, the depth-averaged density within the spinel stability field is roughly 3 kg m^{-3} greater in the non-linear case than in the linear case. Within the garnet stability field, however, the depth-averaged density is slightly greater ($\sim 1 \text{ kg m}^{-3}$) in the linear case. Since the garnet stability field is thicker than the spinel stability field, these two opposite effects approximately cancel each other when averaged through the total thickness of the plate. For instance, the depth-averaged density of the oceanic plate, including the 7-km thick crust (average density $\rho_c = 2900 \text{ kg m}^{-3}$), at 1500 km from the ridge, is ~ 3314 and 3315 kg m^{-3} for the linear and non-linear model, respectively. Strikingly, these values are significantly smaller than the average density of the sublithospheric mantle right beneath the plate ($\sim 3340 \text{ kg m}^{-3}$), contrary to what is typically assumed in geodynamic models (see e.g. Schubert et al., 2001, for a review).

In a recent work, Hynes (2005) also estimated the density distribution of an oceanic plate as a function of composition, temperature, and pressure. Although the method used to incorporate these effects into the density calculation is different from that used in this thesis, the results agree well. The differences between Hynes's results and those presented in this section are attributed mainly to the different thermal models, and to the different chosen depth for the spinel-garnet transition. Hynes (2005) adopted the plate model of Parsons and Sclater (1977) and a deeper spinel-garnet transition, which results in even more buoyant plates. The general agreement between these two models, on the other hand, validates the conclusions outlined above.

The density distribution estimated in OLSM1 has important implications on the

relative stability of mature oceanic lithosphere. To fully explore this, the idealized tilted-bottom OLSM2 model will be used.

5.2.1.2 OLSM2

The OLSM2 is in essence identical to OLSM1 in terms of composition and crustal structure, but with the particular characteristic of having a dipping, smooth lithospheric bottom, assumed to be coincident with the 1300 °C isotherm. This geometry assigns a simple linear relationship between the different thermophysical properties and the local thermal structure. The plate thickens along a 1500 km profile from 50 to 125 km, hence covering a range of plate ages from approximately 20 Ma to literally infinite, except for the HSM, where the 1300 °C isotherm reaches 125 km depth at ~ 80 Ma.

The usual criterion for determining the stability of a compressible medium in the static case is to compare the density gradient in the actual static state with that of a neutrally stable reference state. The latter is characterized by the gradient of its *potential density*, defined as the density attained if a particle is taken to a reference pressure adiabatically and at constant composition (e.g. Kundu, 1990). Therefore, if the density of the actual medium decreases upwards at the same rate or faster than the isentropic neutrally case, the medium is considered to be statically stable.

In order to compare the relative buoyancy of an oceanic plate with respect to the underlying mantle, different approaches have been proposed. In the simplest case, where neither compositional variations nor compressibility is considered between the reference state and the plate, a compositionally homogeneous thermal boundary layer model can be used to estimate the force per unit area, F_{B1} , acting at the bottom of the lithosphere. This gives an expression of the form (e.g. Molnar & Atwater, 1978)

$$F_{B1} = (\rho_a - \rho_c) g h - \frac{1}{2} \rho_a \alpha T_a l g \quad (5.1)$$

where ρ_a and ρ_c are the densities of the asthenosphere and crust, g is the acceleration of gravity, α is the coefficient of thermal expansion, T_a is the temperature of the asthenosphere, l and h , are the thickness of the lithosphere and crust, respectively. The first term in Eq. (5.1) represents the buoyancy of the crust, while the second term is the force per unit area due to the cold lithospheric mantle. Hence, when Eq.(5.1) becomes negative, the plate is gravitationally unstable. Using this expression, Molnar and Atwater (1978) estimated that the oceanic lithosphere becomes unstable after $\sim 25 - 30$ Ma.

Oxburgh and Parmentier (1977) and Davies (1992) included the effect of a relatively thin depleted layer making up the upper subcrustal part of the oceanic plate. Both models assumed a depleted layer with a uniform degree of depletion and constant thickness, although they vary in the actual method to estimate the density of this layer. Neither work, however, explicitly includes pressure effects, phase changes, or detailed modelling of the mineralogical composition of the plate. Oxburgh and Parmentier (1977) used a parameter, δ , which they refer to as the “density defect thickness”, as a measure of the buoyancy of the lithosphere with respect to the undepleted mantle (reference state). This parameter is defined simply as

$$\delta = \int_{l_t}^{l_b} \frac{(\rho_m - \rho)}{\rho_m} dz \quad (5.2)$$

where ρ_m and ρ are the densities of the undepleted mantle at the temperature of the mantle beneath the plate and of the lithosphere at any given temperature, respectively; l_t and l_b the depths at the top and bottom of the lithosphere, respectively. Therefore, a positive value of δ indicates that the lithosphere has an average density less than

the underlying mantle (i.e. the lithosphere is more buoyant). Oxburgh and Parmentier (1977) calculated that oceanic plates older than ~ 40 Ma become gravitationally unstable with respect to the underlying asthenosphere.

Davies (1992) followed a similar approach and defined the age at which the plate reaches neutral buoyancy, τ_n , as

$$\tau_n = \left[\frac{h(\rho_L - \rho_c) + (\rho_D - \rho_L)\delta}{(\rho_L - \rho_M)\gamma} \right]^2 \quad (5.3)$$

where ρ_L , ρ_c , ρ_D , and ρ_M are the densities of the lithosphere, crust, depleted layer, and asthenosphere, respectively, δ the thickness of the depleted layer, h the thickness of the crust, and γ a numerical constant related to the thickness of the thermal boundary. Choosing “representative” average values, Davies (1992) concluded that an oceanic plate reaches neutral buoyancy after only ~ 22 Ma.

Although a direct comparison with these models cannot be made because of the complexity of the model presented here, a similar method to estimate the relative buoyancy of the oceanic lithosphere is adopted. Due to the lack of a homogeneous “asthenosphere” in OLSM2 in terms of its compositional, thermal, and density structure, a simple density comparison between the lithosphere and the underlying mantle is not applicable. Instead, a point-to-point comparison between the OLSM2 model and a reference mantle model is necessary. The latter needs to consider adiabatically advected undepleted mantle brought up to the depth at which the comparison is made. To carry this out, two end-member reference models of an adiabatic mantle were constructed. The first model considers an homogeneous mantle with the Primitive Upper Mantle composition as given in Chapter 2, without considering any phase change. The second model has the same composition, but it takes into account the spinel-garnet phase change. Thus, the first model (hereafter RM-SO) is expected to give upper bound values of relative

buoyancy, while the second (hereafter RM-SI) should give lower bound values. Both reference models have an surface temperature of 1280 °C (i.e. potential temperature) and the geotherms follow an adiabatic gradient of 0.4 °C km⁻¹ (e.g. McKenzie & Bickle, 1988; Schubert et al., 2001).

Once the reference models RM-SO and RM-SI are obtained, the “negative buoyancy”, F_{buoy} of OLSM2 relative to the reference models (i.e. force per unit length perpendicular to a vertical cross-section of a lithospheric column) can be calculated as

$$F_{buoy} = -g \int_A \Delta\rho(x_i) dA \quad (5.4)$$

where $\Delta\rho$ is the density difference between OLSM2 and a particular adiabatic reference model, g is the acceleration of gravity, and A is the area (in a vertical cross-section) of a column of unit width and thickness equal to the depth to the 1300 °C isotherm (note that the magnitude of the total buoyancy of any column is dependent on the chosen width, but its sign and depth-averaged density contrast are not). Therefore if the buoyancy of a certain column is positive, it follows that the lithospheric column is gravitationally stable (i.e. the depth-averaged density of the plate is less than that of the adiabatic reference model).

For comparison, a simple model with the same thermal structure than OLSM2, but with no chemical differentiation at all (i.e. including only the thermal effect) has been tested. When compared with the reference model RM-SO, this experiment should give results consistent with the predictions from simpler models such as the ones discussed above. Fig. 5.8A shows that there is a qualitative agreement. The reason for this agreement is due to the fact that previous models consider the reference model with constant density equal to that at the base of the lithosphere (see above). When more realistic adiabatic models (such as RM-SI) are considered, the density difference between

the lithosphere and the adiabatic reference model at any depth is increased. As a result, the lithosphere becomes unstable only after a few Ma. For instance, Cloos (1993) compared the density structure of oceanic plates with a reference column at a MOR, and concluded that the oceanic lithosphere becomes gravitationally unstable after only ~ 10 Ma (close to the model RM-SI/ND; Fig. 5.8A). This highlights the importance of the chosen reference model in the estimation of plate stability. Since there is still no general consensus on which reference model is more appropriate, the adopted reference model should be always clearly specified before presenting estimations of buoyancy forces.

Another important factor that complicates the comparison between different studies arises from the different thermal models used to estimate the age of the plate (i.e. the faster the predicted cooling, the sooner the occurrence of an instability). If the plate is let to thicken up to ~ 120 km in 140 Myr (e.g. closer to the PM model of Parsons and Sclater (1977)), an experiment with no depletion (RM-SI/ND in Fig. 5.8A) gives an average negative buoyancy of $\sim -8.1 \times 10^7 \text{ N m}^{-1}$ for a lithospheric column at that age. This translates into an average density contrast of $\sim 70 \text{ kg m}^{-3}$ between the lithosphere and the adiabatic reference model RM-SI. This figure is somewhat in agreement with commonly assumed values of 70 - 100 kg m^{-3} (e.g. Schubert & Zhang, 1997; Funicello et al., 2003; Niu et al., 2003).

The situation becomes significantly different when melt depletion is included in the calculations. To study this, two different lithospheric models with the thermal structure of OLSM2 were generated, one following a linear depletion trend and another with a non-linear depletion trend. These two models were then compared separately against the reference models RM-SO and RM-SI. The results are plotted in Fig. 5.8A, using the MJP model for converting thermal thickness into plate age. There are two important results shown in this figure: (a) oceanic plates become gravitationally unstable with respect to the adiabatic reference models RM-SI and RM-SO after 30 and 80 Ma, respectively;

and (b) since the thermal thickness of PMs is prescribed and asymptotic, there is a maximum negative buoyancy that a plate can attain. For plates older than 160 Ma, the maximum negative buoyancy predicted by MJP model is of the order of $-4.0 \times 10^7 \text{ N m}^{-1}$, which translates into an average density contrast of only $\sim 38.5 \text{ kg m}^{-3}$. In this case, if the plate is let to thicken up to $\sim 120 \text{ km}$, a maximum negative buoyancy of $\sim -5.6 \times 10^7 \text{ N m}^{-1}$ is obtained, indicating an average density contrast of $\sim 47.5 \text{ kg m}^{-3}$. This value is 32 % smaller than the RM-SI/ND counterpart, and significantly smaller than commonly assumed values in the literature (see above). In the extreme case represented by the combination of a linear depletion model with the RM-SO reference model, the maximum negative buoyancy and density contrast are of the order of $-1.1 \times 10^7 \text{ N m}^{-1}$ and 10.5 kg m^{-3} , respectively. Notably, if the GDH1 model is used instead as a reference for converting temperature into plate age, oceanic plates become gravitationally unstable with respect to the adiabatic reference models RM-SI and RM-SO after 50 and 160 Ma, respectively. The high temperatures within the plate do not allow a significant increase in the average density of the plate (Fig. 5.8B), giving maximum average density contrasts in the range 0 - 20 kg m^{-3} . It needs to be emphasized that this result represent an upper limit for the stability of the plate, since the GDH1 model also implies higher potential temperatures than that used to construct the adiabatic reference models.

It is important to note here that the above estimates could underestimate the positive contribution of the spinel-garnet phase transition. In all the calculations, the position of this transition was assumed to be described by the experimental results presented in Klemme and O'Neill (2000) for the usual Cr-free $\text{CaO-MgO-Al}_2\text{O}_3\text{-SiO}_2$ system. For a typical thermal structure of an oceanic plate, the spinel-garnet phase change occurs at around 50 km depth (e.g. Fig. 5.6). More recent calculations suggest that the addition of Cr shifts the transition depth towards much higher pressures than previously estimated (Klemme, 2004), increasing the stability field of spinel lherzolite. The thickening of the spinel stability field would translate into greater positive contributions to

the buoyancy of the plate, reducing even more the possibility of reaching a significant negative buoyancy. However, the effect of Cr on spinel stability seems to be small in relatively fertile compositions (Klemme, 2004) as those expected for the oceanic lithosphere. The shifting of the spinel-garnet phase change to depths of ~ 75 km would reduce the average density contrasts estimated above by as much as $\sim 8 \text{ kg m}^{-3}$.

The resulting P-wave synthetic tomography for OLSM1 is shown in Fig. 5.9. Only the non-linear depletion case is shown, since, as expected, the difference between this model and the linear model is almost nil. There are no unanticipated features in this synthetic tomography. Since the temperature effect is dominant on seismic velocities at depths < 100 km, the seismic structure of the plate mimics its thermal structure. P_n velocities increase systematically with plate age from $\sim 7.7 \text{ km s}^{-1}$ close to the ridge, to $\sim 8.2 \text{ km s}^{-1}$ at distances equivalent to a plate age of 80 Ma. Both values are in agreement with seismic data in proximities of MORs (e.g. Canales et al., 1998) and in old oceanic lithosphere (e.g. Gaherty et al., 1999; Bauer et al., 2000; Scherwath et al., 2003). A negative velocity gradient characterizes the lithospheric mantle along the whole transect, varying from $\partial V_P / \partial z \sim -1.3 \times 10^{-2} \text{ s}^{-1}$ close to the ridge, to $\partial V_P / \partial z \sim -4.6 \times 10^{-3} \text{ s}^{-1}$ at 1500 km from the ridge. Seismic velocities decrease monotonically down to the base of the lithosphere, reaching a minimum slightly below it (~ 110 km depth), from which the gradient changes sign and velocities start to follow the normal trend of the adiabatic upper mantle ($\partial V_P / \partial z \sim 3.3 \times 10^{-3} \text{ s}^{-1}$).

The modelled negative velocity gradient can be readily compared with the seismologically detected LVZ under the oceans. Fig. 5.10A shows a comparison between the predicted velocities from OLSM1 for a 90 Ma old oceanic lithosphere and the PA5 seismological model of Gaherty et al. (1999) for the ~ 100 Ma old Pacific plate. The vertical and horizontal P-wave components reported in Gaherty et al. (1999) where used to calculate the mean compressional velocity plotted in Fig. 5.10A. Although a

direct comparison is difficult due of the fact that PA5 does not include phase changes or gradual velocity changes with temperature, it can be seen that OLSM1 is in reasonably good agreement with PA5. The gradient and magnitude of compressional wave velocities predicted by OLSM1 in the mantle underneath the lithosphere are also identical to those in PA5.

For comparison, Fig. 5.10A also includes the velocity estimations by Stixrude and Lithgow-Bertelloni (2005) (hereafter SLB) for a plate of similar age. The SLB model is also based on thermodynamical and mineral physics principles, but the general approach is different from the one used in this thesis (they use a Gibbs minimization scheme for modal abundances and the Voigt-Reuss-Hill theory for the elastic properties) and therefore it can potentially provide an independent validation. The SLB model is very similar to the OLSM1, although it slightly underestimates the velocities with respect to PA5 at depths < 68 km. This discrepancy can be attributed, in principle, to the use of a “hotter” geotherm (such as the ones derived from thermal models with constant k) to calculate the T-dependent elastic properties. More important is the result from both OLSM1 and SLB models that a solid-state velocity reduction at subsolidus temperatures provides a satisfactory quantitative explanation for the commonly observed LVZ beneath oceanic LIDs. Hence, it can be concluded that the occurrence of partial melting as a necessary factor in reducing seismic velocities in the LVZ is not required (Sato et al., 1989; Stixrude & Lithgow-Bertelloni, 2005). This implies that comparisons of local seismic results with theoretical models may overestimate the amount of partial melting if the subsolidus velocity reduction is not considered. For example, 1 % partial melting can reduce seismic velocities by ~ 2 % (e.g. Sato et al., 1989). Consequently, to explain a typical reduction of $\sim 5 - 6$ % in velocity at the LVZ, an amount of partial melting close to 3 % could be argued, while only 0 - 0.5 % could explain the same observation if the solid-state velocity reduction at subsolidus temperatures is considered. This does not imply, however, that small amounts of partial melting cannot occur at all in the

LVZ. As pointed out by Stixrude and Lithgow-Bertelloni (2005), if amounts $\lesssim 1\%$ of partial melt are distributed heterogeneously over a characteristic length scale much less than that of seismic waves, the melt could be “invisible” to seismological models such as the PA5.

The results from an experiment with a thermal structure identical to the one predicted by the GDH1 model for an oceanic plate ~ 100 Ma old (i.e. model OLHPM) are plotted in Fig. 5.10B, together with the seismological models PA5 and PHB3 (Kato & Jordan, 1999). It can be seen in this figure that the lithospheric P-wave velocities predicted by OLHPM are systematically slower than those from PA5 by as much as 3.5 - 6 %, considering the range of variability on reported temperature derivatives of the elastic moduli and appropriate inclusion of anelastic effects (Section 3.6, Chapter 3). These velocities are in fact even slower than those observed in the much younger Philippine Plate (~ 40 Ma), where an extra “attenuation factor” due to an over-depleted LID produces lower seismic velocities than those explained solely by thermal evolution of the lithosphere (Gaherty et al., 1999; Kato & Jordan, 1999). This means that the PHB3 model represents a lower bound for seismic velocities on plates ~ 40 Ma old. The remarkably slow velocities predicted by GDH1 are consequently hard to reconcile with detailed available seismological information for mature oceanic plates, even when uncertainties and/or compositional differences are taken into account. It can be concluded therefore that the thermal structure predicted by the GDH1 model for oceanic plates older than 100 Ma is inconsistent with seismological models, and consequently it cannot be appropriate as a model for “normal” mature oceanic lithosphere.

5.2.2 Continental lithosphere

The purpose of this section is to obtain constraints on compositional, seismological, and tectonic models for Archean and Phanerozoic continental domains. Particular attention

will be given to: (a) the depth-distribution of depletion and the relationship between thermal and compositional boundary layers in Archean domains, and (b) the compositional effects on the gravitational stability of thickened Phanerozoic lithosphere.

5.2.2.1 Archean lithosphere

As discussed in Chapter 2, it is generally accepted that the stability of Archean cratons, which have remained undisturbed since the Precambrian, is assisted by their positively buoyant and highly viscous lithospheric mantle. The magnitude of this effect and the actual mechanism, however, remain an open question. The long-term stability of Archean lithosphere (i.e. its apparent ability to remain undeformed for several mantle overturns times) is difficult for numerical models to explain (see e.g. Lenardic & Moresi, 1999; King, 2005). Both high buoyancy and high viscosities are needed to stabilize cratonic keels in numerical models, but the depth interval and intrinsic causes are still a matter of debate (see King, 2005, for a comprehensive discussion). In the classic “isopycnic” hypothesis of Jordan (1978), a subcratonic keel is not only a thermal boundary layer (TBL), but also a compositional boundary layer (CBL), whose main effect is to offset the increase in density that occurs by conductive cooling.

The concept that the cratonic keel is neutrally buoyant at all depths is consistent with the weak correlation between long-wavelength geoid anomalies and cratons (Shapiro et al., 1999). A cratonic keel 300 km thick is $\sim 450 - 550$ and $200 - 300$ °C colder than the adiabatic mantle at 100 and 200 km depth, respectively. This translates into thermal density changes of ~ 2 and 1 % at these depths, which need to be counterbalanced by compositional heterogeneities in the “isopycnic” hypothesis. Typical density differences from Archean xenoliths are usually higher than these figures ($1.5 - 3$ %) at depths < 140 km, and smaller at greater depths (e.g. Boyd, 1989; Boyd et al., 1997; Griffin et al., 1999b; O’Reilly et al., 2001; Mooney & Vidale, 2003; King, 2005, and references

therein). Isostatic arguments also indicate that cratonic roots are either colder or less depleted than the isopycnic hypothesis (Mooney & Vidale, 2003). In addition, it is unlikely that compositional factors would exactly counterbalance thermal cooling at all depths. King (2005) has recently proposed a model for a cratonic keel that attempts to reconcile petrological and geophysical evidence (see Chapter 2). In this model, the cratonic keel is composed of two boundary layers: (a) a CBL, extending to depths of ~ 175 km, and characterized by being highly depleted (from xenolith evidence) with respect to PUM; and (b) a less depleted (but still more depleted than PUM) TBL that extends to depths of $\sim 250 - 300$ km, corresponding to the seismological keel inferred from seismic studies (Fig. 2.4, Chapter 2). In principle, this hypothesis should also be compatible with geoid observations (Shapiro et al., 1999), since the positive density anomaly from the TBL is offset by the CBL above. Although this keel model seems to be in better agreement with both petrological and geophysical evidence, it has never been quantitatively demonstrated.

From the above discussion and those in Chapters 2 and 4, it is clear that Archean lithosphere is intrinsically buoyant due to its depleted nature. Therefore, from a purely isostatic point of view, it is to be expected that the thicker the lithosphere, the higher the predicted elevation. On the other hand, since thicker lithospheres have lower average temperatures than thin lithospheres, thermal expansivity will somewhat counterbalance the compositional intrinsic buoyancy.

Due to the number of depth-dependent parameters involved in the thermal-isostatic equations of Chapter 4, a simple model that would describe the manner in which the opposite effects of compositional buoyancy and thermal expansivity interact is precluded. To obtain a self-consistent estimation of this relation, an ideal tilted-bottom lithospheric model (base = 1300°C isotherm), with a typical Archean composition, is constructed (hereafter ACSM1). The ACSM1 model is 6000 km long, and it includes a layered crust

with an upper crust 23 km thick and a lower crust 13 km thick (see physical properties in Table 5.1). The thermal thickness of the lithospheric mantle varies from 100 km at $x = 6000$ km to 295 km at $x = 750$ km, from which it remains constant. Fig. 5.11 shows the geometry of the model and its predictions of SHF, 1-D geoid height (Section 4.6, Chapter 4), and elevation. There are two important results in this figure that need to be clarified: (a) the gradual variation in the thermal thickness of the lithosphere is clearly reflected in the SHF (a consequence of assuming a crust with constant thickness) and in the geoid, which change along the transect by $\sim 12 \text{ mW m}^{-2}$ and 34 m, respectively, but is hardly noticeable in the elevation, which changes only by ~ 100 m; and (b) the predicted average elevation of the transect (~ 1800 m) is much higher than the observed elevations in Archean cratons ($\lesssim 500$ m, excepting some sectors in South Africa, India, and Australia, Fig. 4.7a).

The first result is in apparent contradiction with other common methods to calculate absolute elevations of lithospheric sections, which yield a linear relation between the elevation and the thermal thickness of the lithosphere (see e.g. Lachenbruch & Morgan, 1990; Zeyen & Fernández, 1994). It should be noted, however, that in these models the lithospheric mantle density is assumed to vary only with temperature and no compositional differences are included. Furthermore, the lithosphere is assumed to rest on a fluid asthenosphere with uniform density everywhere (3200 kg m^{-3}). These assumptions force a linear relationship between lithospheric thermal thickness and elevation (Lachenbruch & Morgan, 1990), and therefore, the thicker the lithospheric mantle becomes, the greater the subsidence that the column experiences. In the ACSM1 model, on the other hand, the modelled column reaches isostatic equilibrium at the base of the model (see Chapter 4), and consequently, the sublithospheric mantle (PUM) takes part in the isostatic balance. This implies that when the thermal lithosphere is thinned, two separate and opposite effects take place: (i) the density of the lithospheric mantle is reduced (by thermal expansion), exerting a positive contribution to the elevation; and (ii) the

average density of the whole column is increased by replacing lithospheric material with PUM (denser) material, exerting a negative contribution to the final elevation. From the results in Fig. 5.11 it can be seen that these effects almost cancel each other, although the latter is slightly more important, and therefore there is a net (but small) decrease in elevation with lithospheric thinning.

The second result may be a consequence of having used either an average composition that is too depleted (i.e. too buoyant) to be representative of the whole section, or to an incorrect depth distribution of depletion. According to the petrological and geophysical evidence discussed above and in Chapter 2, it seems probable that the high depleted nature of the Archean lithospheric mantle as sampled by xenoliths, is representative of only a limited depth interval, within the CBL, while a more fertile composition exists at deeper levels. To test the hypothesis of a layered depletion, an experiment having the same geometry than ACSM1, but including a stratified two-layer lithospheric mantle is carried out (hereafter ACSM2). In the ACSM2 model, the lithospheric mantle is composed of an upper layer with the same composition of ACSM1 and a lower layer with a much less depleted composition (similar to a typical Phanerozoic domain). The top of the transition between these two layers has been fixed at 175 km depth, and extended downwards for 35 km, where all the thermophysical properties are modelled by two buffer functions in the same manner explained in Section 4.7. The results from this experiment are shown in Fig. 5.12. As expected, the topographic and geoid signal now start to change considerably when the transition between the two mantle layers is reached by the thermal thickness. Within the two-layer domain, a change of ~ 100 km in the thermal thickness translates into a variation of ~ 1100 m in elevation. The elevation of the section at $x = 1200$ (i.e. thermal thickness = 280 km) is ~ 750 m, a value within the range of observed elevations in Archean cratons. When the thermal thickness (i.e. the thickness of the TBL in King's (2005) keel model) is allowed to reach a depth of 295 km, a value of ~ 500 m is obtained for the elevation, closer to, but still

slightly higher than, commonly observed values.

It is clear that modifying the transition depth will have an impact on elevation. The sensitivity of elevation to the depth of CBL is explored by running experiments in which the transition between the mantle layers is raised at regular steps of 10 km, while keeping the same thickness (35 km). The results indicate that elevation increases by ~ 7 m for each km of upward displacement of the transition depth. Therefore, displacing the top of the transition depth to 150 km depth produces elevations of ~ 325 m. A transition zone extending from ~ 150 to 185 km depth is in better agreement with petrological data in many Archean localities where detailed work has been done on mantle stratigraphy (Griffin et al., 1999a, 2003, W. L. Griffin, 2006, pers. commun.). Particular locations with different mantle stratigraphies are expected to deviate from this general picture. However, the requirement of a less depleted (i.e. more dense) lower lithospheric mantle in Archean domains characterized by highly depleted xenolith suites seems to be a robust result.

In this context, it has to be noted that eclogite xenoliths are a common feature in Archean xenolith suites (Griffin et al., 1999a; Kopylova & Russell, 2000; Carlson et al., 2005). Eclogites can be as much as 5 % more dense than Archean peridotites at typical lithospheric conditions (e.g. Aoki & Takahashi, 2004), which implies that 7 - 8 % eclogite can balance the inferred positive buoyancy of Archean sections (Kelly et al., 2003). Although these amounts are within the range of localized eclogite abundances in the cratonic mantle, they are significantly higher than the typical overall abundance of 1 % or less (Carlson et al., 2005). Moreover, mantle eclogites exhibit $\gtrsim 7$ % higher P-wave velocities than normal garnet peridotites (e.g. Ji et al., 2002). Hence, if kilometre-scale bodies of eclogite are present in the lithospheric mantle, they should be resolved by deep seismic imaging. Nevertheless, high-velocity bodies are generally not observed in the continental mantle, except maybe underneath the Slave Craton (Bostock, 1998) (see next

section) and in the shallow uppermost mantle beneath Fennoscandia (E. Kozlovskaya, 2006, pers. commun.).

The depth variation of P-wave seismic velocity predicted by the ACSM2 model at $x = 0$ is shown in Fig. 5.13. For comparison, both PREM (Dziewonski & Anderson, 1981) and *ak135* (Kennett et al., 1995) spherically symmetric models are also shown. When compared against a “normal” adiabatic reference model, the resultant V_P seismic anomalies at depths slices of 100 - 200 and 200 - 300 km are +3.8 and +1.5 %, respectively. When compared against the seismological models at the same depth slices, the anomalies are +3.95 and -0.1 % for PREM, and +2.4 and +0.13 % for *ak135*. Assuming that the $d\ln V_S/d\ln V_P \sim 1.5$ relation given by Bolton and Masters (2001) for the first 220 km applies here, then the above anomalies translate into S-wave anomalies of +5.7 and +2.25 % for the adiabatic reference case, +5.9 and -0.15 % for PREM, and +3.6 and +0.2 % for *ak135*. These figures are in good agreement with the range of values observed in tomographic models underneath Archean cratons (see Fig. 2.4), especially those predicted by the adiabatic reference case and the *ak135* model.

Global seismic tomography models show shear-wave anomalies of +0.5 - +1.0 % down to depths of 350 - 400 km beneath some cratons (e.g. Ritsema & van Heijst, 2000; Ritsema et al., 2004). To explore the effect of a slightly depleted, cold mantle root on seismic velocities, an experiment with a lithosphere 380 km thick is carried out (ACSM2-thick in Fig. 5.13). This experiment indicates that a composition intermediate between typical slightly-depleted Phanerozoic and highly-depleted Archean mantles is necessary in the lower lithospheric mantle layer (below the transition depth between the two mantle layers) to obtain shear wave anomalies of $\sim +0.5$ % at 350 km. Predicted heat flow remains within common values for old cratons ($\sim 37.5 \text{ mW m}^{-2}$). Unfortunately, the finite-element code LitMod cannot be used to model isostatic responses of sections thicker than 300 km in its present form, and hence no self-consistent relationship between

elevation and seismic velocities can be obtained at the depth of interest. Nonetheless, it can be speculated that the negative thermal contribution to elevation due to the thickening of the lithosphere is balanced in some degree by the higher average depletion of the lithospheric mantle necessary to satisfy the seismic evidence. A simple way to estimate this is to assume that the relation between elevation and both thermal structure and depletion derived for depths < 300 km (see above) can still be used at greater depths. In principle, since the depth-derivative of bulk density seems to increase only slightly below ~ 300 km due to the disappearance of orthopyroxene (see Chapter 2), elevations estimated using relations valid at depths < 300 km are expected to be reliable at 350 km depth. Assuming this is true, it can be predicted that the new thermal structure generates a negative contribution to elevation of ~ -1350 m, while the compositional difference generates a positive contribution of $\sim +1515$ m. This means that a 380 km thick section, having the above composition and thermal structure, should display a positive elevation of ~ 165 m, consistent with observations.

In summary, the concept of a cratonic keel being composed of two boundary layers (i.e. a thick thermal boundary layer including a chemical boundary layer in its upper part) has been shown not only to be a necessary condition (from isostatic and seismological arguments) in highly depleted domains, but also to be consistent with petrological and geophysical data. The transition between these two layers appears to be located in the depth range of 150 - 185 km. Shallower or deeper transition depths give elevations that are not consistent with topographical observations in Archean cratons. While the occurrence of $\sim 7 - 8$ vol% eclogites within the lithospheric mantle could modify the above conclusion, it seems to be an unlikely situation in most Archean cratons, as indicated by seismological studies. Observed shear wave anomalies at depths of 350 - 400 km can be reconciled with elevation data when a deep depleted layer with a composition intermediate between typical slightly-depleted Phanerozoic and highly-depleted Archean is included.

5.2.2.2 Thickened Phanerozoic lithosphere

The stability of continental lithosphere in Phanerozoic domains should be markedly different from Archean domains due to its less depleted nature (e.g. Griffin et al., 1999b; Poudjom-Djomani et al., 2001). In particular, in regions of plate convergence and continental collision, lithospheric thickening produces a downward deflection of the isotherms. The rate at which this occurs depends mainly on the balance between the convergence rate, which displaces the isotherms by advection, and thermal diffusion, which smooths out any temperature variation (e.g. Conrad & Molnar, 1997; Pysklywec & Beaumont, 2004). Consequently, it can be expected that if advection dominates over diffusion, there will be a threshold value for the maximum attainable thickness of lithospheric roots, after which the whole lithospheric section becomes gravitationally unstable. Although this concept is well known in the literature, previous models considered thermal effects only, where the lithospheric density is assumed to decrease monotonically with depth until it reaches the “asthenospheric” value (e.g. Bird, 1979; Conrad & Molnar, 1997; Morency et al., 2002; Pysklywec & Beaumont, 2004). Quantitative consideration of the effects of pressure and compositional heterogeneities are lacking.

There are two fundamental models of gravity-driven instabilities for explaining the removal of thickened lithospheric roots in continental domains, namely the *delamination* model (Bird, 1979) and the *unrooting* model (e.g. Houseman et al., 1981; Conrad & Molnar, 1997; Marotta et al., 1998). Although the distinction between these two models is not always acknowledged, they clearly represent different mechanisms (Marotta et al., 1998). In the delamination model of Bird (1979), the cold (i.e. dense) continental lithospheric mantle get disrupted when less dense asthenospheric material is brought up along a conduit, forcing a horizontal viscous flow at the bottom of the crust that decouples the buoyant crust from the dense lithospheric mantle. The lithospheric mantle is then free to sink into the asthenosphere. Due to the geometry of the model, an

asymmetric lever-like shape is predicted, with the side closer to the lithospheric conduit sinking faster (Bird, 1979). On the other hand, the unrooting model is an instance of a typical Rayleigh-Taylor (R-T) instability, involving an exponential growth rate of an initial small perturbation and the total detachment of the lower part of the instability, in a symmetric manner (e.g. Marotta et al., 1998; Pysklywec & Beaumont, 2004).

Both models require a gravitationally unstable (i.e. negatively buoyant) lithospheric column to work. This is readily attained when considering only density changes due to thermal effects. Fig. 5.14 shows a cartoon illustrating the variations in temperature and density assumed in delamination/unrooting models. It is evident that the “cold” lithosphere is gravitationally unstable at *all* times, due to its thermal structure. However, the sinking of a non-thickened lithosphere into the asthenosphere is precluded by its high viscosity. As the lithosphere thickens, the gravitational energy grows continuously, until it is rapidly released and transformed into kinematic energy when the instability is fully developed. The rate at which the potential gravitational energy increases with thermal thickness, as well as its magnitude, will be affected when introducing compositional heterogeneities into the system. Other mechanisms, such as convective erosion (e.g. Morency et al., 2002), entrainment, and engulfment (e.g. Lenardic & Moresi, 1999) of the lithospheric mantle might also take part in the removal of thickened lithospheric roots. However, these mechanisms act mainly by transmitting viscous stresses, and in principle, they require no gravitational instabilities within the lithosphere to work (e.g. Lenardic & Moresi, 1999; Morency et al., 2002; King, 2005). Here, I am interested in exploring the effect of compositional variations on the development of a negatively buoyant lithospheric column necessary to trigger a gravitational instability, and therefore deep convective effects will be ignored.

Fig. 5.15 shows the thermal structure used to simulate a symmetric lithospheric thickening in a compressive tectonic environment. Both the isotherm distribution and

wavelength of the structure are similar to the ones presented in previous models of gravitational instabilities (e.g. Conrad & Molnar, 1997; Marotta et al., 1998; Pysklywec & Beaumont, 2004). By comparison with Fig. 5a of Marotta et al. (1998), the thermal field depicted in Fig. 5.15 would be attained after approximately 60 - 70 Ma of convergence at a rate of 0.2 cm a^{-1} , which coincides with the onset of maximum acceleration (Marotta et al., 1998). The RM-SI model is used as a reference in order to compare the relative stability of a thickened lithospheric root with respect to a normal adiabatic mantle. The total buoyancy of a given column is then calculated in the same manner as in Section 5.2.1.2, using Eq. (5.4). To explore fully compositional effects, three models with the same thermal structure but with different compositions (i.e. varying degrees of depletion) were generated (PCSM1, PCSM2, PCSM3). All models include a crustal layer of constant thickness equal to 35.5 km, and therefore, buoyancy estimations ignore any contribution that may arise from crustal thickening. The omission of this effect gives an upper (lower) bound estimate of the negative (positive) buoyancy. The results from these models are shown in Fig. 5.16 in terms of the density difference ($\Delta\rho$) between the three PCSM models and the reference model as function of depth. The $\Delta\rho$ values are taken at the centre of the instability ($x = 0$ in Fig. 5.15). Included in this figure are the total buoyancy of a column of unit area and 300 km thick, and the buoyancy of the same column produced by the lithospheric mantle only (i.e. no crustal contribution).

In all cases, the total buoyancy remains positive, decreasing its value from PCSM1 to PCSM3, due to the dominant contribution of the crust. When the crustal contribution is removed, the average buoyancy of the lithospheric mantle is negative in PCSM2 (typical Phanerozoic composition) and PCSM3 (undepleted composition), but still positive in PCSM1 (composition intermediate between typical Archean and typical Phanerozoic). A closer examination of the PCSM1 and PCSM2 models reveals that the total average buoyancy of the lithospheric mantle is composed of two parts: an upper dense section and a lower buoyant section. As indicated by the negative average buoyancy of the

lithospheric mantle in PCSM2, the negative contribution of the upper section offsets the positive contribution of the lower section in this model.

From a dynamic point of view, this depth distribution of buoyancy has important implications for the final stability of the entire section. The relative dominance of the lower (positively buoyant) and upper (negatively buoyant) sections on the development of an instability depends mainly on the depth distribution of the viscosity. For instance, if half of the upper dense part is too viscous (i.e. cold) to detach itself from the upper layers, the upward “push” force exerted by the buoyant lower part will tend to support the “deformable” part of the upper section, suppressing the development of an instability. Considering the thermal field depicted in Fig. 5.15, and assuming to the first order that mantle material at temperatures $< 800\text{ }^{\circ}\text{C}$ (effective viscosities $\eta \gtrsim 10^{25}\text{ Pa s}$) is too viscous to exhibit significant deformation over time-scales of 10^7 years, material at depths $\lesssim 100\text{ km}$ would not contribute significantly to the development of a R-T instability. As a consequence, the mantle portion of PCSM1 becomes significantly more buoyant ($\sim 3 \times 10^{10}\text{ N m}^{-1}$), suggesting that this type of lithospheric mantle cannot be removed by gravitational forces alone. On the other hand, the mantle portion of PCSM2 turns out to be only slightly buoyant ($2 \times 10^9\text{ N m}^{-1}$), and therefore, it is more likely that modest temperature perturbations and/or metasomatic processes could trigger the unrooting of the thickened lithosphere.

None of the above applies to the end-member case PCSM3, representative of most models in the literature on gravitational instabilities, where the lithospheric mantle is negatively buoyant at all times and depths (Fig. 5.16).

In brief, when compositional and compressibility effects are taken into account, it seems that mechanisms other than purely thermal are necessary to destabilize the root of a thickened lithosphere with a composition typical of Phanerozoic domains. Processes such as melt injection and subsequent eclogitization, and/or asthenospheric metasoma-

tism might be necessary as driving mechanisms (e.g. Elkins-Tanton & Hager, 2000; Poudjom-Djomani et al., 2001). For example, if a gradual variation with depth is included in the PCSM2 to simulate a large-scale metasomatic refertilization event (Fig. 5.16), the lithospheric mantle becomes negatively buoyant at all depths, hence favouring the removal of the root. The above experiments provide further insight into the importance of considering petrological-geodynamic interactions in the study of gravity-driven mantle flow process.

5.3 Real cases

This section presents the results of two lithospheric transects modelled with LitMod: (a) the Namibian passive volcanic margin, and (b) the Archean Slave Craton.

The first transect was chosen due to the available detailed information of its crustal structure, with the following aims: (i) to examine the lithospheric features of a margin where old oceanic lithosphere is juxtaposed to old continental lithosphere, and (ii) to fill a gap in lithospheric modelling along the Southwestern volcanic margin of Africa. The second transect was chosen mainly due to the comprehensive information on the compositional stratification and thermal state of its lithospheric mantle, making it an ideal place to apply LitMod, and to compare the results with those obtained in Section 5.2.2.1.

Unless indicated otherwise, regional datasets used in this section are: Sandwell and Smith (1997) for free-air gravity anomalies; EGM-96 model (Lemoine et al., 1998), filtered to degree 10 (see Chapter 4), for geoid heights; ETOPO 2 (Etopo2, 2001), with a resolution of 2'x 2', for elevation.

5.3.1 Namibian volcanic margin

5.3.1.1 Geological background

Three Pan-African mobile belts with triple junction geometry characterize the geology of Namibia: The Kaoko belt, flanking the coast in the north; The Damara belt, trending NE-SW, between the Congo and Kalahari Cratons; and the Gariep belt (mostly in South Africa) to the south (Fig. 5.17). Remnants of these Neoproterozoic belts, formed during the amalgamation of South Gondwana (1000 - 450 Ma), are located on the Atlantic coast of South America (Basei et al., 2000). They have been typically interpreted as collisional orogens, although some questions regarding their origin and evolution remain (e.g. Seth et al., 1998; Passchier et al., 2002).

The Damara belt, which spatially separates the other two, represents the eroded core of an aulacogen originated around 900 Ma, which has been later affected by a continental collision between the Congo and Kalahari Cratons in the early Cambrian (Miller, 1983; Goscombe et al., 2003). Its crystalline units are mainly composed of amphibolite-grade metasediments and several post-tectonic granitic intrusions (Miller, 1983). It is overlain by sediments of Permian and Mesozoic age (Karoo Group), and by volcanic rocks (mostly flood basalts) of the Etendeka Group, extruded in the early Cretaceous. This magmatic pulse (age ~ 132 Ma), followed by multiple minor pulses, was also responsible for the extrusion of Paraná lavas in Brazil during the opening of the South Atlantic (Peate et al., 1992). Another important expression of Mesozoic magmatism in this area is the emplacement of more than 20 subvolcanic bodies (Damaraland complexes), which extend from the coast up to ~ 350 km inland (e.g. Mingram et al., 2000). Both the volcanism and the intrusive activity are usually interpreted as a consequence of the activity of the Tristan da Cunha mantle plume (e.g. Milner & le Roex, 1996).

Of particular interest here are the two ring-shaped complexes known as Cape Cross

and Messum intrusions (Fig. 5.17). Both of these intrusions cut Etendeka basalts, although their respective ages do not differ by more than ~ 4 Ma (e.g. Schmitt et al., 2000). The Cape Cross ring complex is located at the present coastline, with more than half of it located offshore. Its shape and extension are clear from magnetic and gravity data (Fig. 5.18). Although there are just a few exposures onshore, its composition appears to be dominated by gabbros, granites, and syenites. The Messum ring complex has an internal structure consisting of three concentric zones: gabbros, anorthosites, and granitoids make up the outer ring; the intermediate zone is mostly composed of granitoids; and the core zone comprises mainly syenitic intrusions (Schmitt et al., 2000).

The early Cretaceous volcanism is associated with the completion of the continental breakup and the opening of the Atlantic Ocean. Although the history of sea floor spreading is well constrained only from anomaly 34 to present (Nürnberg & Müller, 1991), there is general agreement that the oldest magnetic seafloor-spreading anomaly recognized offshore Namibia correlates with M4 (~ 126 Ma) (e.g. Rabinowitz & LaBrecque, 1979; Nürnberg & Müller, 1991). This indicates that the extrusion of lavas of the Etendeka Group and the emplacement of Damaraland complexes commenced just shortly before, or simultaneously with, the onset of seafloor spreading (Gladchenko et al., 1998). This major igneous activity is also supported by seismic data offshore Namibia and Argentina, which have recognized relatively thick wedges of basaltic seaward dipping reflectors (SDRs) on both sides of the South Atlantic (e.g. Gladchenko et al., 1998; Hinz et al., 1999; Bauer et al., 2000).

5.3.1.2 Available geophysical data

Numerous hydrocarbon-related exploration surveys have been carried out on the Namibian continental shelf. These include more than 14,000 km of commercial reflection-refraction seismic profiling, gravimetry, and aeromagnetic surveys (Green, 1983; Maslanyj

et al., 1992; Light et al., 1992; 1993; Clemson et al., 1997; Gladczenko et al., 1997; 1998; Bauer et al., 2000).

Gladczenko et al. (1997, 1998) investigated the deep structure of the crust using commercial seismic data that included four multi-channel seismic lines offshore of the Damara belt, recorded to a maximum of 14 s two-way travel time. They pointed out the occurrence of voluminous basaltic flows related to SDRs to the south of the Walvis Ridge, and the existence of anomalous high-velocity bodies under the transitional crust, interpreted as underplating material. These and other characteristics (e.g. thick initial oceanic crust, intrusives in the sedimentary column), led Gladczenko et al. (1998) to classify the Namibian continental margin, south of the Walvis Ridge, as a typical volcanic margin. A combined seismic-gravity crustal model of their transect 4 (shown in Fig. 5.17; see also Fig. 14 in Gladczenko et al., 1998), covers ~ 300 km from continental, through transitional, to normal oceanic crust. Their density model, derived only from seismic velocities, satisfies the observed gravity anomalies, except for the gravity high associated with the Cape Cross ring-shaped complex, which is not evident in seismic modelling. To fit this feature, a density contrast $> 50 \text{ kg m}^{-3}$ with surrounding rocks was assigned to this intrusive (Gladczenko et al., 1998).

Bauer et al. (2000) presented magnetic and refraction/reflection seismic data on two transects across the Namibian margin. Transect 1 (modelled in this thesis) extends for 500 km, from normal oceanic crust (approx. anomaly M2) up to 100 km inland. It is similar to transect 4 of Gladczenko et al. (1998), making possible a qualitative comparison between them (Fig. 5.17). These authors have modeled magnetic and gravity anomalies, obtaining similar results to those previously found by Gladczenko et al. (1998). The two velocity-depth-density models presented by Gladczenko et al. (1998) and Bauer et al. (2000) are comparable and consistent. The existence of SDRs in the Namibian margin, and high-velocity bodies in the lowermost crust below them, was

confirmed by Bauer et al. (2000). They also suggested that the seismic characteristics of the material beneath the zone of SDRs can only be explained by an igneous composition, and that the transitional crust consists completely of accreted igneous material, with an extended and rifted continental crust almost absent. This led Bauer et al. (2000) to propose that an abrupt continental rupture over a narrow rift controlled the formation of the Namibian margin, in contrast to previous interpretations (e.g. Davison, 1997; see also Holbrook et al., 1994; Geoffroy, 2001). Again, a correction in density of about 50 kg m^{-3} had to be applied to the Cape Cross anomaly in order to fit the observables. More recent studies also corroborate the continuation of Cape Cross and Messum intrusives down to Moho depths (Bauer et al., 2003).

Free-air gravity data in the ocean and continent were obtained, respectively, from Sandwell and Smith (1997) and Vietor et al. (2001). Surface heat flow (SHF) is the least constrained observable. There are only 11 published measurements in the area of interest, both onshore and offshore (Pollack et al., 1993). Nevertheless, the general trend of decreasing SHF from continent to ocean is evident from these measurements (Fig. 5.18), also when the regional database of South Africa is taken into account (Pollack et al., 1993). Values for the oceanic domain range between ~ 30 and 46 mW m^{-2} , with only one extreme value of 57.8 mW m^{-2} , close to the Walvis Ridge. These values are rather low in comparison with actual average estimates of $\gtrsim 50 \text{ mW m}^{-2}$ for deep oceanic basins but they are consistent with values estimated in oceanic areas $> 120 \text{ Ma}$ old (Pollack et al., 1993). Onshore measurements range between ~ 60 and 72 mW m^{-2} , with some isolated values $> 75 \text{ mW m}^{-2}$. These figures are appreciably higher than average values for similar continental areas, but they still are within the range of variability (Jones, 1987; Artemieva & Mooney, 2001). Here I assume an uncertainty of $\pm 15 \text{ mW m}^{-2}$ in SHF, which is also in good agreement with the total uncertainty resulting from errors in the calculation/estimation of the thermal conductivity and radiogenic heat production, poor sampling, and subsurface water circulation (see e.g. Jaupart & Mareschal, 1999).

5.3.1.3 Modelling results

Forward modelling using the finite element code LitMod was applied to the selected transect (transect 1 of Bauer et al., 2000; hereafter NMRS1). For sake of comparison, the same transect was modelled with the original code CAGES, modified to include the temperature-pressure-composition dependent coefficient of thermal expansion (hereafter NMRS2). An initial lithospheric model was constructed based on thermal thickness data obtained in previous works (Artemieva & Mooney, 2001). Results from this preliminary model were then compared with available geophysical data, and modified accordingly to obtain a simultaneous fitting of all the observables.

The crustal thickness and its internal structure is known in reasonable detail as a result of numerous seismic studies performed in the continental margin of Namibia (e.g. Light et al., 1992; 1993; Gladczenko et al., 1997; 1998; Clemson et al., 1997; Bauer et al., 2000; 2003). Only small uncertainties are associated with Moho depths and crustal densities along the transect. Sediments densities and the subsurface shape of the intrusives, on the other hand, are the main sources of uncertainty. Although the Namibian offshore platform does not exhibit large sediment thickness, the uncertainty in sediment densities can appreciably affect the final results (due to their proximity to the surface). Following the results of Gladczenko et al. (1998) and Bauer et al. (2000), I have chosen an average density of 2200 kg m^{-3} for the sedimentary layers (Table 5.2), in agreement with other direct estimates in this margin (Bolli et al., 1978). In the case of Cape Cross and Messum intrusives, there is no clear seismic constraint for their geometry, except that they show a high reflection strength down to Moho depths, suggesting their continuity from the surface down to the base of the crust (Bauer et al., 2000; 2003). Therefore, I have modelled the shape of these bodies to fit the observed free-air gravity anomaly, which is the most sensitive observable to crustal density variations.

The presence of high velocity bodies in the continent-ocean transition zone seems to be a robust result in the Namibian margin. Gladchenko et al. (1998) estimated maximum P-wave velocities of $\sim 7.4 \text{ km s}^{-1}$ for the lowermost transitional crust, corresponding to densities of $\sim 3100 \text{ kg m}^{-3}$. Bauer et al. (2000) computed maximum P-wave velocities of $\sim 7.6 \text{ km s}^{-1}$ for similar bodies, with a resulting density of $\sim 3200 \text{ kg m}^{-3}$. In accordance with these results, I have assigned a density of 3150 kg m^{-3} to the lowermost body, which decreases linearly upwards to the top of the anomalous high velocity zone, where it reaches a value of 3000 kg m^{-3} . Fig. 5.19 shows a comparison of the final crustal model as predicted by LitMod and that presented by Bauer et al. (2000), from which the initial density model was taken. Compressional velocities were converted to densities using global velocity-density databases (Christensen & Mooney, 1995). The Moho depth beneath the Messum intrusive was taken from Bauer et al. (2003). It is evident that no major discrepancies, neither in density nor in structure, are present between the modelled crustal structure and that from Bauer et al. (2000).

It is assumed in the computations that: (a) thermal steady state applies, (b) the density of the lithospheric/sublithospheric mantle is temperature-pressure-composition dependent, (c) local isostasy is appropriate. The first assumption is justified along the entire transect. In the continental domain, the last tectonothermal episode that affected the lithosphere is $> 100 \text{ Ma}$ (Early Cretaceous, see Section 5.3.1.1), and therefore a steady-state conductive regime is approximately applicable. In the oceanic domain, thermal models indicate that departures from thermal equilibrium in old plates ($> 100 \text{ Ma}$) are unimportant (see Section 5.2.1). The second assumption presupposes that the composition of the lithospheric mantle is traceable to some degree. The composition of the continental lithospheric mantle was chosen from xenolith data from various sites in Southern Namibia (Pearson et al., 1994; Franz et al., 1996) and from regional databases in Proterozoic terranes (Griffin et al., 1999b; O'Reilly et al., 2001). In the case of oceanic lithosphere, the general method explained in Chapter 2 and Section 5.2.1 was applied.

The final modal compositions are listed in Table 5.3. When modelling the transect with a variable CTE (NMRS2), the approach depicted in Chapter 3 was adopted to predict the CTE as a function of temperature, pressure, and composition, in both continental and oceanic lithospheres. Also, a constant density asthenosphere has to be assumed in this approach (see Table 5.2).

The third assumption needs some explanation for this particular case. The finite-element code LitMod assumes that isostatic equilibrium is reached by means of local isostasy. The calculations presented in this section show a good long-wavelength correlation between the predicted and observed elevation, which is also controlled by the fitting of the remaining observables. There is, however, one important deviation in predictions from local isostasy in the continental domain associated with the intrusive bodies near the coast, namely Cape Cross and Messum intrusions (Figs. 5.17 and 5.19). These anomalously dense bodies significantly affect the calculated elevation, which is particularly sensitive to lateral density heterogeneities under the local isostasy assumption. Fig. 5.20 shows the resulting topography when the intrusions are considered. Clearly, these features must be supported by other isostatic mechanisms. Also, trying to compensate this departure from the observed elevation by reducing the lithospheric thickness under the intrusions leads to an unrealistic short-wavelength thinning that is not supported by the other observables. The shapes of both ring-complexes are constrained by aeromagnetic and gravity studies (Bauer et al. 2000; 2003), which indicate diameters less than 50 km. Subsurface structures with these densities and sizes are not expected to be compensated, since the flexural rigidity of the lithosphere is able to support the load, preventing any important local deflection (cf. Watts, 2001). The equivalent vertical force due to this density anomaly can be estimated as

$$F = \pi \left(\frac{d}{2} \right)^2 h \Delta \rho g \quad (5.5)$$

where $\Delta\rho$ is the density difference between normal crust and the intrusive, g is the acceleration of gravity, and h and d are the mean height and diameter of the intrusive, respectively. Using representative values for this case ($\Delta\rho = 70 \text{ kg m}^{-3}$, $h = 25 \text{ km}$, $d = 30 \text{ km}$) I obtain a force of the order of $1.2 \times 10^{16} \text{ N}$. This force can be used to estimate the resulting deflection and radius of regionality in a thin shell with an elastic thickness $T_e = 20 \text{ km}$. When the flexural behaviour is taken into account, the maximum predicted deflection is about 40 m, and it is reduced to 10 % of this value at a distance of 100 km. This is clearly beyond the resolution of the data and indicates that the density anomaly due to the intrusives cannot generate any significant local change in the elevation, contrary to what local isostasy predicts. It is also noted that the T_e used above is a lowermost limit suggested for the study region (Stewart et al., 2000). Effective elastic thicknesses $> 20 \text{ km}$, more in agreement with mean values proposed for this area (Stewart et al., 2000), reduce the above estimates even more. Other two small areas, one above the anomalous high-velocity bodies and the other associated with an offshore gravity high, show a small departure from observations (Fig. 5.20). Again, both areas are associated with short-wavelength density anomalies (high-velocity bodies and an edge effect in the oceanic crust; Bauer et al., 2000), and can also be explained in terms of lithospheric flexural support.

The best-fitting model using LitMod (NMRS1) that simultaneously reproduces SHF, geoid height, free-air anomalies, and elevation data, is shown in Fig. 5.21. Model predictions are in very good agreement with observations for both short and long-wavelength patterns. The calculated SHF shows the worst fit to observed values, although it is always within the error margins. In order to fit the average SHF of $\sim 60 \text{ mW m}^{-2}$ in the continental domain, I have used slightly high radiogenic heat production rates in comparison with common values used in lithospheric modelling (Table 5.2). However, both values for upper and lower crust are within the range obtained in the adjacent Proterozoic region of Namaqua mobile belt, where SHF and radiogenic heat production

rates of the order of $61 \pm 11 \text{ mW m}^{-2}$ and $2.3 \pm 1.1 \mu\text{W m}^{-3}$ were estimated, respectively (Jones, 1987). However, due to the relatively high uncertainty associated with this observable, comparisons between observed and predicted values are not conclusive. Calculated elevation shown in Fig. 5.21 includes corrections for flexural isostasy in areas with short-wavelength density anomalies (see above). The results indicate a nearly constant oceanic lithospheric thickness of $\sim 100 \text{ km}$ (depth to the 1300°C isotherm) in the first 100 km of the profile, up to magnetic anomaly M4. This geometry is constrained by the variation pattern of geoid height and absolute elevation, which are particularly influenced by the topography of the LAB. In the continental section the LAB reaches depths of $\sim 180 \text{ km}$, deepening slightly further east where it could attain values $> 220 \text{ km}$ well inside the craton (see e.g. Artemieva & Mooney, 2002). Most of the reduction in lithospheric thickness along the transition region between continental and oceanic domains is produced along a relatively short lateral distance of only 150 km.

The LAB geometry resulting from the best-fitting model using the temperature-pressure-composition dependent CTE approach (NMRS2) is also shown in Fig. 5.21. NMRS2 has an identical crustal structure and crustal physical properties to NMRS1, and fits the observables with the same precision. The main difference between NMRS1 and NMRS2 is the slightly thicker oceanic lithosphere and thinner continental lithosphere predicted by NMRS2. Besides this, the two models are identical.

The final models for thermal structure, CTE distribution, and P-wave velocities are shown and compared in Fig. 5.22. Moho temperatures varies from $\sim 200 - 300^\circ\text{C}$ in the oceanic domain, which is consistent with predictions from cooling models for lithospheres of similar age (Doin & Fleitout, 1996; Parsons & Sclater, 1977; Stein & Stein, 1992), to $\sim 550 - 600^\circ\text{C}$ under the Damara Belt. Although the total change in Moho temperature between the oceanic and continental domains is of the order of 400°C , the average lateral thermal gradient along the Moho is notably small (approx. 1°C

km⁻¹).

The CTE distribution used in NMRS2 is shown in Fig. 5.22B. In the oceanic domain, where the plate is relatively thin and the geotherm steep, the amplitude in the variation of the CTE is important (i.e. the effect of the temperature is more significant), varying non-linearly from $\sim 3.00 \times 10^{-5}$ to $\sim 3.60 \times 10^{-5}$ K⁻¹ at 16 and 110 km of depth, respectively. The higher relative content in olivine with respect to continental lithosphere also favours this situation (Boyd, 1989; Afonso et al., 2005). The depth-averaged CTE is $\sim 3.44 \times 10^{-5}$ K⁻¹, which is within the error margins of previous estimations from inversion techniques (Parsons & Sclater, 1977; Stein & Stein, 1992; Doin & Fleitout, 1996). In the continental domain, the CTE variation pattern is quite different. Values decrease almost linearly from $\sim 3.35 \times 10^{-5}$ to 3.15×10^{-5} K⁻¹ at 42 and 184 km of depth, respectively, with a mean value of $\sim 3.27 \times 10^{-5}$ K⁻¹, somewhat lower than the one in oceanic lithosphere. The small difference between CTE mean values for oceanic and continental domains (~ 5 %) would have permitted in this case the use of a constant value for the whole lithospheric mantle. This is a particular consequence of a local combination of lithospheric thicknesses, temperature and pressure distribution, and composition. However, as Afonso et al. (2005) pointed out, the choice of a constant CTE for different lithospheric domains is not always justified, and representative numbers need to be estimated in each particular case.

Models based on inversion techniques give not only the CTE as an output, but also the age dependence of the SHF and the depth of the ocean floor with respect to the mid-oceanic ridge crest under certain boundary conditions (e.g., plate thickness, and temperature or heat flow at the LAB). Parsons and Sclater (1977) (PS) reported best-fitting values of $3.28 \pm 1.19 \times 10^{-5}$ and $3.1 \pm 1.11 \times 10^{-5}$ K⁻¹ for the North Pacific and North Atlantic, respectively. Their preferred plate thicknesses are 125 ± 10 km and 128 ± 10 km for the same regions. Stein and Stein (1992) (SS) found a slightly smaller

value of $3.1 \pm 0.8 \times 10^{-5} \text{ K}^{-1}$ and an asymptotic plate thickness of $95 \pm 15 \text{ km}$. Doin and Fleitout (1996) (DF) obtained values ranging from 3.34 to $4.2 \times 10^{-5} \text{ K}^{-1}$, with a preferred CTE of $3.85 \times 10^{-5} \text{ K}^{-1}$. Although their asymptotic plate thickness is $> 100 \text{ km}$, their model indicates a lithosphere $\sim 85 \text{ km}$ thick for plates $\sim 120 \text{ Ma}$ old. This reduced lithospheric thickness is mainly a consequence of more recent estimates of around 50 mW m^{-2} for the average heat flow in old oceanic basins. In the DF model, the high CTE assumed in the calculations also favours a thin lithosphere, due to the inverse trade-off between CTE and lithospheric thicknesses. While the PS plate model fits better the observed bathymetry for old oceanic basins, the SS and DF models appears to be in better agreement with SHF data (see discussion in Schubert et al., 2001, p 141).

In NMRS1, the oceanic lithosphere has a depth-averaged CTE value of $\sim 3.44 \times 10^{-5} \text{ K}^{-1}$ and a thickness of $\sim 100 \text{ km}$, while the continental lithosphere reaches a thickness close to 180 km . Fernández et al. (2004a) also estimated thicknesses of $\sim 100 \text{ km}$ in oceanic lithosphere of similar age in the SW Iberian margin by considering a constant CTE value of $3.5 \times 10^{-5} \text{ K}^{-1}$. I have calculated the effect of changing the CTE values in the final model. Potential fields and elevation can be fitted with almost the same precision as in NMRS1 in the three cases (i.e. PS, SS, DF). However, the SHF varies significantly from one model to another. The use of a $\text{CTE} = 3.85 \times 10^{-5} \text{ K}^{-1}$ (DF) implies a reduction of the oceanic lithosphere from ~ 100 to 85 km , and from ~ 180 to 150 km in continental lithosphere to reproduce observable data. The SHF in the oceanic domain increases from $\sim 40 \text{ mW m}^{-2}$ to $\gtrsim 50 \text{ mW m}^{-2}$, representing a difference of $\sim 25 \%$. Using a CTE of $3.1 \times 10^{-5} \text{ K}^{-1}$ (SS) and a thickness of $\sim 90 \text{ km}$ for the lithosphere make more difficult to reconcile the observables than in the previous case. Potential fields can be better modelled with a lithospheric thickness of 100 km only if the density of the crust (mainly the shallowest sedimentary layers) is increased on the average by $\sim 150 \text{ kg m}^{-3}$. Although this value might be considered to be within the uncertainties in sediment densities, an average value $\gtrsim 2300 \text{ kg m}^{-3}$ for oceanic sediments seem to be

too large (i.e. it corresponds with P-wave velocities of $\sim 3.7 - 4.0 \text{ km s}^{-1}$, see Fig. 13 in Bauer et al., 2000).

Another independent validation of the models can be attempted by comparing their predictions for continental lithosphere with estimations from xenolith and geothermal studies. In this manner, extrapolating the CTE values proposed by SS to the continental domain, a lithosphere 155 km thick is necessary to fit the observables. Similarly, applying DF numbers, a comparable thickness of 150 km is found. These estimates are considerably lower than that of $\sim 200 \text{ km}$ proposed by independent models of stable continental lithospheres (e.g. Rudnick et al., 1998; Jaupart & Mareschal, 1999; Poudjom-Djomani et al., 2001), as well as from seismic evidence (Priestley et al., 2006). Although considerable variability is associated with thickness estimations in Proterozoic terrains (e.g. Artemieva & Mooney, 2002), the value of $\sim 180 \text{ km}$ from NMRS1 is closer to these estimations.

A remarkable feature of the Namibian margin is that the seafloor bathymetry near the ocean-continent boundary is about 3500 - 3700 m, contrasting with the $\sim 5700 \text{ m}$ predicted by plate cooling models. This misfit of more than 2000 m is mainly due to the presence of a 2.5 - 3 km thick sedimentary layer and a 4 - 5 km thick oceanic layer 3 (e.g. Gladchenko et al., 1998; Bauer et al., 2000). Considering densities of 2200 kg m^{-3} for sediments and 3000 kg m^{-3} for the oceanic layer 3, the contributions to the seafloor buoyancy are about 1450 m and 550 m, respectively. This suggests that the margin is not affected by local density anomalies, neither within the lithospheric mantle nor at sublithospheric levels, and therefore, plate-cooling models apply. It is also consistent with the assumption that any possible disturbance on the density structure (i.e. thermal structure) of the lithospheric mantle produced by the Tristan da Chuna plume should be negligible.

Fig. 5.22C illustrates the computed lithospheric synthetic tomography. The clearest

result is the distinction in the velocity-depth distributions between the oceanic and continental domains, which supports previous results from mantle seismic tomography studies in ocean-continent transitional areas (Forte et al., 1995). In the continent, the combined effect of a relatively cold geotherm and a thick plate is evident. P-wave velocities in the lithospheric mantle increase linearly from ~ 8.0 at the Moho to ~ 8.2 km s⁻¹ at 200 km of depth, respectively. In the oceanic domain, a general non-linear reduction is observed due mainly to the steeper geotherms. Calculations predict that the P-wave velocity decreases from ~ 8.15 km s⁻¹ immediately below the Moho, to ~ 7.9 km s⁻¹ at 100 km of depth, from which they begin to increase with depth. It is emphasized that : (a) on the oceanic side, predicted P_n velocities are in good agreement with those estimated by Bauer et al. (2000) and other studies in old oceanic lithosphere (e.g. Scherwath et al., 2003); (b) on the continental side, predicted P_n velocities are ~ 1.8 % slower than those estimated by Bauer et al. (2000); (c) compared with *ak135* (Kennett et al., 1995) and PREM (Dziewonski & Anderson, 1981), the predicted P-wave velocity anomalies in continental lithosphere are ~ -0.12 and $\sim +0.17$ %, respectively, between 70 and 210 km of depth; (d) in the oceanic domain, the velocity perturbation is ~ -0.34 % between 20 and 120 km depth in comparison with *ak135*, and ~ -0.9 % at the same depth in comparison with PREM.

I am not aware of any detailed P-wave seismic tomography in this area, and therefore a direct validation of the results is precluded. The most reliable seismic model in the area of interest is the recent S-wave model of Priestley et al. (2006), based on surface wave data with better resolution than previous globally-derived surface wave models. For a depth slice at 150 km depth, this model shows a gradual reduction in S-wave anomalies along the NMRS1 transect from ~ 0.0 % in the continental side, to ~ -1.5 % in the oceanic domain (with respect to the 1-D “smooth PREM” profile; Fig. 3a of Priestley et al., 2006). Assuming that $d \ln V_S / d \ln V_P \sim 1.5$ in the first 220 km of the upper mantle (Bolton & Masters, 2001), Priestley’s model results in P-wave anoma-

lies of ~ 0.0 and -1.0 % in the continental and oceanic side, respectively. Predictions from NMRS1 are therefore in qualitative agreement with Priestley's model. However, predicted Pn velocities in the continental side ($\sim 7.95 \text{ km s}^{-1}$) are still considerably slower than observed values ($\sim 8.1 \text{ km s}^{-1}$, Bauer et al., 2000). There are two possible explanations for this discrepancy: (a) the petrological model (based on xenolith data) assumed in NMRS1 is not appropriate for the uppermost part of the lithospheric mantle; or (b) measurements may be affected by anisotropy in the lithospheric mantle. The first explanation is difficult to assess, since no detailed petrological model is available for this area. In principle, although subject to significant uncertainties, the results of Priestley et al. (2006) support the assumed petrological model. Nevertheless, they give no relevant information on the model's composition at depths $< 50 \text{ km}$. Regarding the anisotropy explanation, although Priestley et al. (2006) showed that the direction of fast horizontally-propagating waves is parallel to the NMRS1 transect, and therefore predicted velocities could be underestimated, the azimuthal anisotropy at depths $< 150 \text{ km}$ is weak (~ 1 %) and it cannot explain alone the discrepancy between predicted and observed Pn velocities. Thus, if the reported anisotropy is representative of the first 150 km , it is concluded that a slightly more depleted composition (less dense) than that suggested by xenolith data is necessary in the uppermost lithospheric mantle to reconcile predicted and observed Pn velocities.

5.3.2 The Slave Craton

5.3.2.1 Geological background

The Slave Craton is a relatively small ($\sim 210\,000 \text{ km}^2$) and well-exposed Archean block within the larger North American craton. The oldest rocks on Earth, more than 4.0 Ga old, occur in this granite-greenstone geological province (e.g. Bowring et al., 1989;

Bowring & Williams, 1999). It is located within the Northwest Territories of Canada, comprising the Contwoyto and Anton domains, and bounded on the east by the Thelon Orogen (~ 2.2 Ga) and on the west by the Wopmay Orogen (1.9 - 2.1 Ga) (Fig. 5.23). Its northern boundary corresponds to the Proterozoic Bear Province and Arctic Platform, and its southern limit is an ancient (1.8 - 2.0 Ga) intracontinental transform fault (Great Slave Lake Shear Zone) that has juxtaposed the Archean rocks of the Slave Province against the Proterozoic rocks of the Churchill Province (Fig. 5.23).

The tectonic history of the Slave Province spans the period from the formation of the Acasta gneiss in the western Anton terrane, ~ 4.0 Ga ago (Bowring et al., 1989), to the final assembly of the craton, ~ 2.5 Ga ago (Kusky, 1989; Davis & Hegner, 1992; Kusky, 1993). Based on crustal ages and structural evidence, Kusky (1989) and Davis and Hegner (1992) interpreted the Acasta gneiss as the remains of a larger Archean terrane or microcontinent that was accreted at ~ 2.6 Ga, via eastward subduction, to a younger accretionary prism and island arc complex, now constituting the eastern Slave. Alternatively, Bleeker (2003) suggested that the eastern Slave may represent a highly attenuated and modified Mesoproterozoic lithosphere generated as a consequence of a rifting process at ~ 2.85 - 2.70 Ga. Its crystalline basement preserves a complex polyphase evolution, involving at least 10 distinct magmatic and/or metamorphic events between 4.0 and 2.85 Ga (e.g. Davis et al., 2003, and references therein). The transition between this period of high magmatic/metamorphic activity and the beginning of basement stability started with the deposition of quartzites and iron banded formations at 2.85 - 2.80 Ga (Bleeker et al., 1999). Major regional tectonic events and plutonism continued through the interval 2.80 - 2.60 Ga (e.g. van der Velden & Cook, 2002), foremost among which are the generation and closure of the Burwash Basin (2.68 - 2.63 Ga; e.g. Ferguson et al., 2005) and the granitic plutonism at 2.63 - 2.60 Ga, ascribed to a widespread thermal anomaly (Davis et al., 2003). The causative process for this thermal disturbance still is a matter of debate. Models to explain this event include lithospheric delamination

(Davis et al., 1994) and post-collisional extension (Kusky, 1993). More recently, Griffin et al. (1999a) suggested that the arrival of a plume head can explain not only the thermal disturbance and consequent plutonism, but also the distinct stratified nature of the lithospheric mantle.

5.3.2.2 Available geophysical and petrological data

Most of the available geophysical information in the area of interest has been obtained in the last 15 years as part of the LITHOPROBE multidisciplinary project, which includes seismic reflection, refraction and magnetotelluric (MT) data collected along ten transects across Canada (see e.g. Cook & Erdmer, 2005). The first multichannel seismic reflection study in the Slave Craton was undertaken as part of the SNORCLE (Slave-Northern Cordillera Lithospheric Evolution) Transect in 1996 (Cook et al., 1998, 1999; Cook & Erdmer, 2005). From east to west, SNORCLE line 1 runs from the Archean Slave Province to the accreted Proterozoic domains of the Wopmay Orogen and Fort Simpson basin (Cook et al., 1998). The initial interpretation of SNORCLE line 1 established the regional features of the crust and uppermost mantle. More recently, a reinterpretation of the main reflectors was given by van der Velden and Cook (2002), who showed a crust characterized by a complex reflectivity pattern, probably indicating tectonic wedging during the late Archean.

Also as part of LITHOPROBE, the SNoRE (SNORCLE Refraction Experiment) 97 seismic refraction/wide-angle reflection experiment was carried out in 1997 along the same previous SNORCLE transect (Fernández Viejo & Clowes, 2003). This study included a total of 594 seismographs, deployed every 1.2 km, with one- and three-component instruments interspersed. Eleven shots with charge sizes between 400 and 3000 kg of explosives were detonated along the line, and two additional shots were sited about 200 km off the line to provide information about the deep lithospheric mantle

structure (Fernández Viejo & Clowes, 2003). A relatively simple velocity structure was inferred for the crust, which is composed of three layers with distinctive velocities, and a nearly horizontal Moho at ~ 33 km depth. The transect modelled in this thesis (line “T” in Fig. 5.23) corresponds to the “segment A” of line 11 in Fernández Viejo and Clowes (2003).

Bostock (1998) used three-component, broadband teleseismic data to investigate the mantle structure below the southern Slave Province down to depths of ~ 250 km. Results showed that a well-developed horizontal mantle stratigraphy characterizes the lithospheric mantle in this region. Varying degrees of seismic anisotropy in the lithospheric mantle, including a layer of depth-localized anisotropy ($\pm 5\%$) at $\sim 70 - 80$ km, were also identified.

Bouguer anomalies and elevation data were taken from the Canadian Gravity Data Base (<http://gdcinfo.agg.nrcan.gc.ca/cat/indexgrave.html>) and from LITHOPROBE Seismic Processing Facility (LSPF) (<http://www.litho.ucalgary.ca>), respectively. Reliable heat flow data in the area of interest are scarce. The only SHF field measurement reported at Yellowknife comes from the work by Lewis and Wang (1992), who estimated values between 53.3 and 54.4 mW m^{-2} . Previous estimates in the northern part of the Slave craton are in the same range (see e.g. Russell & Kopylova, 1999, and references therein). These relatively high values of SHF differ from most paleogeotherm estimations from thermobarometry in xenoliths, which indicate conductive model geotherms corresponding to SHF between $35 - 40$ mW m^{-2} for the Slave Craton (e.g. Griffin et al., 1999a; MacKenzie & Canil, 1999; Menzies et al., 2004). MacKenzie and Canil (1999) pointed out that the discrepancy between measured values and geotherm estimations based on xenoliths can be reconciled if crustal heat production values are raised to average values of ~ 1 $\mu\text{W m}^{-3}$. These figures are somewhat higher than average heat production values in Archean cratons (e.g. Rudnick et al., 1998). However, they are

supported by the high crustal heat production values measured by Thompson et al. (1996) in crustal rocks of the Central Slave, which has been shown to be as high as 5 to 15 $\mu\text{W m}^{-3}$.

There has been much work done on mantle xenoliths from the Slave craton in the past eight years. Due to the recent discovery of its diamondiferous potential, numerous kimberlite pipes are being exploited in the Slave Province, providing an unique opportunity to examine material from the mantle beneath the craton. In an analysis of xenoliths and heavy mineral concentrates from the Lac de Gras area, Griffin et al. (1999a) mapped the thermal and compositional structure of the lithospheric mantle beneath the Central Slave. Results revealed a lithospheric mantle characterized by a distinct two-layer compositional structure: a shallow ultradepleted layer and a deeper less depleted layer. The sharp boundary between them is found at an approximate depth of 140 - 150 km. Griffin et al. (1999a) interpreted the upper layer as a remnant of an ancient ultradepleted oceanic/arc lithosphere that was underthrust during the accretion of the Hackett and Contwoyto terranes. The deeper layer, on the other hand, was interpreted as plume material accreted from the lower asthenosphere at ~ 2.6 Ga. This interpretation is consistent with the widespread post-tectonic magmatism during the the same period (see above), as well as with the presence of abundant lower-mantle inclusions in diamonds from the region (Griffin et al., 1999a). Kopylova and Russell (2000) showed that the compositional structure of the Slave varies between the central and northern areas. The transition between the Archean ultradepleted shallow mantle layer and the Archean-Proterozoic deeper layer shallows towards the north, where it may reach depths of 80 - 100 km. Although the causative tectonic process for this stratification is a subject of debate, the layered nature of the lithospheric mantle beneath the Slave craton has been documented in many works (Bostock, 1998; Griffin et al., 1999a; Kopylova & Russell, 2000; Menzies et al., 2004).

5.3.2.3 Modelling results

The selected transect corresponds to the first segment of SNORCLE line 1 (van der Velden & Cook, 2002) and to “segment A” of line 11 in Fernández Viejo and Clowes (2003). The transect runs overall E-W along 140 km, passing through the Contwoyto and Anton terranes (Fig. 5.23). The refraction study included four shots, which sampled the entire crust and uppermost upper mantle of these Archean domains. Crustal compressional velocities show a three-layer distribution: (1) an uppermost thin layer ($\sim 1 - 2$ km thick) exhibiting values between $5.4 - 5.6 \text{ km s}^{-1}$, (2) a middle layer (~ 20 km thick) with velocities between $6.2 - 6.5 \text{ km s}^{-1}$ at about 20 km depth, and (3) a lower layer (~ 10 km thick) with average velocities of $\sim 6.7 \text{ km s}^{-1}$. Values close to 6.9 km s^{-1} are estimated right above the Moho, which is located at 33 km depth throughout the whole profile. Generally speaking, velocities are somewhat lower in the eastern part of the transect, corresponding to the Contwoyto terrane. Using global velocity-density databases for crustal rocks (Christensen & Mooney, 1995), the following average densities are estimated for the upper, middle and lower layers, respectively: 2650, 2850, and 2950 kg m^{-3} . The density structure of the crust is modelled here with a two-layer crust, in which density is allowed to vary continuously with depth in both layers. Since the uppermost layer is very thin, and the density is varied with depth in such a way that it matches the density distribution derived from seismic velocities, the inclusion of a third layer is not necessary. Accordingly, the upper layer (i.e. layers 1 and 2 of the seismic model) comprises the first 23 km, with a depth-dependent density varying from 2670 kg m^{-3} at the surface to a maximum value of 2945 kg m^{-3} at 23 km depth. The lower layer (layer 3 of the seismic model) extends to the Moho, with an upper density value of 2920 kg m^{-3} and a lowermost value of 2990 kg m^{-3} . These values are incremented by a 1 % in the Anton terrane, where velocities tend to be higher. The rest of the thermophysical parameters used in this model (hereafter SCRS1) are listed in Table 5.4.

The initial composition of the lithospheric mantle and its stratigraphy have been taken partially from Griffin et al. (1999a), since the Lac de Gras area is close to the modelled transect. This study indicates a minimum lithosphere thickness (based on Y-depleted garnets) of $\sim 200 - 220$ km. Accordingly, a LAB located at 210 km depth was used in SCRS1. W. L. Griffin (pers. commun.) provided a detailed compositional model for the area (hereafter GMC06), with mineral modes estimated from both Y and Cr in garnets. This method permits to recalculate the major element composition of any xenolith based on the obtained median whole-rock Al_2O_3 , which in turn is used to estimate the mineral modes. However, the estimation from Cr-in-garnet tends to overestimate whole-rock Al_2O_3 , especially at relatively shallow depths where garnet and chromite coexist, while the Y-in-garnet estimation may underestimate the whole-rock Al_2O_3 (W. L. Griffin, pers. commun.). Therefore, the average of these two methods (Cr and Y in garnet) was used in the SCRS1 model (Table 5.4). The transition between the upper and lower layer was set at 150 km depth.

Fig. 5.24 shows the geotherm as predicted by SCRS1, together with xenolith data from both central (Griffin et al., 1999a; Menzies et al., 2004) and northern Slave (Kopylova et al., 1999). In this case, the T-dependent thermal conductivity at temperatures $> 550^\circ\text{C}$ was modelled with Eq. (4.2c). This is intended to account for the increase in thermal conductivity with pressure in thick lithospheres (Hofmeister, 1999; Jaupart & Mareschal, 1999). Fig. 5.24 shows that the thermal structure predicted by SCRS1 is in good agreement with xenolith data, suggesting that the thermal parameters and lithospheric thickness are appropriate. However, the SHF and the elevation of the model are inconsistent with observations. In particular, although the thermal structure of the lithospheric mantle is consistent with xenolith data, the elevation as predicted by SCRS1 is overestimated by ~ 1800 m, while the SHF is underestimated by $\sim 10 \text{ mW m}^{-2}$ (but consistent with xenolith-derived geotherms). This clearly points towards a compositional and a crustal factor as responsible for the discrepancy in elevation and SHF, respectively.

The latter factor will be considered first.

If the geotherms estimated for the Slave Province from thermobarometry on xenoliths are representative of the steady-state conductive regime in the mantle, then the thermophysical parameters and the thermal lithospheric thickness cannot be changed too much from the ones used in SCRS1. Geotherms constructed from xenoliths in kimberlites are commonly thought to provide information on lithospheres that are relatively thermally unperturbed (O'Reilly & Griffin, 1996; Rudnick et al., 1998; Carlson et al., 2005). However, the choice of thermobarometers is critical. Menzies et al. (2004), for example, provided an instructive analysis of how different combinations of thermobarometers give different geotherm estimations. In particular, these authors showed that the apparent change in the geotherm with depth reported by Griffin et al. (1999a) is not discernible beyond the resolution of various thermobarometers. On the other hand, as shown in Fig. 5.24, the preferred estimations of Menzies et al. (2004) for xenoliths from the Lac de Gras area depict a geotherm that is consistent with those estimated in other works within the Slave Province (Griffin et al., 1999a; Kopylova et al., 1999). All of the above suggests that the thermal structure predicted by SCRS1 for the lithospheric mantle cannot be significantly changed to reproduce a SHF in agreement with observations ($\sim 53 - 54 \text{ mW m}^{-2}$). However, as previously mentioned, an average crustal heat production value of $\sim 1 \mu\text{W m}^{-3}$, more consistent with local field measurements in crustal rocks (Thompson et al., 1996), could increase the SHF towards values close to the observed ones. Changing the depth-averaged heat production value of the crust to $1 \mu\text{W m}^{-3}$ in SCRS1 changes the SHF to 52 mW m^{-2} , without modifying appreciably the thermal structure of the lithospheric mantle. Although this average crustal heat production value is somewhat higher than the maximum value estimated by Rudnick et al. (1998) for Archean terranes ($\sim 0.67 \mu\text{W m}^{-3}$), it is well known that many other measurements in areas dominated by igneous-metamorphic rocks also give crustal heat production values of the order of $1 - 3 \mu\text{W m}^{-3}$ (e.g. Jones, 1987; Rudnick et al., 1998;

Jaupart & Mareschal, 1999). Hence, it is not surprising that the results from SCRS1 with a higher crustal heat production show that SHF values measured in the Slave craton are dominated by the heat production of the crust, not being representative of a lithospheric-scale feature. This is also consistent with global tomography studies, which show fast anomalies down to depth of $\sim 250 \pm 50$ km in the Slave craton (e.g. Ritsema & van Heijst, 2000; Ritsema et al., 2004, see also the difference between Fig. 2.4A and 2.4B).

The magnitude of the overestimated elevation indicates that the mantle composition used in SCRS1 cannot be representative of the whole lithospheric section, and therefore it provides important constraints to petrological models. There are at least two possible causes for the apparent high buoyancy of the model: (a) the algorithms used to estimate the modal content of the mantle are based on regressions that are biased by large number of xenolith suites from the Kaapvaal craton, which exhibit high orthopyroxene/olivine ratios between 0.2 - 0.4 (W. L. Griffin, pers. commun., see also Chapter 2), and (b) no eclogites were included within the mantle. The first item is somehow difficult to address in a quantitative form. This is mainly because most of the available xenolith datasets are also strongly biased by the samples from the Kaapvaal craton (see discussion in Chapter 2). More recent studies in the Siberian (e.g. Boyd et al., 1997, W. Griffin, pers. commun.) and North Atlantic cratons (Bernstein et al., 1998), show that the high orthopyroxene/olivine effect is much less obvious in these areas. If this is also true for the Central/Southern Slave, the buoyancy will decrease not only due to the higher content of dense olivine, but also because the garnet content would have to increase to make up for the lost CaO and Al₂O₃ that reside in the orthopyroxene. Interestingly, the actual modal count in peridotite xenoliths from the lower layer of Griffin et al. (1999a) shows that it has a significantly lower orthopyroxene/olivine ratio (~ 0.16) than that in GMC06 (0.37). Modal counting of depleted peridotite xenoliths presented in Kopylova and Russell (2000) show values between 0.24 - 0.30. The modal content of orthopyroxene

estimated by Kopylova and Russell (2000) varies from a maximum of ~ 26 vol% in the shallow layer to ~ 15 vol% at depths greater than 140 km. These figures are significantly different from those reported by MacKenzie and Canil (1999), who estimated an average orthopyroxene/olivine ratio of ~ 0.51 and an average orthopyroxene modal content of ~ 30 vol% for the first 170 km in the Central Slave Province.

It is clear from the above that estimates based on xenolith suites vary significantly. However, there are two important observations that need to be considered. Firstly, it seems possible that the modal estimates of GMC06 overestimate the orthopyroxene/olivine ratio of the lithospheric mantle, at least in the lower layer. Secondly, the existence of an ultradepleted upper layer (above 150 km depth) is a robust result. In accordance with this, a new model (hereafter SCRS2) that includes an upper layer with orthopyroxene/olivine ratio 0.29 and a lower layer with a composition matching that in Table 2 of Griffin et al. (1999a) is considered (see Table 5.4). Also, the SCRS2 model has a LAB 15 km deeper than SCRS1, in better agreement with seismological evidence (see above), and a depth-averaged crustal heat production of $1 \mu\text{W m}^{-3}$. The geotherm, SHF, and elevation predicted by SCRS2 are shown in Fig. 5.24. As expected, the thermal structure of the model does not change significantly, and therefore the SHF and the mantle geotherms are still in agreement with experimental data. The predicted elevation, on the other hand, is still overestimated by ~ 1300 m. Slight changes in the composition of the upper layer, as allowed by the petrological information, do not make the result much better. This forces the conclusion that another compositional effect, such as the occurrence of eclogites in the lithospheric mantle, is necessary to reconcile the above discrepancies.

As a matter of fact, the omission of eclogites in petrological models of the Slave Craton lithospheric mantle might be a serious shortcoming, as indicated by both xenolith analysis and seismic evidence. Eclogite samples are known to be abundant across the

Slave Province, where locally they can comprise more than 70 % of the mantle-derived xenoliths (Griffin et al., 1999a; Kopylova et al., 1999; Kopylova & Russell, 2000). They may be derived from oceanic crust subducted during the assemblage of the Slave craton (e.g. Kusky, 1993, 1989; van der Velden & Cook, 2002). Seismic evidence for a thin (~ 10 km) subhorizontal layer of eclogite at approximate depths of 70 - 80 km was also presented by Bostock (1998), and corroborated by Fernández Viejo and Clowes (2003). At pressures and temperatures corresponding to these depths, eclogitized oceanic crust can reach densities of $\sim 3540 \text{ kg m}^{-3}$ (e.g. Aoki & Takahashi, 2004), and consequently it has a significant impact in the total buoyancy of a lithospheric section (e.g. Kelly et al., 2003). When an eclogite layer 13.5 km thick with an average density of 3540 kg m^{-3} is included in SCRS2, elevation is drastically reduced to values that are only ~ 300 m greater than average observed elevations. This discrepancy is entirely within the uncertainties arising from the thermal model, compositional heterogeneities, transition depth, and total eclogite content. It is interesting to note that the thickness of the eclogite layer used above is higher than normal oceanic crust, but consistent with the generally accepted idea that higher temperatures inferred for the Archean would have produced thicker oceanic crust.

The preferred best-fitting model (hereafter SCRS3) that simultaneously reproduces SHF, geoid height, Bouguer anomalies, xenolith data, and elevation data, is shown in Fig. 5.25; the predicted geotherm is shown in Fig. 5.24. The only differences between SCRS2 and SCRS3 are the inclusion of: (a) a 10 km thick eclogite layer at 75 km depth, and (b) a buffer body between the lithospheric and the sublithospheric mantle, across which composition (and temperature) varies non-linearly from typical sublithospheric to purely lithospheric. The thickness of this body is 20 km.

Seismic surveys of the Slave craton show that its lithospheric mantle is slightly faster with respect to spherically symmetric models (e.g. Bank et al., 2000; Frederiksen et al.,

2001; Fernández Viejo & Clowes, 2003). In particular, the P-wave seismic tomography of Bank et al. (2000) revealed that the highest velocities in the Slave are found in the region covered by the SCRS3 transect. This high-velocity anomaly extends down to depths of $\sim 200 - 300$ km, with peak values of $\sim +1.6$ % with respect to *iasp91* (i.e. *ak135*, Kennett et al., 1995) at ~ 100 km depth (Bank et al., 2000). This is consistent with the relatively high mantle velocities reported by Fernández Viejo and Clowes (2003) at these depths. Predictions of P-wave seismic velocities from SCRS3 are shown in Fig. 5.26, together with those from the *ak135* spherically symmetric model and from the petrological model of Kopylova et al. (2004). Over the depth interval 50 - 200 km, SCRS3 predicts an anomaly of $\sim +1.47$ % with respect to the *ak135* model, in good agreement with the results of Bank et al. (2000). The velocities predicted by SCRS3 are closer to the upper bound values estimated by Kopylova et al. (2004) for the Slave lithospheric mantle. This is not surprising, since the estimations of Kopylova et al. (2004) are an average for the whole Slave craton, while the SCRS3 transect is located in the region with fastest mantle velocities.

The existence of a ENE - WSW seismic anisotropy in the Slave upper mantle has been revealed by SKS splitting analyses (Bostock, 1998; Bank et al., 2000; Snyder et al., 2003). The splitting axes are oriented along the present-day plate motion of North America, generally though to be the responsible for the lattice preferred orientations of olivine and pyroxenes necessary for generating anisotropy in the mantle (Bank et al., 2000; Snyder et al., 2003). Allowance for anisotropy in P-wave velocity calculations significantly expands the range of velocities permitted by petrological models (Kopylova et al., 2004). Unfortunately, reliable estimations on the absolute magnitude and depth distribution of seismic anisotropy in this area are lacking. However, since the SCRS3 transect is approximately perpendicular to the splitting axis direction, it could be speculated that the velocities predicted by SCRS3 may represent upper bound values.

Table 5.1: Thermophysical parameters used in ACSM1

Layer	$A [\mu\text{W m}^{-3}]$	$k [\text{W m}^{-1} \text{K}^{-1}]$	Density $[\text{kg m}^{-3}]$
Upper crust	1.1	2.5	$2670 \times (1 + 1.3 \times 10^{-10} P [\text{Pa}])$
Lower crust	0.2	2.1	$2900 \times (1 + 1.6 \times 10^{-11} P [\text{Pa}])$
Lithospheric mantle	0.01	^a	^b

^a Modelled as explained in Chapter 4.

^b Modelled as explained in Chapters 3 and 4 with Ol/Opx/Cpx/Grt = 70/17/6/7 assuming $\text{mg}\# = 93$.

Table 5.2: Thermophysical parameters used in NMRS1

Lithology	$A [\mu\text{W m}^{-3}]$	$k [\text{W m}^{-1} \text{K}^{-1}]$	Density ^a $[\text{kg m}^{-3}]$
Marine sediments	0.9	2.3	2200
Cont. upper crust	1.8	2.5	2750
Cont. lower crust	0.7	2.1	2900
Cape Cross mafic intrusion	0.8	2.2	2970
Messum mafic intrusion	0.8	2.2	2970
Transitional upper crust	0.4	2.4	2870
Lower oceanic crust	0.2	2.2	2980
High veloc. zone	0.4	2.1	3000
Underplating	0.03	2.1	3150 ^b
Lithospheric mantle	0.008	^c	3200 ^d

^a From Christensen and Mooney (1995).

^b Density varies linearly upwards until the top of the body, where it reaches a value of 3000 kg m^{-3} .

^c Modelled as explained in Chapter 4.

^d Only when modelling with the CTE; otherwise, as explained in Chapters 3 and 4.

Table 5.3: Lithospheric mantle modal compositions (vol%) used in NMRS1

Lithospheric domain	Olivine	Orthopyroxene	Clinopyroxene	Garnet	Spinel
Continental garnet field ^a	66	17	9	8	
Continental spinel field	67	20	12		1
Oceanic ^b					

^a Assuming mg# = 91.

^b Modelled as explained in Chapters 2 and Section 5.2.1 assuming a linear depletion model.

Table 5.4: Thermophysical parameters used in Slave Craton models

SCRS1	A [$\mu\text{W m}^{-3}$]	k [$\text{W m}^{-1} \text{K}^{-1}$]	Density [kg m^{-3}]	Ol/Opx/Cpx/Grt ^d
Upper crust	1.0	2.5	$2670 \times (1 + 1.6 \times 10^{-10} \text{ P [Pa]})$	
Lower crust	0.3	2.1	$2920 \times (1 + 2.5 \times 10^{-11} \text{ P [Pa]})$	
Upper Layer ^a	0.016	^b	^c	74.5/23.6/0.1/1.8
Lower Layer ^a	0.016	^b	^c	69.9/26.3/0.3/3.5
SCRS2	A [$\mu\text{W m}^{-3}$]	k [$\text{W m}^{-1} \text{K}^{-1}$]	Density [kg m^{-3}]	Ol/Opx/Cpx/Grt ^d
Upper crust	1.3	2.5	$2670 \times (1 + 1.6 \times 10^{-10} \text{ P [Pa]})$	
Lower crust	0.4	2.1	$2920 \times (1 + 2.5 \times 10^{-11} \text{ P [Pa]})$	
Upper Layer ^a	0.016	^b	^c	76/21.9/0.1/2
Lower Layer ^a	0.016	^b	^c	79/13/1/7

^a In the lithospheric mantle

^b Modelled as explained in Chapter 4.

^c Modelled as explained in Chapters 3 and 4.

^d Assuming mg# = 93 and 92 in the upper and lower layers, respectively.

Figure 5.1: A) Age-dependent seafloor topography. Depth data for the Atlantic, Pacific, and Indian oceans are from Johnson and Carlson (1992). Unfilled symbols represent “outlier” data affected by local variations. Data for the North Pacific are from Parsons and Sclater (1977). The two dotted lines indicate the root mean square error for the data in Johnson and Carlson (1992). The dashed envelope is one standard deviation from the mean value for the data presented in Stein and Stein (1992). GDH1 = Plate model of Stein and Stein (1992); PSM = Plate model of Parsons and Sclater (1977); HSM = Half-space cooling model. The thick-dashed grey line is the best fit of the data when the “outlier” points are neglected. B) Heat flow data and predictions from different models. Black dots are measurements from Stein and Stein (1992). Rectangular boxes are data from Lister et al. (1990). The dashed envelope is one standard deviation from the mean value for the data presented in Stein and Stein (1992). C) Heat flow zoom-in for plate ages > 100 Ma. Symbols for the three models as in (A).

Figure 5.2: Location map of the modelled oceanic transect (dashed black line). Contour lines indicate bathymetry in meters.

Figure 5.3: Modelling results of surface heat flow (SHF), geoid height, free-air gravity anomalies (F.A.), and elevation for the synthetic oceanic transect OLSM1. The lower panel shows the lithospheric structure of the best fitting model. Grey dots and vertical bars denote observed values and associated scatter, respectively. Black lines represent outputs from the model.

Figure 5.4: Thermal structure of the synthetic model OLSM1. Predicted 200, 600, 1000, and 1300 °C isotherms by the models MJP (McKenzie et al., 2005), GDH1 (Stein & Stein, 1992), and HSM are indicated for the respective crustal age at 90, 65, and 35 Ma. Shown plate ages are from Mueller et al. (1997).

Figure 5.5: Comparison between MJP and OLSM1 models for oceanic lithosphere. A) Thermal structure predicted by the MJP model. The 200, 600, 1000, and 1300 °C isotherms are highlighted. Black crosses indicate the depth of the 200, 600, 1000, and 1300 °C isotherms predicted by: i) the OLSM1 model for lithospheric ages of 10 ($x = 1400$ km) and 65 ($x = 500$ km) Ma; ii) a flat-bottom model with the same thermal thickness that the asymptotic thickness of MJP (at 200 Ma). Predicted depth and heat flow by the above synthetic models are shown for the same locations. B) Age-dependent seafloor topography. Symbols as in Fig. 5.1. Grey dots indicate seafloor depth and associated scatter of the modelled transect, respectively. Predictions by OLSM1 at 10, 65, and 80 Ma are shown.

Figure 5.6: Density structure of OLSM1 assuming a linear depletion model. The contour lines indicate density values in kg m^{-3} . The dotted yellow line indicates the approximate location of the spinel-garnet phase change. The dotted red line is the 1300 °C isotherm. The density profile at $x = 0$ km is shown in the lower right corner.

Figure 5.7: Density structure of OLSM1 assuming a non-linear depletion model. All symbols as in Fig. 5.6. The density profile at $x = 0$ km is shown in the lower right corner.

Figure 5.8: Time evolution of the buoyancy for oceanic plates. A) RM-SI = RM-SO = Adiabatic reference models, L = linear depletion model, NL = non-linear depletion model, ND = no depletion. B) Time evolution of the buoyancy for an oceanic plate with a thermal structure as given by the GDH1 model.

Figure 5.9: P-wave synthetic tomography of an oceanic plate as predicted by OLSM1. Contour lines are compressional velocities in km s^{-1} . P_n velocities (sub-Moho) varies along the transect from $\sim 7.7 \text{ km s}^{-1}$, close to the MOR, to $\sim 8.2 \text{ km s}^{-1}$ at old oceanic lithosphere. The dotted yellow line indicates the depth of the 1300 °C isotherm.

Figure 5.10: Comparison of V_P predicted by OLSM1 with those from seismological and theoretical models for an oceanic plate $\sim 90 - 100$ Ma old. A) PA5 is the seismological model of Gaherty et al. (1999) for the Pacific. The dotted lines indicate the uncertainty associated with PA5. SLB is the theoretical model of Stixrude and Lithgow-Bertelloni (2005) for a plate ~ 100 Ma old. B) Comparison of the V_P predicted by a model with an identical thermal structure to that given by GDH1 for a plate 100 Ma old (OLHPM, shaded area) with those from seismological models. The two dash-dotted lines represent extreme values due to uncertainties in thermal and compositional parameters. PHB3 is the model of Kato and Jordan (1999) for a young section of the Philippine Plate (~ 40 Ma).

Figure 5.11: Modelling results of surface heat flow (SHF), geoid height, and elevation for the synthetic model ACSM1. The lower panel depicts the lithospheric structure.

Figure 5.12: Modelling results of surface heat flow (SHF), geoid height, and elevation for the synthetic model ACSM2. The lower panel depicts the lithospheric structure, including the boundary between the two distinct compositional layers. The small curvature of this boundary towards the right is a consequence of the modelling approach, which identifies compositional boundaries as isobaric planes.

Figure 5.13: P-wave velocities predicted by ACSM2 at $x = 0$ (lithospheric thickness = 295 km). ACSM2-thick is a similar model but with a thermal thickness of 380 km.

Figure 5.14: Cartoon of variations in temperature and density through the lithospheric and sublithospheric mantle used in delamination/unrooting models. (Figure based on Fig. 1 and 4 of Conrad and Molnar (1997) and Marotta et al. (1998), respectively.)

Figure 5.15: Thermal structure of a thickened lithosphere in a compressive environment.

Figure 5.16: Buoyancy of a 300-km thick column at the centre of thickened continental root. PCSI1 has an average composition intermediate between typical Archean and typical Phanerozoic. PCSI2 has a typical Phanerozoic composition. PCSI3 has a fertile (PUM) composition (no depletion). $\Delta\rho = (\rho_l - \rho_{am})$; ρ_l and ρ_{am} are the densities of the lithosphere and adiabatic reference model, respectively. Mantle buoyancy only, depth-averaged density contrast of the mantle portion only ($\bar{\rho}$), and total (crust + mantle) buoyancy (numbers within brackets) are indicated for the three models. Buoyancy is in N m^{-1} ; density contrast is in kg m^{-3} .

Figure 5.17: Location map of the modelled transect across the Namibian volcanic margin (solid black line). Dotted lines at both sides of the main transect represent additional refraction and reflection seismic profiles used to constraint the crustal structure (A, transect 4 of Gladczenko et al., 1998; B, transect 2 of Bauer et al., 2000.). Contour lines indicate bathymetry in meters.

Figure 5.18: Maps of observables of the Namibian volcanic margin. A) free-air gravity anomalies, contours every 20 mGal; B) geoid height, contours every 1 m; C) elevation, contours every 500 m; D) surface heat flow (SHF), contours every 10 mW m⁻². Black dots indicate SHF measurements used to produce the map. Solid lines indicate the location of the modelled transect.

Figure 5.19: Crustal structure used to model the present-day lithospheric structure of the Namibian volcanic margin (upper panel) compared with the original seismic model, from which density values were taken (lower panel). Densities in the upper panel are the preferred values for modelling, consistent with the seismic velocities and direct measurements in the Namibian margin. Corresponding model parameters are listed in Table 5.2.

Figure 5.20: Resulting elevation considering local and flexural isostasy. Grey thick line denotes observed values and associated scatter; dotted line represents elevation predicted by local isostasy; solid line denotes elevation corrected for flexural isostasy with a plate of effective elastic thickness $T_e = 20$ km.

Figure 5.21: Modelling results (NMRS1) of SHF, geoid height, free-air gravity anomalies, and elevation for the Namibian volcanic margin. The lower panel shows the lithospheric structure of the best-fitting model. Grey dots and vertical bars denote observed values and associated scatter. Black lines represent outputs from the model. Thin dotted line denotes the geometry of the 1350 °C isotherm predicted by NMRS2.

Figure 5.22: Modelling results for (A) thermal structure (NMRs1), (B) coefficient of thermal expansion (NMRs2), and (C) P-wave velocities (NMRs1) in the Namibian volcanic margin. The thick dashed line in (B) and (C) represents the trace of the 1350 °C isotherm.

Figure 5.23: Location map of the modelled transect in the Slave Craton (solid white line labelled "T"). Thick dashed line indicates the approximate boundary of the Slave Province. Thin dashed line indicates the trace of the Great Slave Lake Shear Zone. Topography in meters.

Figure 5.24: Model geotherms for three different models of the Southern/Central Slave. Parameters used to obtain these geotherms are listed in Table 5.4. Black squares, black circles, and open circles are xenolith thermobarometry data from Griffin et al. (1999a), Kopylova et al. (1999), and Menzies et al. (2004), respectively. When present, horizontal and vertical bars denote scatter from several data. Predicted SHF and elevation are indicated for each model.

Figure 5.25: Modelling results (SCRS3) of SHF, geoid height, Bouguer gravity anomalies (B.A.), and elevation for the Slave transect. The lower panel shows a simplified cartoon of the lithospheric structure. Grey dots and vertical bars denote observed values and associated scatter. Black lines represent outputs from the model.

Figure 5.26: Comparison of P-wave seismic velocities predicted by SCRS3 with those from the seismological model *ak135* (thick solid line; Kennett et al., 1995) and the petrological model of Kopylova et al. (2004) (grey areas). Bars denote the extent of seismic anisotropy expected in peridotites (5 %) and eclogites (2 %) estimated by Kopylova et al. (2004). Thin solid line is the prediction from SCRS3 without an eclogitic layer; dotted line includes a 13.5 km thick eclogitic layer at 80 km depth with an anisotropy of 3 % (Figure modified from Kopylova et al., 2004).

CHAPTER 6

Mantle Instabilities and Initiation of Subduction

6.1 Introduction

For the past 30 years, the accepted view about the relative stability of the oceanic lithosphere with respect to the underlying mantle has been that in which a mature oceanic plate becomes significantly more dense ($\Delta\rho \sim 70 - 100 \text{ kg m}^{-3}$) than the underlying mantle (see Chapter 5). As a result of this large density contrast, mature oceanic lithosphere was thought to founder and sink spontaneously into the interior of the Earth through the creation of a trench, marking the initiation of a subduction zone (cf. e.g. Schubert et al., 2001). This view, adapted from laboratory and theoretical studies on thermal convection, was rapidly adopted by many authors. The final expression of this model, in which a major (i.e. large) oceanic basin is created before it can be recycled into the mantle, is represented in the so-called Wilson Cycle, which gave a geological evolutionary framework to the new plate tectonics paradigm. However, soon after the inception of this model, several authors started to realize that the transformation of a passive into an active margin by spontaneous foundering of old, and therefore dense, oceanic lithosphere was difficult to reconcile with information from laboratory data on the rheology of lithospheric rocks (e.g. McKenzie, 1977; Cloetingh et al., 1982). Although the pioneering work that set the basis for these concept was developed more than 30 years ago, little further exploration into the problems of identifying and quantifying available driving forces was considered subsequently. In view of new composition-pressure-temperature-dependent models for oceanic lithosphere, such as those presented in Chapter 5 and elsewhere (e.g. Phipps Morgan, 1997; Hynes, 2005), the widely accepted idea of an oceanic lithosphere significantly more dense than the underlying mantle requires a thoughtful re-examination, along with its implications for subduction initiation.

In this chapter, I first review previous concepts and models on subduction initiation, and discuss their consistency with the new evidence presented in this thesis for the evolution of oceanic lithosphere. I then present further calculations on the density distribution of oceanic plates, available driving forces favouring subduction initiation, and resisting forces preventing it. I later use these calculations to evaluate the necessary conditions for the initiation of a subduction zone, and propose a new scenario that incorporates all of the above in a consistent manner. Finally, a discussion of a number of potential criticisms to the proposed new scenario is given.

6.2 Previous models and concepts

There are basically two competing models for explaining the nucleation of a subduction zone: forced or induced (INSZ) and spontaneous (SNSZ) (e.g. Gurnis et al., 2004; Stern, 2004). The INSZ model requires externally applied compressive stresses at a plate boundary as the driving mechanism (e.g. McKenzie, 1977; Toth & Gurnis, 1998; Hall et al., 2003; Gurnis et al., 2004). The SNSZ model, on the other hand, is entirely driven by a gravitational instability, commonly thought to be originated by the cooling of oceanic lithosphere (e.g. Stern & Bloomer, 1992; Canright & Morris, 1993; Fowler, 1993; Kemp & Stevenson, 1996; Solomatov, 2004a; Stern, 2004). In principle, the mode of subduction initiation can be inferred from the geological record, since the two models predict different features at the beginning of subduction. For example, according to the INSZ model, strong compression in both the overriding and subducting plates will predate the initiation of a subduction zone. The formation of a new trench by this mechanism involves forced convergence, elastic buckling of the plates, rapid uplift on the hanging wall, and subsidence on the footwall (Gurnis et al., 2004). In a SNSZ model, however, strong extension of the overriding plate and subsequent trench roll-back is expected (Stern, 2004). Although the INSZ model is consistent with present-day tectonics

in several locations in the Western Pacific, evidence from ophiolitic complexes and associated boninites (high-Mg andesites produced by high degrees of hydrous partial melting of harzburgites) support a SNSZ model (cf. e.g. Stern, 2004). Moreover, as Stern (2004) pointed out, pre-Cenozoic subduction zones must have started by a SNSZ-type mechanism at least once without a priori plate convergence in order to begin the plate tectonic regime. It seems thus possible that the two mechanisms occur on the Earth. However, whether they are distinct expressions of a single driving mechanism or totally different processes remains a matter of debate.

Whatever the mode of subduction initiation, its dynamics are governed by the balance between driving and resisting forces. The origin and magnitudes of the forces that may dominate in the process of initiating and sustaining a subduction zone have been investigated by a number of workers (see e.g. Gurnis et al., 2004 for a recent review). McKenzie (1977) was among the first to establish a formal relationship between resisting and driving forces. The general concept is expressed as a force balance between the forces resisting trench formation and those favouring it. McKenzie (1977) considered four main forces controlling the behaviour of the trench system: 1) a *ridge push* (D_R) that drives flow away from a MOR, 2) a *slab pull* (D_S) exerted by the incipient slab, 3) a *frictional force* (F_E) due to the friction on the thrust plane between plates, and 4) a *bending force* (F_B) arising from the work that must be done against elastic and gravitational forces to bend the lithosphere. For an instability of this type to grow and evolve into a “self-sustaining” subduction zone, the following inequality must be satisfied

$$D_R + D_S > F_E + F_B \quad (6.1)$$

Although the particular meaning of the above four forces, or even the existence of some of them, may change among different possible scenarios for the initiation of

subduction, the main concept of a force balance controlling the growth and development of the instability is general and constitutes the core of all models of subduction initiation.

Many different ideas and approaches have been proposed to explain the initiation of subduction. These models can be grouped into four basic categories:

- (a) Analytical and numerical models based on the mechanics of faulting (e.g. McKenzie, 1977; Turcotte et al., 1977; Cloetingh et al., 1982, 1989; Mueller & Phillips, 1991; Erickson & Arkani-Hamed, 1993; Kemp & Stevenson, 1996; Schubert & Zhang, 1997; Niu et al., 2003)
- (b) Analogue laboratory experiments (e.g. Shemenda, 1994; Becker et al., 1999; Facenna et al., 1999; Leroy et al., 2004; Mart et al., 2005)
- (c) Thermomechanical numerical models with horizontal compression or sedimentary loads (e.g. Toth & Gurnis, 1998; Branlund et al., 2001; Regenauer-Lieb et al., 2001; Doin & Henry, 2001; Hall et al., 2003; Gurnis et al., 2004; Billen & Hirth, 2005)
- (d) Analytical and numerical thermal convection models (e.g. Fowler, 1985, 1993; Canright & Morris, 1993; Solomatov, 2004a, 2004b)

6.2.1 Analytical and numerical models based on the mechanics of faulting

This first group of models studied the basic mechanisms responsible for the initiation of subduction, and gave first-order constraints on the magnitude of the involved forces. Using simple physical arguments, McKenzie (1977) estimated that a gravitational instability would grow and become self-sustaining if external driving forces cause a net convergence of $\sim 130 - 180$ km, at which point D_S starts to offset the resisting forces. Turcotte et al. (1977) analyzed the possibility of initiating subduction in an extensional

environment. In this case, the force F_E does not exist, but is replaced by a driving force arising from the “flooding” of mantle rocks on top of the oceanic crust. These authors concluded that the lithosphere will bend and descend into the mantle only if dense mantle rocks can penetrate and override the lithosphere. Unfortunately, they were unable to explain how such a scenario could occur. Cloetingh et al. (1982, 1989) evaluated the lithospheric strength of passive margins and found that ageing of passive margins alone does not make them more suitable for initiating subduction. This is simply a consequence of the strengthening of the lithosphere as it gets colder (i.e. older). This difficulty in initiating subduction led them to propose that extensive sediment loading of young oceanic lithosphere may be the only effective mechanism for the initiation of subduction and closure of small ocean basins. However, they could not explain how major subduction zones, such as the circum-Pacific ring, would form. This model also fails to predict why those places where extensive sedimentation has affected young oceanic lithosphere (e.g. Mississippi Delta, Ganges Delta, Amazonian Delta) do not experience subduction. Mueller and Phillips (1991) and Erickson and Arkani-Hamed (1993) also evaluated lithospheric strengths in several tectonic settings (intraoceanic, passive margins, transform faults, fracture zones, spreading centres) and concluded that lithospheric failure of mature oceanic lithosphere is unlikely to be driven by common available tectonic stresses, namely ridge push. Some special circumstances were proposed for making subduction initiation a viable process. Erickson and Arkani-Hamed (1993) argued that fluid pressures exceeding hydrostatic levels and/or thermal weakening of the lithosphere by plumes or sediment blanketing could be important mechanisms favouring the initiation of a trench, although they recognized that lithospheric resistance is always greater than available forces arising from the ridge push. They also discussed the possibility of a transform margin that is oblique to the current ridge push force (e.g. the Grand Banks Transform Margin) acting as a kernel for producing a translithospheric fault. These authors further suggested that major pulses of plate reorganizations could be enough to trigger subduction at these passive margins, but they did not provide quantitative

estimations of these effects. Indeed, episodes of major tectonic activity, such as the India-Asia collision in the Tertiary, do appear to cause important changes in plate motions, trench jumps, and propagating rifts. The Macquarie Ridge Complex, for instance, is considered to be the most convincing case of incipient subduction as a consequence of ridge rotation and transverse shortening (e.g. Lebrun et al., 2003), although it is not clear if such a system will actually evolve into a self-sustained subduction zone (e.g. Lebrun et al., 2003; Niu et al., 2003). In any case, it is still unclear if the initiation of a new subduction zone is a consequence or a trigger of these episodes of plate reorganization (e.g. King et al., 2002; Lowman et al., 2003).

The same basic idea originally proposed by Turcotte et al. (1977) was more recently resurfaced by Kemp and Stevenson (1996) and further expanded by Schubert and Zhang (1997). The first work was focused on the forces responsible for the tensional failure of the margin and the subsequent mantle flooding of the lithosphere. The two main assumptions behind the model of Kemp and Stevenson (1996) are: (a) the subsidence of the oceanic lithosphere adjacent to a passive margin is inhibited by an intrinsic shear resistance (i.e. the oceanic plate is totally welded to the continent), leading to a flexural profile, even in the total absence of sedimentation; and (b) after the creation of a rift at the ocean-continent boundary, the sublithospheric mantle is able to rise and override the lithosphere over a distance of several tenths of kilometers. These authors highlighted that the principal issue with this scenario is whether the mantle flooding onto old oceanic lithosphere can actually occur. The criterion provided by Kemp and Stevenson (1996) to evaluate this takes the form

$$\frac{gh_o^3(h_oq)^2}{\kappa\nu} \geq 1 \quad (6.2)$$

where g is the acceleration of gravity, κ the thermal diffusivity, h_o the hydrostatic head

of the mantle (i.e. the maximum equilibrium height of the mantle column above the seafloor), q is a parameter of the system ($\sim 10^{-5} \text{ m}^{-1}$), and ν the kinematic viscosity. Assuming h_o values of 3 - 4 km, Eq. (6.2) implies that there will be enough mantle flooding only if mantle viscosities are very small ($< 10^{19} \text{ Pa s}$), and therefore, the foundering of the lithosphere would be only marginally possible even in the most favourable circumstances (Kemp & Stevenson, 1996).

Besides the difficulty of satisfying the criterion expressed in Eq. (6.2) with commonly accepted values of mantle viscosities, there are a number of other issues that make the above scenario even more unlikely, but have not been explicitly considered by Kemp and Stevenson (1996). Foremost among these are the neglect of viscous resistance and thermal thinning of the lithosphere during rifting, the conceptually incorrect assumption of an homogeneous mantle rising to depths comparable to those of MORs without experiencing changes in composition and density, and the unjustified assumption of a perfectly welded ocean-continent boundary. In this respect, the scenario depicted by Kemp and Stevenson (1996) does not differ considerably from intraoceanic rifting. Both abandoned and currently propagating intraoceanic rifts in mature oceanic lithosphere have been documented in the Pacific (e.g. Lonsdale, 2005). The result of such a tensional regime developed in oceanic lithosphere is always the development of a belt several hundred km wide, where stretching and fracturing result in a MOR-type setting, rather than the foundering of the lithosphere by extensive mantle flooding. There is no documentation of sublithospheric mantle flooding onto the seafloor. This is simply the consequence of the evolution of a mantle volume on its way towards the surface. The column of material that will actually rise to a depth of ~ 3 km above the seafloor in a mature oceanic basin is mainly composed of basaltic-type rocks, due to the extensive decompression melting that occurs. Making the reasonable assumption of a normal oceanic crust ~ 7 km thick produced in the rifting, it is clear that the only material that could flood onto the ocean floor, even when no thermal thinning is accounted for, would be mainly basalt. The

piling of basaltic rocks can isostatically load the lithosphere (e.g. in volcanic islands or passive margins), but they cannot produce a gravitational instability due to the flexural strength of the lithosphere (e.g. Turcotte et al., 1977). Regarding the assumption of a perfectly welded ocean-continent boundary, it needs to be mentioned that although a flexural response is usually present across passive margins, there is compelling evidence that the oceanic side can reach its compensation depth without being inhibited by a shear resistance along the ocean-continent boundary (e.g. Southern Australia, Bay of Bengal, Vøring Margin).

Niu et al. (2003) acknowledged the role of lateral compositional differences in the lithosphere as a dominant factor in the initiation of subduction within oceanic lithosphere. Based on a comparison between Tonga and Mariana fore-arc peridotites and abyssal peridotites, these authors concluded that subduction could start at the boundary between an oceanic plateau and normal oceanic lithosphere, as long as enough compression from ridge push was available. The petrological argument is similar to the one presented in Section 5.2 of Chapter 5. The more depleted oceanic plateau is relatively more buoyant than normal oceanic lithosphere, and therefore it would tend to be more stable than the latter. Their idea of lateral compositional heterogeneities as a dominant factor favouring subduction initiation is appealing. However, the quantitative mechanical approach adopted by Niu et al. (2003) is rather simplistic and key assumptions are unjustified. Elastic resistance, which has been shown to be an important factor in subduction scenarios (e.g. McKenzie, 1977; Hall et al., 2003; Gurnis et al., 2004, see also Section 6.2.3), is not considered. In their calculations, the existence of a pre-existent translithospheric discontinuity coinciding with the petrological boundary separating the relatively buoyant material from the less buoyant material is assumed at all depths (cf. Fig. 4 of Niu et al., 2003). This petrological boundary was further forced to coincide with the different angles of potential faults. This is highly unlikely to occur, and no evidence of any kind was provided by Niu et al. (2003) to support this assumption. Perhaps

more important is the fact that, although compositional differences are presented as the main factor controlling the initiation of subduction, they are ignored in the calculation of the negative buoyancy. When $\Delta\rho$ values of 20 - 35 kg m⁻³, more in agreement with the results from Chapter 5 (see also Section 6.3.1), are included in their equations, the estimated negative buoyancy and resulting stresses decrease by as much as a factor of 2 - 3.

6.2.2 Analogue laboratory experiments

Analogue laboratory experiments provide interesting insights into the mechanical problem of initiating subduction. Nevertheless, they do not always embody all representative features of a natural system. Shemenda (1994), Becker et al. (1999), and Faccenna et al. (1999), for instance, used a typical experimental set-up where the oceanic lithosphere is composed of either a single or a double layer (typically dry sand and/or silicone putty) significantly more dense ($\Delta\rho$ equivalent to $\sim 65 - 100 \text{ kg m}^{-3}$ in nature) than the upper mantle, which is modelled with a low-density and low-viscosity material (usually glucose syrup). These studies usually involve a compressive stress component perpendicular to the margin, simulated with a piston that moves at a constant velocity. The continental lithosphere is decoupled from the oceanic counterpart by a pre-existent discontinuity, dipping towards the continent between 90° and 45° from the horizontal.

Given the above physical properties, the general behaviour of the system can be easily predicted. In a first stage, the gravitational energy is continuously increased as the material is being compressed. Due to the density difference between the continental and the oceanic plate, the latter tends to underthrust the former, creating a gravitational instability with respect to the lighter material beneath it. Eventually, the negative buoyancy of the slab overcomes the viscous resistance of the mantle, leading to the “sudden” release of gravitational energy. This marks the typical accelerating phase

of a Rayleigh-Taylor instability (hereafter R-T instability). Despite minor effects associated with different material rheologies, this is exactly how laboratory systems evolve (Shemenda, 1994; Becker et al., 1999; Faccenna et al., 1999). However, according to the results presented in Chapter 5, the density values chosen to be representative of mature oceanic lithosphere in laboratory experiments seem to be too high, leaving some of the interpretations open to questions.

An extreme case of simplification is exemplified by the centrifuge models of Mart et al. (2005). These authors considered the oceanic lithosphere to be $\sim 21\%$ more dense than the continental counterpart within an equivalent thickness of 120 km. Assuming a normal average density value of $\sim 3320 \text{ kg m}^{-3}$ for a 150 km thick Archean lithosphere (Chapter 5), the above difference means that the oceanic lithosphere would have an average density of $\sim 4015 \text{ kg m}^{-3}$. This value is generally thought to be reached by the sublithospheric primitive mantle at depths of $\sim 600 \text{ km}$ (e.g. Kennett et al., 1995). The density contrasts assumed by Mart et al. (2005) are extremely high and completely inconsistent with results presented in Chapter 5 and in many other works. For the asthenosphere, these authors assumed a density equal to that used for the oceanic lithosphere, also in disagreement with results presented in Chapter 5. No justification or evidence for using these extreme values was provided. Moreover, the experiments were not isostatically compensated before the beginning of the centrifuge runs, and therefore the results are biased by the tendency of the system to achieve isostatic equilibrium during the running of the experiment. Mart et al. (2005) concluded, based on their experiments, that the initiation of subduction is a natural consequence of the lateral density variation between oceanic and continental lithosphere, and that the requirement of compressional stresses or a negatively buoyant oceanic lithosphere are not necessary conditions for subduction initiation, since their experiments evolve spontaneously towards subduction at the passive margin. However, a logical corollary of these conclusions is that all mature passive margins should be subducting at present, which is

clearly not the case.

6.2.3 Thermomechanical numerical models with horizontal compression or sedimentary loads

Two-dimensional numerical models have been partially successful in reproducing the main characteristics of a subduction zone, including its initiation. The usual approach is to force plate convergence kinematically, either at a passive margin (e.g. Toth & Gurnis, 1998; Doin & Henry, 2001; Billen & Hirth, 2005) or at a fracture zone (e.g. Hall et al., 2003; Gurnis et al., 2004), and analyze the balance between driving and resisting forces to elucidate the possibility of the creation of a new subduction zone. Using this scheme, estimates of the force required to create a new subduction zone typically exceed those available from ridge push. As a result, to generate a self-sustained system in agreement with the inferred structure of subduction zones, pre-existent very low-resistance fault zones across the lithosphere must be included. In addition to this, favourable orientations of these weak zones must also be prescribed (e.g. Toth & Gurnis, 1998; Billen & Hirth, 2005). Alternatively, vertical loading due to sedimentation in combination with different rheological laws can be used to estimate the necessary conditions for whole-lithospheric failure (e.g. Branlund et al., 2001; Regenauer-Lieb et al., 2001). However, these models only deal with the conditions for the generation of a lithospheric-scale fault, without actually exploring the problem of subduction initiation.

The main results from numerical experiments can be summarized as follows:

- (a) For a forced-convergence system to become self-sustained, a minimum initial convergence of 130 - 150 km needs to be driven by external forces, and the average fault zone stress must be below ~ 20 MPa.

- (b) The force balance is dominated by the state of elastic flexure of the plate, and the rate-dependent (viscous) resistance to lithospheric deformation is negligible.
- (c) Under some particular rheological conditions, realistic sedimentary loads could produce a translithospheric fault zone along a passive margin.

The first item (a) implies fault zones with effective coefficients of friction much less ($0.0 < \mu \leq 0.02$) than common measured values for real rocks ($0.4 < \mu < 0.8$) (e.g. Ranalli, 1995). Taking compressive stresses to be positive, the total shear resistance of a fault zone of depth z_r is

$$F_r(\theta, z) = \frac{\mu}{\sin \theta} \int_0^{z_r} [\sigma_n(\theta, z) - p_f] dz \quad (6.3)$$

where θ is the angle the fault makes with the horizontal, μ the coefficient of friction, σ_n the resolved normal stress on the fault plane, p_f the fluid pressure, and z the vertical coordinate. Assuming that $\sigma_n \sim g\rho z$, a fault dipping 45° from the horizontal, with $\mu = 0.4$ (representative of serpentinites), a hydrostatic p_f , and extending to $z_r = 50$ km, supports fault-averaged shear stresses exceeding 130 MPa. Even when small values $\mu = 0.1 - 0.2$, as inferred from stress orientations and heat flow anomalies along the San Andreas fault (see e.g. Kemp & Stevenson, 1996, and references therein) and in the Nankai subduction thrust (Brown et al., 2003), are used in Eq. (6.3), the shear resistance is still a factor of 3 - 7 too high to lithospheric faulting. This outcome has led several authors to suggest that overpressurization and/or other “hidden” weakening factors are necessary conditions to nucleate subduction (Toth & Gurnis, 1998; Hall et al., 2003; Gurnis et al., 2004). However, the existence of these conditions at passive margins and fractures zones, and their time evolution, remain unknown.

The second item (b) is simply related to the fact that the long-term strength dom-

inating the evolution of an oceanic plate and subduction initiation is mainly located within the brittle/elastic layer. Stresses in the underlying mantle are able to relax, providing a negligible contribution to the total resistance (e.g. Hall et al., 2003).

The third item (c) has been proposed by Branlund et al. (2001) and Regenauer-Lieb et al. (2001), based on a new parametrization of the rheological laws used to describe the mechanical behaviour of lithospheric materials. Based on the work by Kohlstedt et al. (1995), these authors adopted a strength profile for the oceanic lithosphere defined by a three-layer structure, instead of the commonly assumed two-layer structure. The uppermost brittle layer is described by Byerlee's law (e.g. Kohlstedt et al., 1995; Ranalli, 1995); the intermediate "ductile" layer is governed by a low-temperature plasticity constitutive law (Peierls mechanism), and its thickness is determined by the Goetze criterion (Chapter 4, Kohlstedt et al., 1995); the lower creep layer follows the common power-law creep constitutive law. Without explicitly dealing with the problem of subduction initiation, these authors focused on the vertical load necessary to break the lithosphere through its whole thickness. This could be accomplished by placing an accretionary prism $\sim 10 - 15$ km thick (i.e. forces $\sim 2 \times 10^{13}$ N m⁻¹) onto a mature passive margin (Branlund et al., 2001). As expected, this situation is favoured by the addition of a wet-type rheology (Regenauer-Lieb et al., 2001).

These results show that the previous idea regarding the impossibility of breaking old oceanic lithosphere by sedimentary loading (e.g. Cloetingh et al., 1982, 1989, Muller & Phillips, 1991) could be the result of an oversimplification of the lithosphere's rheology. Branlund et al. (2001) and Regenauer-Lieb et al. (2001) suggested that lithospheric failure by sedimentary loading is the first stage in subduction initiation. However, accepting that old oceanic lithosphere could be broken by large sedimentary loads, it remains to be explained why there is no subduction in any of the passive margins where, according to the model's predictions, the lithosphere should be broken. For instance, in the Texas

Gulf Coast, the Amazon cone, the eastern margin of India, and in the eastern margin of North America, the accretionary prisms have already exceeded the necessary thickness for breaking the lithosphere ($\gtrsim 15$ km thick), but none of them shows bathymetric, seismic, or volcanic evidence of being affected by incipient subduction.

6.2.4 Analytical and numerical thermal convection models

Both analytical and numerical models of thermal convection have been applied to address the problem of subduction initiation (e.g. Fowler, 1985, 1993; Canright & Morris, 1993; Solomatov, 2004a). These models include the possibility that sublithospheric convection plays an important role in the initiation of subduction. The general idea behind convection models with strongly temperature-dependent rheologies is that the fate of the thermal boundary layer (i.e. lithosphere) depends on the convection pattern beneath it.

The works of Fowler (1985, 1993) presented a boundary layer theory applied to the case of a vigorous convection beneath a thick, virtually stagnant lid. The stresses below and within the lid were found to increase gradually from the interior of the convective cell toward the surface of the convective layer, where they undergo a large jump in a thin stress boundary layer (only when a free-slip condition is applied to the top of the model). The origin of these large stresses is due to the horizontal balance between the force produced by the shear stresses acting on the base of the lid and the normal stresses acting over the lid thickness (i.e. $\partial\sigma_{xy}/\partial y = -\partial\sigma_{xx}/\partial x$; x and y are coordinates in the 2-D vertical plane). Since predicted normal stresses within the stress boundary layer can be significantly in excess of typical yield strengths of rocks, Fowler (1993) modified his previous viscous model and assumed a viscoplastic rheology to account for the finite yield stress of lithospheric materials. Viscoplastic fluids, also called “yield stress” fluids, have the property of behaving like a solid below some critical stress value (the yield stress), and as a viscous fluid when the yield stress is exceeded. This means that the

stresses generated by convection beneath the lid will reach the plastic yield stress at some depth (close or within the stress boundary layer) at which the material yields in a plastic manner. The thickness of the plastic zone increases as the yield stress is reduced, until at some critical yield stress, it reaches the base of the lid. Fowler (1993) considered that at this point, the lid can become mobile and take part of the circulatory motion (i.e. subduction initiates). The explicit criterion for the initiation of subduction is sensitive to the viscosity η_a of the upper mantle. Many different approaches give upper mantle viscosity estimates between 10^{19} to 10^{21} Pa s (Ranalli, 1995; Schubert et al., 2001, and references therein). Using representative numbers for the Earth's mantle, Fowler (1993) found that the critical yield stress necessary to start subduction is only reached for $\eta_a > 10^{21}$ Pa s. That is to say, subduction would be only marginally feasible in an Earth-like planet.

Solomatov (2004a) has applied Fowler's analytical theory in numerical simulations to investigate the possibility of initiation of subduction by small-scale convection. Using scaling laws for thermal convection, he showed that the thickness of the plastic zone should occupy 40 to 70 % of the lithosphere instead of its entire thickness, as Fowler's model assumed. He also found that the critical yield stress which would allow for initiation of subduction by small-scale convection is only about 3 MPa (Solomatov, 2004a, 2004b). This value is one order of magnitude smaller than stresses estimated by numerical models, heat flow measurements, and plate boundary strength (see above). Therefore, the requirement of such a small yield stress makes initiation of subduction by small-scale convection rather unlikely.

Fowler's and Solomatov's models provide evidence on the role that sublithospheric convection could play in the final fate of the oceanic lithosphere. However, they include an internal inconsistency in their rheological assumptions, which makes difficult to appraise the validity of their conclusions. Implicit in their models is the assumption that

stresses can be modelled with a temperature-strain rate-dependent creep law throughout the whole model. Consequently, very high stresses are predicted in a shallow stress boundary layer, where the temperature, strain rate, and viscosity are low, low, and high, respectively. However, the mechanical behaviour of lithospheric rocks at low to moderate temperatures and pressures does not follow a simple creep law, but is better described by a viscoelastic rheology (Turcotte & Schubert, 1982; Ranalli, 1995; Hall et al., 2003). The total deviatoric shear strain rate in a viscoelastic (Maxwell) material is

$$\dot{\epsilon} = \frac{\dot{\sigma}}{2\mu_M} + \frac{\sigma}{2\eta_M} \quad (6.4)$$

where μ_M and η_M are the Maxwell rigidity and Maxwell viscosity, respectively, σ the applied deviatoric stress, and $\dot{\sigma}$ its time derivative (Ranalli, 1995). According to Eq. (6.4), when the viscosity reaches values of the order of 10^{26} - 10^{30} Pa s, corresponding to temperatures between 550 - 750 °C for realistic ranges of olivine rheological parameters and convective stresses, the behaviour of the material is essentially elastic for normal convective time-scales. This implies that the stress transfer problem at temperatures $\lesssim$ 750 °C cannot be solved assuming the same constitutive rheological law for the material below this isotherm, and the brittle/elastic strength of the lid should be explicitly taken into consideration. This is also suggested by the results of Hall et al. (2003) and Gurnis et al. (2004) discussed above. When the elastic component of Eq. (6.4) is assumed to dominate the stress transfer within the upper lithosphere, the enormous amplification of stresses obtained by Fowler (1985, 1993) and Solomatov (2004a) disappears.

In summary, it is evident that the identification and interpretation of the general mechanism or mechanisms responsible for initiating subduction remain highly controversial and poorly understood. The difficulty arises not only because of the intrinsic complexity of the problem, but also because of the lack of consensus regarding basic

concepts behind the models, such as appropriate rheology, tectonic setting, dominant stress regime, driving forces, and density distribution. More importantly, most of the models focus on the issue of demonstrating that subduction initiation is a possible process, given certain conditions thought to be representative of some particular settings (e.g. mature passive margins). However, any model that attempts to explain the initiation of subduction must explain also the absence of it in those setting where the model predicts that subduction should take place.

All of the above models assume, explicitly or implicitly, that mature oceanic lithosphere is much more dense than the underlying mantle. In this scenario, the development of a significant gravitational instability is easily achieved, favouring the foundering of the lithosphere. This widely accepted idea was already shown to be in conflict with detailed composition-pressure-temperature-dependent models for oceanic lithosphere, such as those presented in Chapter 5 of this thesis and elsewhere (Hynes, 2005). The occurrence of frictionless discontinuities, necessary to force the slab to go down using expected ridge push values ($< 3.0 \times 10^{12} \text{ N m}^{-1}$), is also problematic. Even for the small values of friction coefficients (0.1 - 0.2) inferred in some plate boundaries (e.g. Brown et al., 2003), a typical fault zone supports average stresses that preclude subduction initiation (Hall et al., 2003). Also, it is not clear whether average fault zone stresses estimated from faults that have been active for many Ma are representative of incipient faults.

In the following section, I will analyze these two common assumptions (i.e. large negative buoyancy of mature oceanic lithosphere and the relation between ridge push and frictional resistance) separately, and show how they affect the relative stability of an oceanic plate with respect to subduction initiation.

6.3 Stability of oceanic lithosphere

6.3.1 Density structure as a function of age and depth

It was shown in Chapter 5 that the depth-averaged density of the oceanic lithosphere never exceeds the value reached by the sublithospheric mantle right beneath the lithosphere. Furthermore, maximum depth-averaged density contrasts between mature oceanic plates (using the MJP model for converting thermal thickness into plate age) and the adiabatic reference models were shown to be $< 40 \text{ kg m}^{-3}$. It is important, however, to identify which parts of the lithosphere contribute to this overall positive buoyancy and which ones could promote the development of an instability. To better understand the physical processes in this problem, models that isolate different parts of the physics must be formulated. To accomplish this, vertical profiles of density contrasts between the synthetic model OLSM2 and the reference mantle models RM-SI and RM-SO, at three different ages (25, 50, and 90 Ma), are constructed. Both cases of linear and non-linear depletion are analyzed.

The comparison between the non-linear depletion model and the reference model RM-SI is shown in Fig. 6.1A. The crust clearly represents the main contribution to positive buoyancy at all ages. In fact, for the cases of a 50 and 90 Ma old plate, it is the only buoyant part of the lithosphere. This is not strictly the case for plates younger than ~ 35 Ma, where there exist a positive contribution at the base to the plate. This is due to the differences in depletion between the OLSM2 and RM-SI models, which in young plates slightly offsets the negative contribution caused by thermal differences. The effects of the spinel-garnet transition are evident in the two jumps at ~ 50 and ~ 75 km depth. The former is the result of the phase transformation taking place within the plate, which is clearly displaced towards deeper levels at younger ages (i.e. exothermic reaction; see Fig. 5.7). The latter is a consequence of the downward shifting of the

phase transition in the adiabatic RM-SI reference model.

In accordance with the results from Chapter 5, no significant changes are observed when the linear depletion model is used instead (Fig. 6.1B). In both cases, maximum $\Delta\rho$ values of $\sim 100 \text{ kg m}^{-3}$ in the lithospheric mantle are marginally reached in a thin layer below the Moho. Depth-averaged $\Delta\rho$ values for the lithospheric mantle are $\sim 58 \text{ kg m}^{-3}$ for the 90 Ma old case. When the RM-SO reference model is used, the curves are displaced toward smaller values of $\Delta\rho$, but the general pattern remains the same (Fig. 6.1C - 6.1D). The only noticeable difference is the lack of a jump at $\sim 75 \text{ km}$ depth in old plates. This effect is obviously absent in these cases since RM-SO does not include the spinel-garnet phase change. Depth-averaged values of $\Delta\rho$ in the lithospheric mantle range between ~ 27.5 and 31.0 kg m^{-3} for the 90 Ma old case. For a plate of similar age that has not experienced any depletion at all, depth-averaged values of $\Delta\rho$ can be as large as $\sim 90 - 95 \text{ kg m}^{-3}$ (Fig. 6.1D). If the density distribution in a MOR column is used as a reference model, the above values estimated with the reference model RM-SI are increased by only $5 - 6 \text{ kg m}^{-3}$. This is because the density distribution at a MOR exhibits considerable departures from the RM-SI only at depths $\lesssim 30 \text{ km}$, where partial melting becomes significant (i.e. $> 5 \%$, Chapter 4).

As previously mentioned, these estimations are not representative of the whole plate, since they do not include the positive crustal effect. When the crust is included in the calculation of the total buoyancy, the above figures are significantly reduced ($\sim 50 - 90 \%$), and in some cases the lithosphere as a whole becomes positively buoyant. The depth-averaged $\Delta\rho$ value for the whole lithosphere (i.e. crust included) when depletion is considered in a 90 Ma old plate, is $\sim 30 \text{ kg m}^{-3}$ for the RM-SI case, and $\sim 0 - 3 \text{ kg m}^{-3}$ for the RM-SO case. Even in the case of no depletion, values $\lesssim 60 \text{ kg m}^{-3}$ for the total buoyancy are obtained. These are estimations for a plate generated in a purely passive MOR (see Chapter 4). Any active component at the time of plate generation

would result in a greater average depletion, reducing even more the negative buoyancy of the lithosphere. When this factor is combined with the possible underestimation of the depth of the spinel-garnet transition (Chapter 5; cf. also Klemme, 2004), the $\Delta\rho$ values estimated above are likely to represent upper bounds of attainable negative buoyancy.

A first approximation on how the above figures would affect previous estimations of the stability of mature oceanic lithosphere can be achieved following the analytic theory presented by Schubert and Zhang (1997). This model considered the foundering of the edge of a lithospheric plate shortly after the initiation of subsidence created by a negatively buoyant load. The latter is represented as the gravity force arising from the density difference between the lithosphere and the underlying asthenosphere $\Delta\rho$, considered to be a viscous half-space of constant density, ρ , and viscosity, η . The solution for the foundering velocity, as given by Schubert and Zhang (1997), reads

$$v_z = \left(\frac{1}{6e}\right) \left(\frac{\Delta\rho}{\rho}\right)^4 \left(\frac{\rho g d^2}{\eta}\right) \left(\frac{d}{x_n}\right)^2 \quad (6.5)$$

with

$$x_n = \frac{1}{4} \left(\frac{4D}{\rho g}\right)^{1/4} \quad (6.6)$$

where e is the base of natural logarithms, g the acceleration of gravity, d the thickness of the lithosphere, and D its flexural rigidity. As usually found in stability problems, Eq. (6.5) shows that the velocity with which the edge of the plate founders is strongly dependent on the density contrast. Using a $\Delta\rho \sim 90 \text{ kg m}^{-3}$, and other commonly accepted values for the above parameters, Schubert and Zhang (1997) estimated a maximum foundering velocity of $\sim 7.5 \text{ mm a}^{-1}$, which means that it would take $\sim 13 \text{ Ma}$

for the upper corner of the plate to reach a depth of 100 km below the level of the surrounding seafloor. This value is somewhat in agreement with estimations of the order of a few Ma for the time over which the Pacific plate changed its direction of motion, which has been attributed to the initiation of the Izu-Bonin-Mariana subduction zone (see references in Lowman et al., 2003). When $\Delta\rho$ values of 10 and 35 kg m⁻³, more in agreement with the above estimations for the whole lithosphere, are used in Eq. (6.5), foundering velocities of $\sim 7.5 \times 10^{-4}$ and 0.16 mm a⁻¹ are obtained, respectively. These velocities indicate that the upper corner of the plate would reach 100 km depth after 10 - 0.62 Ga, eliminating then the possibility of initiating subduction by this mechanism.

This conclusion applies also to the case of passive loading by sedimentation, as long the lithosphere maintains its mechanical integrity. Although the lithosphere could fail throughout its whole thickness by this process (e.g. Regenauer-Lieb et al., 2001; Branlund et al., 2001), it would not sink into the mantle because its depth-averaged density becomes smaller the greater the sediment pile is. A similar argument was presented by Turcotte et al. (1977) based on the stability of an elastic plate. However, if delamination of its lower part is possible, the sinking of this unstable section could be a viable process, although it can be never the cause for the foundering of the whole plate.

The average $\Delta\rho$ values obtained above are likely to affect the estimations of the evolution of the negative buoyancy of sinking slabs as well (i.e. models where the subduction is already taking place). This force has proven to be the dominant factor controlling a self-sustained subduction system (e.g. McKenzie, 1977; Hall et al., 2003), and representative estimations are therefore of primary importance. Since the analytical estimation of McKenzie (1977) of the minimum forced convergence (i.e. negative buoyancy) to generate a self-sustained system is similar to those obtained in more recent and detailed calculations (e.g. Hall et al., 2003; Gurnis et al., 2004; Mahatsente & Ranalli, 2004), it can be used to recalculate this convergence using the average $\Delta\rho$ values obtained

above. There is, however, one important factor that needs to be taken into account before a direct comparison can be made. Contrarily to what happens in the evolution of normal oceanic lithosphere, subducted lithosphere is greatly affected by compressibility and phase changes effects. This is due to the fact that in a subducting slab with an average velocity of $2.0 - 5.0 \text{ cm a}^{-1}$, the rate of pressure increase at a particular point within the slab is more important than the rate of thermal diffusion (cf. Schubert et al., 2001). As a consequence, a significant part of the slab experiences quasi-adiabatic compression, which increases the density of the mineral assemblage. Also, the subducted oceanic crust starts to transform into high-density eclogite at depths of $\sim 60 \text{ km}$ (e.g. Hacker, 1996; Aoki & Takahashi, 2004), progressively increasing the negative buoyancy of the slab. The blueschist/eclogite reaction is usually assumed to be completed at $\sim 100 \text{ km}$, but this depth depends on the actual hydration state of the slab (e.g. Hacker, 1996). For simplicity, I assume here that the transition is sharp and that it takes place at an average depth of 75 km .

A simple model that considers all of the above (hereafter SLSM1), plus the depletion factor, was constructed using LitMod. Snapshots of the thermal structure of a vertical slab 120 km thick at depths of 150 , 180 , and 250 km are shown in Fig. 6.2. Although the thermal structure of SLSM1 is highly idealized, and surely unreliable in the crustal part, it is representative of more than 80% of the slab, according to other more accurate calculations (e.g. Doin & Henry, 2001; Mahatsente & Ranalli, 2004). Moreover, since the calculation of the crustal buoyancy is carried out independently, the thermal structure on the crustal part of SLSM1 does not affect significantly the final estimation of the slab buoyancy. A further cross-check was also performed between SLSM1 and the model of Mahatsente and Ranalli (2004), considering the different subduction angle between the models. The latter includes compressibility effects, but neither compositional differences between lithospheric and surrounding mantle nor eclogitization. It was found that when these effects are removed in SLSM1, the negative buoyancy predicted by both models

at similar depths are almost identical, suggesting that the simple thermal structure of SLSM1 is a good proxy for studying the properties of a subducting slab. With this in mind, the minimum forced convergence to start a self-sustained subduction system was obtained by calculating the negative buoyancy of the slab at the three different depths, and comparing them with those computed by McKenzie (1977).

Based on the force balance expressed in Eq. (6.1) for a plate 120 km thick, McKenzie (1977) estimated a minimum convergence of 130 km for a vertical slab (i.e. tip of the slab at 250 km depth), assuming a constant density contrast of 57.5 kg m^{-3} . This figure corresponds to a minimum buoyancy force $D_S \sim 8.8 \times 10^{12} \text{ N m}^{-1}$. Since SLSM1 includes a depleted oceanic slab (intrinsically more buoyant), it can be expected that the predicted minimum forced convergence will be larger than that given in previous works. Fig. 6.3 illustrates the results. Surprisingly, predictions from SLSM1 ($\sim 140 - 170 \text{ km}$ of convergence) are not considerably different from those given in McKenzie's work. This apparent contradiction can be explained as follows. The model of McKenzie (1977) considers only thermal anomalies in an homogenous material, but neither depletion, compressibility, or eclogitization were included. The thermal effect alone gives an overestimation of the real buoyancy, since depleted material is intrinsically more buoyant. However, eclogitization and quasi-adiabatic compressibility have an opposite effect on the final buoyancy. If these opposite and competing effects are of similar magnitude, a model that takes into account only the thermal contribution would provide an approximately valid estimation of the total buoyancy. According to the results from SLSM1, this seems to be the case. Instead, thermal models that include only two of the three main factors controlling the magnitude of the negative buoyancy (e.g. thermal + depletion, thermal + compressibility/eclogitization) are "unbalanced", and therefore they would either overestimate or underestimate the negative buoyancy of the slab. This is the main cause for the discrepancies found between the SLSM1 model and that of Mahatsente and Ranalli (2004) (Fig. 6.3).

Summarizing, analysis of systems that include composition-compressibility-thermal effects indicate that these factors play a key role in the stability of the oceanic lithosphere, making it more resistant to mechanisms previously thought to initiate subduction. This suggests that models that consider only thermal effects are not appropriate for modelling subduction initiation. On the other hand, for the case of a slab already subducting, models based on thermal differences only seem to be a valid approximation for estimating the total negative buoyancy of the slab. Results from both purely thermal models and those including compressibility, eclogitization, and depletion (SLSM1), are consistent in terms of the minimum amount of lithospheric material that needs to be forced into the mantle to generate a self-sustained subduction.

6.3.2 Force Balance: Ridge push vs fault resistance

Ridge push forces arise from the negative buoyancy associated with the cooling of the oceanic lithosphere as it moves away from a MOR (e.g. Parsons & Richter, 1980; Turcotte & Schubert, 1982). They are commonly assumed to be the main factor responsible for the general state of compression in old oceanic lithosphere and for passive margin reactivation, compression, and/or failure (e.g. Parsons & Richter, 1980; Mueller & Phillips, 1991; Faccenna et al., 1999).

It is straightforward to estimate the ridge push when a particular model for the evolution of the oceanic lithosphere is assumed. Calculations based on the half-space cooling model gives a relation of the type (Turcotte & Schubert, 1982)

$$D_R = g\rho_r\alpha\Delta T \left[1 + \frac{2}{\pi} \frac{\rho_r\alpha\Delta T}{(\rho_r - \rho_w)} \right] \kappa t \quad (6.7)$$

where g is the acceleration of gravity, ρ_m the asthenosphere density, α the CTE, ΔT the

temperature difference between the asthenosphere and the plate surface, ρ_w the density of the sea water, ρ_r a reference density at the bottom of the lithosphere, κ the thermal diffusivity, and t the age of the lithosphere. To a good approximation, Eq. (6.7) can be simplified to

$$D_R = g \Delta\rho \kappa t \quad (6.8)$$

where $\Delta\rho$ is the density difference between the base and the top of the plate. In this model, the ridge force increases linearly with age. Estimations for D_R using Eqs. (6.7-6.8) range between 6×10^{12} and 7×10^{12} N m⁻¹ for a 200 Ma old plate (Parsons & Richter, 1980; Turcotte & Schubert, 1982). If a plate cooling model is assumed instead, D_R approaches an asymptotic value of about 3×10^{12} N m⁻¹ (e.g. Parsons & Richter, 1980).

Again, these estimates are based purely on thermal cooling. A detailed density model of a MOR that includes thermal, compositional, partial melting, and compressibility effects was obtained in Chapter 4. Therefore, it would be instructive to calculate the ridge push force that this model predicts and compare it with previous estimations. To do this, a force balance is performed in an identical manner as in Parsons and Richter (1980) and Turcotte and Schubert (1982), but considering the thermal and density structure of the OLSM1 model (Figs. 5.4 and 5.6). Fig. 6.4 illustrates the geometry used to derive the ridge push force. The forces involved in the system are the integrals of the lithostatic pressures on the boundaries of the plate. Hence,

$$F_M = g \int_0^{z_{max}} \rho_m(z) z dz \quad (6.9a)$$

$$F_W = g \int_0^{z_W} \rho_W z dz \quad (6.9b)$$

$$F_P = \int_{z_W}^{z_{max}} P_L dz \quad (6.9c)$$

where P_L is given by

$$P_L = g\rho_W z_W + g \int_0^{z'} \rho_l(z) dz' \quad (6.10)$$

and z_{max} is the depth to the base of the plate, z_W the water depth (from the ridge crest), $z' = z - z_W$, and $\rho_m(z)$, $\rho_l(z)$, ρ_W the depth-dependent densities beneath the MOR, within the plate, and of seawater (constant), respectively. Taking the densities obtained in Chapter 4 and 5 for the MOR, a plate ~ 100 Ma old, $\rho_W = 1030 \text{ kg m}^{-3}$, $z_W = 3000 \text{ m}$, and $z_{max} = 106 \text{ km}$ (the asymptotic depth of the 1300°C isotherm), Eqs. (6.9a) - (6.9c) give asymptotic values $F_M \sim 1.78 \times 10^{14}$, $F_W \sim 4.5 \times 10^{10}$, and $F_P \sim 1.75 \times 10^{14} \text{ N m}^{-1}$. The asymptotic net horizontal force (i.e. ridge push) on the lithosphere is obtained by combination of these three forces

$$D_R = F_M - F_W - F_P = 2.95 \times 10^{12} \text{ N m}^{-1} \quad (6.11)$$

equivalent to an average normal stress of $\sim 28.6 \text{ MPa}$. If the structure corresponding to a ~ 25 Ma old plate is used instead, together with representative values of $\rho_W = 1030 \text{ kg m}^{-3}$, $z_W = 1000 \text{ m}$, and $z_{max} = 60 \text{ km}$ (depth of the 1300°C isotherm), a value $D_R = 9.0 \times 10^{11} \text{ N m}^{-1}$ (average normal stress of 15.2 MPa) is obtained. In both cases, predictions from the present model are almost identical to those from other plate models (Fig. 6.5), suggesting that compositional, partial melting, and compressibility effects are not of primary importance in the estimation of the ridge push. Indeed, an inspection of Eqs. (6.9a), (6.9b), (6.9c), and (6.10) indicates that the results depend

mainly on the integral limits, and are not significantly sensitive to small changes in the average densities.

If the ridge push force is only supported by the brittle/elastic layer over the long time scale, asymptotic average horizontal normal stresses in mature oceanic lithosphere can reach values of 42, 53, and 74 MPa depending on whether the thickness of the elastic layer is defined by the 800, 600, or 400 °C isotherm. The first two values are in the same range as estimations in trenches and fracture zones, respectively (Watts, 2001), and therefore they are more likely to be appropriate for thermally undisturbed oceanic lithospheres, such as those found in most passive margins. Considering the variation in orientation of potential planes of failure, the area per unit length on which the ridge push force would be acting is

$$A' = \frac{A}{\sin \theta} \quad (6.12)$$

where A is the thickness of the elastic layer and θ as in Eq. (6.3). Hence, the depth-averaged normal and shear stresses on that plane are

$$\sigma_{RP} = \frac{D_R \sin \theta}{A'} \quad (6.13)$$

$$\tau_{RP} = \frac{D_R \cos \theta}{A'} \quad (6.14)$$

Assuming that the average normal stress at any depth is the sum of Eq. (6.13) and the average lithostatic pressure ($\rho g z_{max}/2$), that the fault has no cohesion, and that the fluid pressure is hydrostatic, the average shear resistance of a fault in the case of an elastic layer defined by the 600 °C isotherm is ~ 53 and 108 MPa for friction coefficients

of 0.1 and 0.2, respectively (Fig. 6.6). The latter values represent the smallest friction coefficients measured in laboratory (e.g. Brown et al., 2003). Fig. 6.6 shows that for the case above, the shear resistance is on the average ~ 30 to 70 MPa greater than the available average shear stress arising from the ridge push.

In order to reduce the shear resistance to values comparable to those from the ridge push, either a friction coefficient one order of magnitude less ($\mu \sim 0.03$) than the smallest estimations in rocks or pore fluid factors λ (i.e. the ratio between fluid pressure and lithostatic pressure) much greater than hydrostatic throughout the whole section ($\lambda \sim 0.8$) are needed. Alternatively, a combination of these factors could also satisfy this condition. However, there is no direct evidence for the existence of these extreme conditions along passive margins, fracture zones, or transform margins. Zoback and Townend (2001), for example, showed that the pore fluid pressure in several tectonic environments is often near hydrostatic down to depth of ~ 12 km. The present-day situation along the Norwegian margin is relevant to this matter, since the ridge push component in the regional stress field is considerably large ($\sim 2 \times 10^{12}$ N m $^{-1}$) and enhanced by isostatic rebound (e.g. Fejerskov & Lindholm, 2000). Structural interpretations and *in situ* measurements are consistent with high compressional stresses dominating in this margin (between 20 - 30 MPa in the first 10 km from the surface). If representative friction coefficients and pore fluid factors for this margin were 0.05 and 0.75, respectively, shear resistance of faults as long as 20 and 40 km would be ~ 6 and 9 MPa, respectively, and consequently deviatoric stresses higher than these values should not be present. This is in disagreement with *in situ* stress observations (Fejerskov & Lindholm, 2000). In contrast, when an average hydrostatic value for pore fluid factor is considered together with a friction coefficient of ~ 0.1 , 20 to 40 km-long faults support average shear stresses of 21 - 37 MPa, more consistent with observations and estimations of the ridge push. Because the uncertainties in μ and λ are still quite large, a conclusive assessment of representative fault shear strengths is precluded. However, coefficients of friction smaller than 0.05

seem to be too low for being representative of translithospheric faults. If it is assumed that near hydrostatic fluid pressures are appropriate, then coefficients of friction of the order of 0.1 - 0.2 give fault shear strengths that are consistent with measurements in different tectonic settings (10 - 60 MPa).

6.4 A new model for the initiation of subduction

Three main conclusions can be drawn from the discussion in the previous section: (a) models that require a large depth-averaged negative buoyancy (i.e. $60 < \Delta\rho < 100 \text{ kg m}^{-3}$) in mature oceanic lithosphere cannot be used to account for the initiation of a subduction zone; (b) available forces are too small to effectively cause convergence along “normal” fault zones; and (c) inactive approximately frictionless fault zones are difficult to reconcile with laboratory and field observations.

Most of the models that attempt to explain the initiation of subduction are based on a balance of forces that are originated within the lithosphere, either by compositional variations, differential loading, or differential cooling. All these forces, however, are ultimately a consequence of mantle convection. It is therefore logical to think that sublithospheric mantle dynamics could play an important role in both the creation and the destruction of lithospheric plates. In this section I present a simple analytical theory that seeks to explain how an oceanic plate can be initially broken and pulled into the mantle by a R-T instability, until the system becomes self-sustaining. This model is more consistent with the evidence presented in this thesis for the oceanic lithosphere. The reasons for pursuing an analytical theory are twofold. First, besides having the advantage of being simpler than numerical models, analytical studies permit to assess in a simple way the first-order reliability of the proposed physical scenario. Second, analytical models provide scaling information on the fundamental relations among the factors controlling the evolution of the system under study, which can be used later to imple-

ment more complicated models. In an analytical model, however, many assumptions and simplifications have to be made. Yet, by using well-established physical concepts and realistic interactions between them, the first-order features of the system can be obtained with reasonable confidence.

6.4.1 Statement of the problem

The scenario analyzed is envisaged in Fig. 6.7, which depicts a brittle/elastic layer, representing the long-term stress supporting layer, on top of a highly viscous fluid in which a R-T instability is being developed. This is possible because the material making up the lowermost part of the oceanic lithosphere is essentially of the same composition as the underlying mantle (Section 5.2.1 in Chapter 5). Hence, thermal anomalies translates directly into buoyancy anomalies. For a certain critical wavelength, the instability will grow until it reaches a quasi-steady state, at least for a certain finite period of time (cf. Schubert et al., 2001). The development of the downgoing plume produces two adjacent cells where hot material is brought up in order to conserve mass and momentum in the system. Due to the geometry of the flow, zones of high shear develop between the downgoing plume and the upgoing return flow, where deformation will be strongly concentrated if the material follows a stress-dependent rheology. The elastic upper lithosphere also experiences relatively high shear stresses at the same position, in addition to a longitudinal tensile stress due to the bending of the elastic plate. This tensile stress will decrease the effective strength of any potential fault plane to be activated. Because there is a vertical gradient in the shear stress transmitted from the viscous part to the brittle/elastic layer, a horizontal gradient in the longitudinal stress will also develop within the latter (i.e. ∂

$\sigma_{xy}/\partial y = -\partial\sigma_{xx}/\partial x$; x and y are the coordinates in the 2D vertical plane). The resulting longitudinal stresses are compressive above the downwelling and tensile above

the forced upwellings. Thermal and mechanical thinning occurs at both sides of the cold plume (Fig. 6.7B). If the asthenospheric material reaches depths of $\sim 80 - 60$ km, partial melting occurs, weakening these zones even more. Due to second-order random perturbations (e.g. proximity to a passive margin, other plumes, mantle inhomogeneities, etc), eventually one side starts to concentrate the deformation more than the other, until a clear asymmetry between the upgoing section and the downgoing plume is reached (Fig. 6.7C). At this point, most of the negatively buoyant material is concentrated in one side of the zone where most of the upwelling (and incipient partial melting) occurs. When this happens, widespread partial melting (boninitic magmatism) and extension takes place in the top side of the incipient trench, while the gravitational force of the cold plume provides enough energy to decouple and bend the lithosphere at the other side (Fig. 6.7D). By now, thermal relaxation has further increased the negative buoyancy of the plate by cooling the upper parts of it above the instability. The negatively buoyant edge of the incipient slab is now supported only by one side of the elastic lithosphere, which further bends and is pulled into the mantle, marking the initiation of a subduction zone (Fig. 6.7E).

The above description of the instability is based on well-established observations in laboratory, numerical, and analytical models of R-T instabilities (e.g. Canright & Morris, 1993; Fowler, 1993; Conrad & Molnar, 1997; Marotta et al., 1998; Solomatov & Moresi, 2000; Schubert et al., 2001; Pysklywec & Shahnas, 2003; Solomatov, 2004a; Zaranek & Parmentier, 2004). Indeed, although available convection computational codes cannot simulate simultaneously all the above processes, the proposed scenario is in agreement with results from recent convection experiments in which failure of the lithosphere is allowed (e.g. Auth, 2001). Unfortunately, neither fully coupled thermomechanical numerical simulations nor scale models of the above scenario are yet available.

In the following analysis I will first describe the governing equations, give general

solutions for them, and find useful relationships between the main parameters. Then I will perform a first-order energy balance to show that the model is energetically feasible and to constrain the minimum wavelengths of the instabilities. These estimated wavelengths can be thought of as the minimum attainable size by the instability necessary to drive the system. If the physical description is correct, they should be qualitatively comparable to the ones obtained in convection experiments, and at least, similar to those predicted by perturbation methods. The stress transfer problem between the viscous and elastic parts of the lithosphere, and the generation of a translithospheric fault will be addressed subsequently. Finally, the sinking of the lithosphere due to its negative buoyancy will be analyzed.

6.4.2 Flow of the viscous layer

The geometry of the model is schematized in Fig. 6.8. The viscous and the elastic layers are coupled at the interface, where stresses and velocity vectors are continuous. The effect of gravity is implicitly included in the prescribed velocity field, which is the result of the body force. In other words, the instability is modelled kinematically. For the dimensions of the region of interest, compressibility has negligible effects on the flow pattern and consequently is not included. Since the Prandtl number (ratio of the kinematic viscosity to the thermal diffusivity) of the Earth's mantle is practically infinite, it is appropriate to neglect inertia or time-dependent terms in the equations of motion. Also, a Newtonian viscosity is assumed, which greatly simplifies the manipulation of the equations without losing generality for the major features of the flow. Although average velocities and dimensions of plumes are typically modified by the inclusion of a non-Newtonian rheology (see Section 6.5), both analytical and numerical experiments show that the main characteristics of a R-T instability do not experience first-order changes, either in the flow pattern or in the stresses spatial distribution (e.g. Canright

& Morris, 1993; Solomatov & Moresi, 2000; Schubert et al., 2001). It is recognized that a power-law rheology would favour to some extent the mechanical erosion in regions of high shear. This means that deformation of the lithosphere will be greater in these regions, producing a stronger weakening effect, and reducing even more its mechanical thickness. It is important then to identify these regions in the general flow pattern driven by the cold plume.

In Cartesian coordinates, the governing equations for a viscous incompressible flow with no body forces are (see e.g. Kundu, 1990; Schubert et al., 2001)

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (6.15)$$

$$-\frac{\partial P}{\partial x} + \eta \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = 0 \quad (6.16)$$

$$-\frac{\partial P}{\partial y} + \eta \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) = 0 \quad (6.17)$$

where u and v are the horizontal and vertical components of the velocity field, respectively, and η is the viscosity of the medium. The viscous deviatoric stresses are given by

$$\tau_{xx} = 2\eta \frac{\partial u}{\partial x} \quad (6.18)$$

$$\tau_{yy} = 2\eta \frac{\partial v}{\partial y} \quad (6.19)$$

$$\tau_{xy} = \eta \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \quad (6.20)$$

I look for a solution that assumes a sinusoidal dependence on x for the vertical component of the velocity. This assumption is based on results from numerical models of gravitational instabilities, and it will be justified *a posteriori* by the success of the final solution to describe a flow with identical features that those predicted by more rigorous numerical models (see below). Accordingly, I choose

$$v_{(x,y)} = -v_o f(y) \cos \left(\frac{2\pi x}{\lambda} \right) \quad (6.21)$$

where v_o is the vertical component of velocity at $x = 0$ and $y = H$ (Fig. 6.8), and $f(y)$ is an unknown dimensionless function to be determined that describes the variation of the velocity in the y -direction. From Eqs. (6.15), (6.18), (6.19), and (6.21), we can write

$$\frac{\partial u}{\partial x} = v_o \frac{df}{dy} \cos \left(\frac{2\pi x}{\lambda} \right) \quad (6.22)$$

Integrating

$$u(x, y) = v_o \frac{\lambda}{2\pi} \frac{df}{dy} \sin \left(\frac{2\pi x}{\lambda} \right) + c_1 \quad (6.23)$$

From symmetry ($u(0, y)$), c_1 is required to be zero. From Eqs. (6.18) - (6.23)

$$\tau_{xx} = 2\eta v_o \frac{df}{dy} \cos \left(\frac{2\pi x}{\lambda} \right) = -\tau_{yy} \quad (6.24)$$

$$\tau_{xy} = \eta v_o \frac{\lambda}{2\pi} \left[f(y) \left(\frac{2\pi}{\lambda} \right)^2 + \frac{d^2 f}{dy^2} \right] \sin \left(\frac{2\pi x}{\lambda} \right) \quad (6.25)$$

Eliminating the pressure term from Eqs. (6.16) and (6.17) by cross-differentiating and subtracting yields

$$\frac{\partial^2 \tau_{xy}}{\partial x^2} - \frac{\partial^2 \tau_{xy}}{\partial y^2} - 2 \frac{\partial^2 \tau_{xx}}{\partial x \partial y} = 0 \quad (6.26)$$

Using Eqs. (6.24) and (6.25) I obtain the differential equation for $f(y)$

$$\frac{\lambda}{2\pi} \frac{d^4 f}{dy^4} - \frac{4\pi}{\lambda} \frac{d^2 f}{dy^2} + \left(\frac{2\pi}{\lambda} \right)^3 f = 0 \quad (6.27)$$

or

$$\frac{d^4 f}{dy^4} - a \frac{d^2 f}{dy^2} + b f = 0 \quad (6.28)$$

where

$$a = 2 \sqrt{b} \quad ; \quad b = \left(\frac{2\pi}{\lambda} \right)^4 \quad (6.29)$$

Eq. (6.29) is a homogeneous fourth-order differential equation that can be solved by standard methods (e.g. Kreyszig, 1988). The auxiliary equation takes the form

$$\lambda^4 - 2 \sqrt{b} \lambda^2 + b \quad (6.30)$$

which can be solved by the well-known quartic equation method to obtain the roots

$$\lambda_1 = \lambda_2 = \frac{1}{2} R \quad ; \quad \lambda_3 = \lambda_4 = -\frac{1}{2} R \quad (6.31)$$

where $R = \sqrt{4\sqrt{b}}$. Therefore the general solution of Eq. (6.27) is

$$f(y) = A e^{\alpha y} + B y e^{\alpha y} + C e^{-\alpha y} + D y e^{-\alpha y} \quad (6.32)$$

where A , B , C , and D are constants that need to be determined from boundary conditions (this will be done in Section 6.4.5), and $\alpha = R/2$.

6.4.3 Deformation of the elastic layer

6.4.3.1 General solution

The general equation for elastic flexure under combined vertical and horizontal (i.e. in-plane) forces is (Eq. (4.15))

$$q(x) = D \frac{d^4 w(x)}{dx^4} + N \frac{d^2 w(x)}{dx^2} + \Delta \rho g w \quad (6.33)$$

where $w(x)$ is the deflection, $q(x)$ is the loading function, D the flexural rigidity, N the horizontal force per unit length acting on the direction of the x axis, and $\Delta \rho$ the density difference between the average density of the elastic layer and that of water. Referring to Fig. 6.8 and Eqs. (6.21), the loading function is represented as

$$q(x) = -q_o \cos\left(\frac{2\pi x}{\lambda}\right) \quad (6.34)$$

Eq. (6.33) is a fourth-order, non-homogeneous differential equation, and therefore its general solution is of the form $w(x) = w_H(x) + w_P(x)$, where $w_H(x)$ is the solution of the homogeneous part and $w_P(x)$ is the solution of the non-homogeneous part (Kreyszig, 1988). The former is derived in Appendix A; the latter can be guessed on the basis of the form of the non-homogeneous part (i.e. the loading function). I try

$$w_P(x) = w_o \cos\left(\frac{2\pi x}{\lambda}\right) \quad (6.35)$$

Differentiating Eq. (6.35) and substituting into Eq. (6.33) yields

$$w_o = \frac{-q_o}{\left[D\left(\frac{2\pi}{\lambda}\right)^4 - N\left(\frac{2\pi}{\lambda}\right)^2 + \Delta\rho g\right]} \quad (6.36)$$

Eq. (6.36) shows that, when the wavelength of the deformation tends to infinity, the topography tends to the isostatic value ($w_o \Delta\rho g = -q_o$). At shorter wavelengths, the elastic resistance of the lithosphere prevents total isostatic compensation (see also Turcotte & Schubert, 1982). The ratio between Eq. (6.36) and the infinite-wavelength case (w_o / w_∞) is plotted in Fig. 6.9 as a function of the wavelength for an elastic plate with $E = 70$ GPa, $\nu = 0.25$, $\Delta\rho = 2300$ kg m⁻³, and different elastic thicknesses. It is found that the topography is 50 % compensated if the wavelength is $\sim 240, 325$, or 400 km for a plate $20, 30$, and 40 km thick, respectively. It is also evident from this figure that the contribution of a horizontal force (i.e. N) with a magnitude representative of the ridge push ($1 - 5 \times 10^{12}$ N m⁻¹) is negligible.

Applying proper boundary conditions for an infinite elastic plate with a finite distributed load to Eq. (6.33) leads to the conclusion that $w_H(x) = 0$, and therefore the full solution in this case is (see Appendix A)

$$w(x) = w_P(x) \quad (6.37)$$

6.4.3.2 Elastic stresses

Strains due to bending alone result in normal stresses across the elastic layer that are given by (Turcotte & Schubert, 1982)

$$\sigma_{xx} = \frac{E}{(1 - \nu^2)} \epsilon_{xx} = -\frac{E}{(1 - \nu^2)} y \frac{d^2 w}{dx^2} \quad (6.38)$$

where E is the Young's modulus, ν is the Poisson's ratio, ϵ_{xx} is the longitudinal strain, and $y = 0$ is taken in the middle of the layer. Using Eq. (6.35 - 6.37), Eq. (6.38) gives

$$\sigma_{xx} = \frac{E}{(1 - \nu^2)} y w_o \left(\frac{2\pi}{\lambda} \right)^2 \cos \left(\frac{2\pi x}{\lambda} \right) \quad (6.39)$$

Therefore, for the geometry illustrated in Fig. 6.8, the maximum longitudinal stresses are attained at points where the curvature of the plate is either a maximum or a minimum (i.e. where the viscous flow is entirely vertical).

In addition to the bending stresses, a deformation of the type depicted in Fig. 6.8 will also generate homogeneously distributed tensional strains and stresses, arising from the difference in length between the deformed and the undeformed state (only when the

lateral boundaries of the plate are not allowed to experience horizontal displacements). For small deflections, this difference can be described as (Timoshenko & Woinowsky-Krieger, 1959)

$$\epsilon_{xx} = \frac{s - \lambda}{\lambda} \approx \frac{1}{2\lambda} \int_0^\lambda \left(\frac{dw}{dx} \right)^2 dx \quad (6.40)$$

Substituting Eq. (6.37) into (6.40) yields

$$\epsilon_{xx} = -\frac{1}{2\lambda} w_o^2 \left(\frac{2\pi}{\lambda} \right)^2 \int_0^\lambda \sin^2 \left(\frac{2\pi x}{\lambda} \right) dx \quad (6.41)$$

Using trigonometrical identities, Eq. (6.41) can be rewritten as

$$\epsilon_{xx} = -\frac{1}{2\lambda} w_o^2 \left(\frac{2\pi}{\lambda} \right)^2 \int_0^\lambda \left[\frac{1 - \cos 2 \left(\frac{2\pi x}{\lambda} \right)}{2} \right] dx \quad (6.42)$$

which has the solution

$$\epsilon_{xx} = -w_o^2 \left(\frac{2\pi}{\lambda} \right)^2 \quad (6.43)$$

The normal stresses arising from this longitudinal strain can be calculated substituting Eq. (6.43) into Eq. (6.38).

The integrated shear stress along a vertical plane is given by (Turcotte & Schubert, 1982)

$$V_{(x)} = D \frac{d^3 w}{dx^3} = D w_0 \left(\frac{2\pi}{\lambda} \right)^3 \sin \left(\frac{2\pi x}{\lambda} \right) \quad (6.44)$$

From Eq. (6.44) it can be seen that shear stresses will reach their maximum magnitude at the midpoints between the down-going and up-going plumes. It will be shown that this shear force is not important unless large deflections take place.

6.4.4 Energy balance

If the generation of an instability in the lowermost part of the lithosphere is the main factor responsible for the deformation, failure, and sinking of the oceanic lithosphere, it is expected that the gravitational energy associated with this instability (and lateral upwellings) must reach a critical value before it can trigger subduction. One way to estimate this critical value is to compare the total available gravitational energy with that dissipated in deforming the underlying mantle, in shearing (frictional and viscous) of a potential fault plane, and by viscous dissipation during the deformation of the viscous part of the lithosphere (e.g. Conrad & Hager, 1999). Elastic deformation does not dissipate energy, but requires work done by an external force. When an instability of a certain wavelength starts to develop, both the negative buoyancy force and the potential energy increase. If the configuration is stable and isostatically compensated, the only work done by the total buoyancy force on the system is the deformation of the overlying elastic layer. If the system is experiencing motion, and consequently viscous dissipation, the available energy from buoyancy forces to do work on the elastic layer is decreased. In the limit case where all the released potential energy is being dissipated by deforming a limited region of viscous material and the surrounding mantle, there would not be enough energy to drive the motion of the fault and bend the elastic layer.

If the initiation of subduction by the proposed mechanism is feasible, then it requires

that (Conrad & Hager, 1999)

$$\Phi_B \geq \Phi_{mc} + \Phi_f + \Phi_l \quad (6.45)$$

where Φ_B , Φ_{mc} , Φ_f , and Φ_l are the total rate of potential energy release by the downgoing plume, and the viscous dissipation rate in the surrounding mantle, in the fault, and in the viscous part of the lithosphere, respectively. All dissipation terms are per unit length perpendicular to the direction of flow ($\text{J s}^{-1} \text{m}^{-1}$). Instabilities that do not satisfy Eq. (6.45), cannot initiate subduction because the available gravitational energy due to their negative buoyancy is rapidly dissipated by the aforementioned deformation mechanisms. It should be noted that this does not preclude the growth of smaller instabilities. It only means that in order for the instability to overcome all the dissipative processes at a lithospheric scale, there is a critical size that must be attained. In what follows, I give first order estimations of the above energy terms and show that under realistic circumstances the postulated mechanism for initiating subduction is energetically viable.

A lower bound value for the total gravitational body force can be obtained by considering changes in density arising only from thermal anomalies. The omission of compressibility gives a highly conservative estimate of the total gravitational body force. For a cold thermal plume of the type illustrated in Fig. 6.8, this force can be approximated as

$$F_B = g \rho \Delta T \alpha \frac{l_p}{2} \lambda \quad (6.46)$$

where l_p is depth of the tip of the plume. The factor $1/2$ arises from integrating a sinusoidal function that describes the shape of the plume. The total rate of potential

energy release provided by the plume is, to the first order, (Turcotte & Schubert, 1982).

$$\Phi_B = F_B \frac{v_o}{2} \quad (6.47)$$

where v_o is, as before, the vertical component of velocity at $x = 0$ and $y = H$.

For an isoviscous mantle, the fluid deformation within a convective cell, such as that generated on both sides of the downgoing plume, produces shear stresses that dissipate energy by doing work on the boundaries of the cell. For the case in Fig. 6.8, a lower bound value for this dissipation rate can be estimated as (Turcotte & Schubert, 1982)

$$\Phi_{mc} = 2 l_p \left(\frac{2 v_o^2 \eta_c}{\lambda} + \frac{\bar{u}^2 \lambda \eta_c}{l_p^2} \right) \quad (6.48)$$

where η_c is the viscosity of the surrounding mantle and $\bar{u}$ is a representative depth-averaged horizontal velocity.

The shear strain rate across a viscous fault zone is simply

$$\dot{\epsilon}_f = \frac{1}{2} v_r / w_f \quad (6.49)$$

where v_r is a representative slip velocity and w_f is the fault zone width. The average shear stress within this fault zone is therefore given by

$$\bar{\tau}_f = 2 \eta_f \dot{\epsilon}_f \quad (6.50)$$

where η_f is the average viscosity of the fault zone. In the case of a purely frictional fault, the strength is given by Eq. (6.3) divided by the length of the fault. The energy dissipation per unit area in a frictional fault is $\tau_{friction} v_r$. The rate at which energy is dissipated in a translithospheric fault plane is the combination of these two effects

$$\Phi_f = \overline{\tau_f} v_r l_{fv} + \tau_{friction} v_r l_{ff} \quad (6.51)$$

where l_{ff} and l_{fv} are the lengths of the frictional and viscous part, respectively. The thermomechanical coupling between the heat generated by this mechanism and its effect on fault weakening is ignored here. It will be implicitly included in the value of η_f .

The rate at which work is done on the viscous part of the lithosphere and plume is (Conrad & Hager, 1999)

$$\Phi_l = 2 \int_x \int_y \eta_l \dot{\epsilon}_{ij} \dot{\epsilon}_{ij} dy dx \quad (6.52)$$

where η_l is the average viscosity of the viscous part of the lithosphere and $\dot{\epsilon}_{ij}$ is the strain rate. Eq. (6.52) shows that the viscous dissipation is directly proportional to the square of the velocity gradients and is therefore more important in regions of high shear. Naturally, it is also dependent on the area affected by deformation and on the average viscosity of the medium. Integrating as before over a sinusoidal function that describes the shape of the plume and considering representative constant strain rates, Eq. (6.52) can be explicitly written as

$$\Phi_l = 2 \eta_l \frac{l_p \lambda}{2} \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 + \frac{1}{2} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 \right] \quad (6.53)$$

When the rate of available energy provided by gravitational instability satisfies the condition (6.45), then subduction can start if the buoyancy force is enough to bend the elastic part of the lithosphere. In the scenario depicted in Fig. 6.8, the total work done to bend the elastic plate can be approximated as (neglecting horizontal forces)

$$W_e = \frac{1}{2} \int_0^\lambda q(x) w(x) dx \quad (6.54)$$

Substituting Eqs. (6.34) into Eq. (6.54) and integrating by parts gives

$$W_e = \frac{D}{2} \left[\left(w \frac{d^3 w}{dx^3} - \frac{dw}{dx} \frac{d^2 w}{dx^2} \right) \Big|_0^\lambda \right] + \frac{D}{2} \int_0^\lambda \left(\frac{d^2 w}{dx^2} \right) dx + \frac{1}{2} g \Delta \rho \int_0^\lambda w^2 dx \quad (6.55)$$

Using Eq. (6.37) yields

$$W_e = \frac{D}{2} \int_0^\lambda \left(\frac{2\pi}{\lambda} \right)^4 w_o^2 \cos^2 \left(\frac{2\pi x}{\lambda} \right) dx + \frac{1}{2} g \Delta \rho \int_0^\lambda w_o^2 \cos^2 \left(\frac{2\pi x}{\lambda} \right) dx \quad (6.56)$$

which can be solved using trigonometric identities to give

$$W_e = \frac{D}{4} w_o^2 \left(\frac{2\pi}{\lambda} \right)^4 \lambda + \frac{1}{4} g \Delta \rho w_o^2 \lambda \quad (6.57)$$

Substituting Eq. (6.36) into Eq. (6.57) and rearranging, the final expression for the work done by the force q_o in bending the elastic plate is

$$W_e = \frac{q_o^2 \lambda}{4 \left[D \left(\frac{2\pi}{\lambda} \right)^4 + \Delta \rho g \right]} \quad (6.58)$$

Consequently, the total average force needed to generate this bending is

$$\overline{F_e} \sim \frac{W_e}{2w_o} \quad (6.59)$$

and it must be provided by the negative buoyancy of the gravitational instability. The force in Eq. (6.59) is the total force to produce the complete wavelength undulation of the elastic plate. However, in the case of a plate that has been already broken (Stage D in Fig. 6.7), the resistance of the elastic plate to the same load decreases approximately by a factor of two (Turcotte & Schubert, 1982, pp. 127). It will be shown below that realistic-size instabilities can provide enough negative buoyancy to bend the lithosphere with a radius of curvature similar to those observed in current subduction settings.

The algebraic difference between Φ_B and the other dissipation terms is shown in Fig. 6.10 for plumes with $\lambda = 200, 300$, and 400 km. The results plotted in this figure suggest that the critical wavelength necessary to promote a translithospheric fault zone with realistic plume lengths (200 - 300 km) is $\gtrsim 350$ km. Despite the crudeness of the analysis, this general result agrees with other estimations from more rigorous numerical experiments on the onset of convection and mantle instabilities (e.g. Solomatov & Moresi, 2000; Korenaga & Jordan, 2003; Solomatov, 2004a; Zaranek & Parmentier, 2004). Nevertheless, the simple energy balance performed here cannot be used to estimate the maximum possible wavelengths. Critical possible wavelengths for the onset of convection depend strongly on the dimensions and scaling adopted in each particular experiment. For the case of upper mantle convection, it is now generally accepted that the maximum wavelength that would trigger sublithospheric convection cannot be much greater than 400 - 500 km (Solomatov & Moresi, 2000; Zaranek & Parmentier, 2004). Otherwise, conductive smoothing would suppress the growth of the instability. It is also commonly observed that, in order to conserve mass and energy, the initial thick-

ness of the plume is reduced by 50 - 60 % when the instability is fully developed. To simulate this more realistic behaviour, the energy balance is calculated for a sinusoidal plume with an initial $\lambda_{in} = 450$ km and a final $\lambda_{qs} = 260$ km ($\lambda_{qs}/\lambda_{in} \sim 0.57$) when it reaches 350 km depth. Again, since the greater viscous dissipation due to a longer plume is counterbalanced by a greater available gravitational energy, it is found that Eq. (6.45) is satisfied before reaching the maximum depth (Fig. 6.10). Note that this is only done to imitate the thinning of the plume with depth. In reality, the wavelength of the system does not change much (i.e. downwelling and return upwellings axes remain approximately at the same initial distance).

The choice of representative first-order values for the parameters controlling the dissipative terms is of primary importance. An exploration of parameter space indicates that the main parameters controlling the energy balance are the average mantle viscosities and the downwelling velocities. Of these, the lithospheric viscosity has the strongest impact on the results. On the contrary, the outcomes are not significantly modified for a wide range of average fault frictional stresses between 30 - 100 MPa. This result seems to relax somewhat the condition of very weak faults required by other models. The parameters chosen to obtain Fig. 6.10 are based on commonly accepted values from the literature, and are shown in Table 6.1. In particular, the chosen viscosity of the surrounding mantle, η_c , is an average taken from rheological estimations for dry and wet olivine at depths between 100 and 300 km (Karato & Wu, 1993) and post-glacial rebound data (Lambeck & Johnston, 1998). The value for the viscous part of the lithosphere, η_l , is the average of two extreme values considered to be the limits for the lithospheric mantle: 10^{18} Pa s to the lowermost lithosphere (i.e. asthenosphere) and 10^{26} Pa s to the upper boundary. The former is consistent with asthenospheric values from many different approaches and the latter is the cutoff value at which the lithosphere become essentially rigid (typically reached at temperatures of $\sim 550 - 750$ °C, (see e.g. Schubert et al., 2001). The average downwelling velocity directly control Φ_B and Φ_{mc} , and

indirectly Φ_l and Φ_f through the strain rates and v_r , respectively. The latter necessarily has to be much lower than v_o , since velocities decrease upwards. A safe assumption used in Fig. 6.10 assigns to v_r a value 40 % of v_o , although it is recognized that this number could overestimate the real slip velocity and fault dissipation. A decrease in the average downwelling velocity translates into a proportional decrease of the four terms in Eq. (6.45), and the general conclusions should therefore remain the same.

In line with the results from this simple energy balance, it appears possible that a gravitational instability with a wavelength between 300 - 450 km can provide enough energy to break, bend, and pull down normal oceanic lithosphere, thus triggering subduction initiation. It remains yet to be shown, at a more local scale, that stresses acting in the ductile viscous part of the lithosphere, as well as stresses within the elastic layer, are indeed able to overcome the resistance offered by fault friction and elastic bending. Also, the more favourable places where this might occur need to be identified. This is the purpose of the next section.

6.4.5 Viscous and elastic deformations and stress transfer

Analyzing the geometry of the system and the mechanical coupling between the layers, appropriate boundary conditions can be obtained to solve the relevant equations. In particular, four boundary conditions are needed to solve Eq. (6.27). Referring to Fig. 6.8, the following boundary conditions apply

$$f(0) = 0 \quad (6.60a)$$

$$\left. \frac{df}{dy} \right|_{(y=0)} = 0 \quad (6.60b)$$

$$f(H) = 1 \quad (6.60c)$$

The first two boundary conditions specify the no-slip top surface (i.e. $v(x, 0) = u(x, 0) = 0$). This implicitly stipulates that the surface responds instantaneously to whatever perturbation is applied beneath it. It also specifies that normal viscous stresses generated by vertical velocity gradients at the base of the elastic layer are nil (i.e. $\partial v / \partial y = 0$ at $y = 0$). The third condition simply specifies that $v(0, H) = -v_o$. The fourth boundary condition can be obtained by equating the hydrostatic pressure head associated with the resulting topography, $w(x)$, to the total normal stress at the upper boundary of the viscous layer. This is possible because the resulting topography and deformation of the elastic layer are a consequence of the flow beneath it, and hence any topography variation must be dynamically supported by the viscous flow. Since the vertical displacements are expected to be small in comparison to the thickness of the elastic layer and wavelength of deformation, it is appropriate to equate these stresses at $y = 0$. Therefore

$$\rho g w(x) = -p + 2\eta \left. \frac{\partial v}{\partial y} \right|_{(y=0)} \quad (6.61)$$

The last term is zero because of condition (6.60b). The pressure p at $y = 0$ can be found by combining Eq. (6.23) with Eq. (6.16) and integrating with respect to x

$$p(x, 0) = -\eta v_o \left(\frac{\lambda}{2\pi} \right)^2 \cos \left(\frac{2\pi x}{\lambda} \right) \left. \frac{d^3 f}{dy^3} \right|_{(y=0)} \quad (6.62)$$

Using Eqs. (6.35) - (6.37), the fourth boundary condition is found to be

$$\left. \frac{d^3 f}{dy^3} \right|_{(y=0)} = \frac{w_{\circ} \rho g}{\eta v_{\circ} \left(\frac{\lambda}{2\pi} \right)^2} \quad (6.63)$$

Eqs. (6.60a),(6.60b), (6.60c), and (6.63) are therefore used to solve Eq. (6.27), giving the following expressions for the four constants

$$A = -C = \frac{1 + H D 2 \sinh(\alpha H)}{\gamma} \quad (6.64)$$

$$B = -D - 2 A \alpha \quad (6.65)$$

$$D = -\frac{(\Gamma - \Lambda)}{\Upsilon} \quad (6.66)$$

where

$$\Gamma = \frac{w_{\circ} \rho g}{\eta v_{\circ} \left(\frac{\lambda}{2\pi} \right)^2} \quad (6.67)$$

$$\Lambda = -\frac{4 \alpha^3}{\gamma} \quad (6.68)$$

$$\Upsilon = \frac{8 H \alpha^3 \sinh(\alpha H)}{\gamma} \quad (6.69)$$

$$\gamma = 2 \sinh(\alpha H) - 2 H \alpha e^{\alpha H} \quad (6.70)$$

It is recognized that Eqs. (6.60a),(6.60b), (6.60c), and (6.63) are not the only boundary conditions that can be applied to this problem. However, they are the simplest that keep the main features of a flow pattern such as the one of interest.

The final velocity field for the viscous layer, as predicted by Eqs. (6.21), (6.23), with Eqs.(6.32) and (6.64) - (6.70), is shown in Fig. 6.11C. For comparison, the velocity field from a more rigorous numerical experiment (Korenaga & Jordan, 2003) on gravitational instabilities is also shown. The latter also assumed a Newtonian-type viscosity. It is clear from this figure that the main features of the flow are well described by the present analytical model. The free parameters controlling the results are the velocity v_o , the mean viscosity η of the medium, and the maximum load q_o (or w_o). Constraints on the ranges of these parameters can be readily obtained from the numerous convection models in the literature. Moreover, if the velocity field is restricted to reproduce results from numerical models, then possible values for the three parameters are not independent anymore. This is illustrated in Fig. 6.12, which plots the vertical component of velocity as a function of depth for several combinations of v_o , η , and q_o , at $x = 0$. As expected, it is clear that as q_o increases, either v_o or η also have to increase to maintain a realistic velocity profile. This is entirely consistent with the physical problem analyzed here. For instance, if the viscosity is too low, even high velocities cannot generate high surface stresses, since most of the viscous strain-generated stresses are relaxed within the low viscosity layer and not transmitted to the surface. In this case, the elastic layer would be essentially detached from the flow beneath it.

Numerical experiments suggest that gravitational instabilities can generate peak surface normal stresses of the order of 10 - 50 MPa and average vertical velocities of 3 - 10 cm a⁻¹ (Marotta et al., 1998; Pysklywec & Shahnas, 2003; Solomatov, 2004a). Although velocities of the order of 1 - 3 m a⁻¹ were reported for individual cold plumes (e.g. Solomatov & Moresi, 2000), the actual velocities of the flow right underneath the

elastic layer are unlikely to reach such high values (this is mainly due to the variation in viscosities). The magnitude of the dynamic topography induced by gravitational instabilities has been recently estimated by Pysklywec and Shahnas (2003) for a number of cases with different viscosity contrasts between the lithosphere and underlying mantle (a Newtonian-type viscosity was also adopted in this study). Their experiments A1 and B1 are relevant here due to the similarities with the model studied in this section. They estimated peak values of dynamic topography (i.e. at the collapse of the instability) of around 1 - 2 km below the surface of the model above cold plumes, consistent with normal stresses of ~ 30 and 60 MPa, respectively. Characteristic wavelengths of these cold plumes were found to be $350 < \lambda < 440$ km, in agreement with those found in Section 6.4.4 and other studies. The estimated topography, however, was calculated assuming that the surface is free to deform in a viscous manner, reaching isostatic equilibrium at each step. The elastic rigidity of the lithosphere was not considered. From the discussion in Section 6.4.3.1, it is clear that total isostatic equilibration is only possible for very long wavelengths (Fig. 6.9). The results of Pysklywec and Shahnas (2003) should represent therefore upper limits to the actual dynamic topography. Considering the wavelengths from their experiments and the results from Fig. 6.9, the actual deflection of the surface should be $\sim 85, 60, 40$ % of their values for an elastic plate 20, 30, and 40 km thick, respectively.

Bearing in mind these ranges of possible values for the free parameters v_o , η , and q_o (or w_o), the stress distribution within both the viscous and the elastic layers can be calculated using Eqs. (6.24), (6.25), (6.39), (6.43) and (6.44). The stresses acting on the elastic part of the lithosphere arise from the viscous stresses beneath it (Fig. 6.14). I focus on the uppermost 50 km of the viscous layer, and calculate the stress distribution in this region. The shear stress that will be transmitted to the elastic part are calculated at $y = 0$ (i.e. at the interface). The normal vertical stresses can be estimated from Eq. (6.34), assuming realistic values for q_o (10 - 50 MPa, see above). Because of the non-

linear shape of the vertical component of the velocity with depth, a representative value for v_o in the uppermost 50 km of the viscous layer must be significantly smaller than the average values for the whole instability. An inspection of Figs. (6.12A) and (6.12D) suggest that an appropriate v_o value should be around two orders of magnitude smaller than values used for the whole instability. Since the average temperature of this layer is also lower than that for the whole instability, the average viscosity need to be increased accordingly. Considering a normal range of oceanic geotherms, the average viscosity of this region is estimated to range between 10^{23} - 10^{24} Pa s (e.g. Schubert et al., 2001).

Fig. 6.13A depicts the general pattern and range of magnitudes for the shear viscous stresses at the top of the viscous layer (i.e. $y = 0$). Fig. 6.13B shows the maximum deflection of a plate as a function of the elastic thickness for different q_o values. Parameters used in these experiments are summarized in Table 6.2. Numerical simulations conform to the simple pattern followed by the shear stresses near the cold plume (see e.g. Fig. 2 in Lowman et al., 2003). Expected peak shear stresses at the top of the viscous layer range from 20 to 400 MPa, while horizontally-averaged values are in the 12 - 240 MPa range. Numerical experiments on gravitational instabilities indicate that shear stresses developed near cold plumes are smaller but of the same order than the normal stresses right above the plume (e.g. Marotta et al., 1998). Therefore, the upper bound value in Fig. 6.13A seems to be too large to be considered a representative magnitude. Another argument against the validity of peak shear stresses > 50 - 60 MPa comes from a rheological point of view. Firstly, such high stresses will generate enough heat by viscous dissipation to weaken this region significantly (e.g. Turcotte & Schubert, 1982). This will in turn reduce the strength of the material (i.e. thermomechanical erosion of the lithosphere), and thus the attainable stresses. Secondly, it is expected that the power-law component of the viscosity will become dominant at high shear stresses (Ranalli, 1995). This has a similar (but more pronounced) softening effect than viscous heating, and it precludes shear stresses from becoming too high. Accordingly, it can be safely

assumed that maximum attainable shear stress would range between 10 - 50 MPa, which translates into horizontally-averaged values of $\sim 6 - 30$ MPa, respectively.

To describe the state of deviatoric stress within the elastic layer resulting from the viscous flow below it, I start with the equilibrium equations in two dimensions (cf. e.g. Ranalli, 1995)

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} = 0 \quad (6.71a)$$

$$\frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{xy}}{\partial x} + \rho g = 0 \quad (6.71b)$$

The stresses within the elastic layer are hereafter denoted by σ , to differentiate them from the viscous stresses τ . I adopt here the geological sign convention *sensu* Twiss and Moores (1992), where normal compressive stresses are positive and tensile normal stresses negative. However, since the y axis is here taken to be positive downwards, the appropriate convention for shear stresses is the engineering convention (cf. Twiss & Moores, 1992).

To the first order, Eq. (6.71a) can be rewritten as

$$\frac{\partial \sigma_{xx}}{\partial x} \approx - \left. \frac{\tau_{xy}}{T_e} \right|_{y=0} \quad (6.72)$$

where T_e is the elastic thickness of the plate, and the suffix $y = 0$ means that the shear stress τ_{xy} is calculated at the base (top) of the elastic (viscous) layer. Substituting Eq. (6.25) into Eq. (6.72) and integrating with respect to x gives

$$\sigma_{xx} \approx \eta v_o \left(\frac{\lambda}{2\pi} \right)^2 \cos \left(\frac{2\pi x}{\lambda} \right) \left[f(y) \left(\frac{2\pi}{\lambda} \right)^2 + \frac{d^2 f}{dy^2} \right] \Big|_{y=0} \frac{1}{T_e} + c_1 \quad (6.73)$$

where c_1 is a constant of integration. Since the lateral boundaries of the plate ($x = 0, \lambda/2$) are assumed to experience no displacement in the x -direction, the horizontal gradient in σ_{xx} puts the boundary at $x = 0$ under deviatoric tension, while the boundary at $x = \lambda/2$ is under deviatoric compression. Applying the boundary conditions $\epsilon_{xx} = 0$ at $x = 0, \lambda/2$, and taking compressive deviatoric stresses to be positive, Eq. (6.73) can finally be written as

$$\sigma_{xx} \approx -\eta v_o \left(\frac{\lambda}{2\pi} \right)^2 \cos \left(\frac{2\pi x}{\lambda} \right) \left[f(y) \left(\frac{2\pi}{\lambda} \right)^2 + \frac{d^2 f}{dy^2} \right] \Big|_{y=0} \frac{1}{T_e} \quad (6.74)$$

Following the same arguments, it can be proven that, to a first approximation, the horizontal gradient of σ_{xy} is negligible in comparison with the vertical gradient of the lithostatic pressure. The same applies to the vertical gradient of the normal stress exerted by the flow. Therefore, Eq. (6.71b) simply becomes the lithostatic equation

$$\sigma_{yy} \approx \rho g y \quad (6.75)$$

Eqs. (6.74) and (6.75), together with those obtained in Section 6.4.3, represent the stresses acting on the elastic part of the lithosphere. Provided the deflection is small in comparison with the elastic thickness of the plate (as it is the case in lithospheric flexure), the linear superposition of these stresses along the x - and y - directions defines the total stress distribution in the plate (cf. e.g. Sokolnikoff, 1956; Timoshenko & Woinowsky-Krieger, 1959). The longitudinal stresses acting on the elastic layer are

depicted in Fig. 6.14. They include the compressional stress arising from the ridge push, the flexural bending stresses, the extensional stress due to the undulation of the plate, and the tensional/compressional stress due to the basal shear traction. The ridge push is a homogeneously distributed stress, and in the present context, can be considered constant. Unless indicated otherwise, a conservative constant value of $1.0 \times 10^{12} \text{ N m}^{-1}$ will be assumed throughout the calculations. The bending stresses are given by Eq. (6.39) with $y = 0$ at the midplane of the elastic plate. The extension arising from the undulation of the plate is (Eqs. (6.38) and (6.43))

$$\sigma_U = \frac{-E}{(1-\nu^2)} w_o^2 \left(\frac{2\pi}{\lambda} \right)^2 \quad (6.76)$$

Therefore, taking tensile stresses negative, the total (elastic) longitudinal stress is

$$\begin{aligned} \sigma_{xx}^T = \sigma_R - \frac{E}{(1-\nu^2)} w_o \left(\frac{2\pi}{\lambda} \right)^2 \cos \left(\frac{2\pi x}{\lambda} \right) y_e \\ - \frac{\tau_{xy}^o}{T_e} \left(\frac{\lambda}{2\pi} \right) \cos \left(\frac{2\pi x}{\lambda} \right) - \frac{E}{(1-\nu^2)} w_o^2 \left(\frac{2\pi}{\lambda} \right)^2 + \rho g y \end{aligned} \quad (6.77)$$

where σ_R is the stress from the ridge push, $y_e = 0$ at the midplane and positive upwards, and

$$\tau_{xy}^o = \eta v_o \left(\frac{\lambda}{2\pi} \right) \left[f(y) \left(\frac{2\pi}{\lambda} \right)^2 + \frac{d^2 f}{dy^2} \right] \Big|_{y=0} \quad (6.78)$$

is the maximum basal shear stress (from Eq. 6.25 at $x = \lambda/4$). Note that both y_e and y represent depth in meters, but they are measured in different coordinate systems ($y_e = 0$ at the midplane and positive upwards; $y = 0$ at the surface of the plate and is

taken positive downwards). This convention simplifies the treatment of the equations. The last term in Eq. (6.77) denotes the lithostatic component. Strictly, a perfect elastic medium develops horizontal stresses that are only a fraction of the vertical stress ($\sim 1/4 \sigma_{yy}$), and depend on the effective Poisson ratio (cf. e.g. Sokolnikoff, 1956; Turcotte & Schubert, 1982). However, in a lithospheric context, it is more realistic to assume that the initial state of stress prior to any deformation is lithostatic (Turcotte & Schubert, 1982).

The isotropic component of the stress field (i.e. average pressure) is

$$P = \frac{(\sigma_{xx}^T + \sigma_{yy})}{2} \quad (6.79)$$

The deviatoric components are obtained by subtracting Eq. (6.79) from the total x - and y - components (Eqs. (6.77) - (6.75)).

The shear stress from bending only can be obtained by differentiating Eq. (6.39) with respect to x , substituting into Eq. (6.71b), and integrating between $y_e = -T_e/2$ and $y_e = T_e/2$ with the condition $\sigma_{xy} = 0$ at $y = -T_e/2$ and $y = T_e/2$. This yields

$$\sigma_{xy} = -\frac{3}{2T_e} V_{(x)} \left[1 - \left(\frac{2y_e}{T_e} \right)^2 \right] \quad (6.80)$$

where $V_{(x)}$ is given by Eq. (6.44). The total shear stress is the sum of Eq. (6.80) plus the shear from the basal traction

$$\sigma_{xy}^T = -\frac{3}{2T_e} V_{(x)} \left[1 - \left(\frac{2y_e}{T_e} \right)^2 \right] - \frac{\tau_{xy}^\circ}{T_e} \sin \left(\frac{2\pi x}{\lambda} \right) y \quad (6.81)$$

The vertical shear stress due to flexure, which has a maximum at $x = \lambda/4$ (Eq. 6.80), and the vertical normal stresses arising from the flow are also depicted in Fig. 6.14. Before presenting quantitative estimations for each of these stresses (Section 6.4.6), I will briefly discuss qualitatively their separate effects on potential translithospheric faults.

The stress arising from the ridge push puts the plate in compression. This increases both the available shear stress to produce slip and the average normal stress along any fault plane. The most favourable plane to be reactivated by these stresses would be one with the orientation that makes the difference between the competing effects of normal and shear stresses a minimum (usually around $30^\circ - 40^\circ$ to the maximum compressive stress).

The stresses arising from bending are symmetric with respect to the mid-point of the elastic plate (Fig. 6.14; cf. Turcotte & Schubert, 1982). Where the plate is deflected downwards ($x = \lambda/2$), the bending stresses are compressive in the upper half of the plate and tensile in the lower half. The opposite situation applies where the plate is deflected upwards ($x = 0$; $x = \lambda$). Along vertical planes, bending stresses integrate to zero with depth, and therefore make no contribution to the average shear resistance of a translithospheric fault. However, since they vary along the x -direction, planes other than vertical contain a net contribution from these stresses. They play a major role in defining the overall stress distribution within the plate, and consequently the most suitable places for a reactivation to occur.

The tensional stresses due to the undulation of the plate are a consequence of assuming that the ends of the plate cannot experience displacement in the x -direction. This condition would be relaxed if at least one of the ends could move freely in response to the applied forces. In a plate tectonics context, this situation requires a weak lithospheric-scale discontinuity, such as a MOR, that would allow the whole plate to experience horizontal displacement without exerting significant resistance. Assuming a

wavelength $\lambda = 400$ km, Eq. (6.43) predicts horizontal extensions of 24 and 80 m for deflections of 500 and 1000 m, respectively. These translates into average tensile stresses of 4.5 and 15 MPa (Eq. (6.38) with $E = 70$ GPa and $\nu = 0.25$). Since these stresses are tensile throughout the whole plate, they decrease the normal stress of all potential fault planes, diminishing their shear resistance to slip.

The longitudinal stresses arising from the basal viscous shear stresses are symmetric with respect to a vertical plane at $x = \lambda/4$, and antisymmetric with respect to a vertical plane at the axis of the cold plume (i.e. $x = \lambda/2$). Their magnitude is strongly dependent on the horizontal distance on which the basal shear stresses act, as well as on the thickness of the elastic plate (Eq. (6.74)). This has two important implications in the context of initiating subduction. Firstly, it indicates that small wavelength instabilities would be unable to produce significant stresses within the plate. Secondly, thick lithospheres are less affected by basal tractions than thin lithospheres. Since these stresses are roughly horizontal, their contribution to the reactivation of faults parallels that for the ridge push. Because of their symmetry within $0 < x < \lambda/2$, they have the same maximum magnitude, but different sign, at the points $x = 0$ and $x = \lambda/2$ (i.e. above the upwelling and above the downwelling).

The vertical normal stresses transmitted from the plumes to the elastic plate tend to reduce the shear strength of potential fault planes above the cold plume by reducing the effective normal stress resolved onto them (i.e. they pull away potential fault planes). The opposite applies above the upwellings, where the effective normal stress is increased on potential fault planes of any orientation (Fig. 6.14). The resultant shear stresses, however, are the same in these two regions. This situation favours the reactivation of faults above the cold plume rather than above the forced upwellings.

6.4.6 Plate shear strength and whole-lithosphere failure

The long-term strength of the lithosphere resides mainly in its brittle/elastic layer, since viscous creep cannot support stresses over geologic time-scales (cf. Turcotte & Schubert, 1982; Kemp & Stevenson, 1996). Provided that the lithosphere has randomly oriented pre-existent planes of weakness on which slip can occur (a common assumption in lithospheric modelling), its total shear resistance F_R can be defined as the integrated frictional resistance of a given translithospheric fault. Similarly, the total available shear force F_A is defined here as the integrated shear stress resolved onto the fault plane. This is possible due to the fact that randomly oriented planes of weakness tend to coalesce into a single major “plane” which orientation depends on the actual stress field. When the available shear force F_A overcomes F_R on a particular fault plane, slip can take place along the entire fault, allowing decoupling of the whole lithosphere. It is acknowledged that the available shear stress varies with position, and in zones of high stresses, local failure can take place. However, local yielding generates a concentration of stresses in the remaining intact parts of the lithosphere, making them more prone to further yielding. Subduction can only start when slip occurs across the entire lithosphere. It is then reasonable to assume that a necessary condition for the initiation of subduction is that the total available shear force on a particular fault plane equals the total shear resistance resolved onto it.

Calculating the total stress distribution within the plate allows the estimation of the total available shear stress on any particular plane, as well as its shear resistance. These values depend on the fault length, the average normal stress, and the coefficient of friction of the fault (cohesionless pre-existing fractures are assumed here due to the high uncertainty in the coefficient of friction). The change in fault length with orientation must be explicitly considered in the calculations. This is not only because the stresses resolved onto it depend on the angle of the fault, but also because the stress field, and

consequently the available stresses, changes with position. Fig. 6.15 shows the σ_{xx}^T field for four cases with different combinations of basal shear tractions and bending. Since the lithostatic component is by far the largest, it was removed from the total σ_{xx}^T to emphasize the lateral variability of these stresses. The instability responsible for these stresses has a wavelength $\lambda = 400$ km. It can be seen that bending alone produces the expected vertically and horizontally symmetric stress pattern (Fig. 6.15B). When bending and basal shear tractions are combined, an asymmetric stress distribution is obtained (Fig. 6.15C and 6.15D). The stresses are now magnified in the upper two-thirds of the plate, and reduced in the lower third. The stress fields predicted by the present analytical theory have been corroborated with a finite-element code (JL Analyzer 10.0; <http://www.autofea.com/Download-FEA-software.htm>).

The problem of locating the most favourable translithospheric faults to be reactivated within an heterogenous stress field is two-fold. Firstly, potential fault planes can be obtained by plotting the directions of the principal stresses σ_1 and σ_2 . The Coulomb criterion requires that shear failure planes contain the intermediate principal stress (in a 2-D geometry the intermediate principal stress is perpendicular to the x,y -plane) and that the fracture plane makes an angle less than 45° to the maximum principal stress σ_1 (depending on the coefficient of friction; cf. e.g. Twiss & Moores, 1992). Secondly, according to the shear criterion adopted above, the balance between F_R and F_A must be evaluated for each of these potential faults to identify those in which the ratio $F_A/F_R > 1$.

The magnitudes and orientations of σ_1 and σ_2 are obtained from the stress components as (cf. e.g. Twiss & Moores, 1992; Ramsay & Lisle, 2000)

$$\sigma_1 = \frac{1}{2} \left[\sigma_{xx}^T + \sigma_{yy} + \sqrt{4(\sigma_{xy}^T)^2 + (\sigma_{xx}^T - \sigma_{yy}^T)^2} \right] \quad (6.82a)$$

$$\sigma_2 = \frac{1}{2} \left[\sigma_{xx}^T + \sigma_{yy} - \sqrt{4(\sigma_{xy}^T)^2 + (\sigma_{xx}^T - \sigma_{yy})^2} \right] \quad (6.82b)$$

$$\tan \theta_1 = -\frac{\sigma_{xy}^T}{\sigma_1 - \sigma_{yy}} \quad (6.82c)$$

where θ_1 is the angle (measured counterclockwise) between the horizontal and σ_1 . The directions of σ_1 and σ_2 are plotted in Fig. 6.16A, together with the orientations of potential faults. The predictions of orientation and movement sense are based on the assumption that they are inclined 40° to the principal stress σ_1 trajectories (equivalent to a coefficient of friction ~ 0.2) and on the sign of the resultant shear stress. The colour background of Fig. 6.16A represents the principal stress difference ($\sigma_1 - \sigma_2$) for the case of a deflection $w_o = 500$ m and a maximum basal shear stress $\tau_{xy}^o = 20$ MPa. The general pattern exhibited by the orientations of σ_1 and σ_2 is clearly dominated by the stress distribution due to elastic bending. Due to the combined effects of bending, basal shear, and ridge push, the largest principal stress difference is located in the upper part of the plate at $x = \lambda/2$ (above the downwelling), where reactivation of reverse faults are favoured according to the spatial stress distribution. Indeed, shear stresses resolved onto translithospheric fault planes such as those shown in Fig. 6.16A have the same sign along the entire plane, except in the lowermost part of the elastic layer. This particular situation makes these fault planes ideal places for translithospheric failure (along a reverse-type fault). On the other hand, shear stresses resolved onto potential translithospheric fault planes at $x = 0$ (above the forced upwellings) have opposite signs in the upper and lower parts of the plate, respectively. Consequently, normal faulting is favoured in the upper parts of the plate, where $\sigma_1 - \sigma_2$ is also larger, while reverse faulting is promoted in the lower parts. In other words, these fault planes are kinematically inconsistent. Although local faulting is possible, especially in the upper parts, it can be anticipated that whole lithospheric failure above the upwellings would

not be feasible.

Having localized the planes most prone to reactivation, it remains to be estimated which fault is more likely to be reactivated based on the balance between the available total shear force F_A and the total shear resistance of the fault F_R . It is important here to clarify that even when gently dipping faults ($< 20^\circ$ from the horizontal) can have ratios $F_A/F_R > 1$ (a consequence of having low normal stresses resolved onto them), the orientations of σ_1 and σ_2 precludes them to actually form (see above). Therefore, the ratio F_A/F_R is only meaningful for the particular range of possible fault orientations predicted by the actual pattern of σ_1 and σ_2 . For the present case, Fig. 6.16B indicates that angles $70^\circ < \theta < 20^\circ$ are physically irrelevant, and consequently they are omitted in the calculations. It is acknowledged that fault planes are likely to be curved along some section of the fault rather than maintaining a constant orientation. This is expected to result in a slight difference between the actual value of F_A/F_R along a particular fault plane and that estimated for an average constant orientation. However, the curvature effect cannot be responsible of first-order discrepancies in the value of F_A/F_R , since local translithospheric fault orientations do not vary significantly from their length-averaged orientation (e.g. Fig. 6.16A).

The ratio F_A/F_R is plotted in Fig. 6.17 as a function of the fault orientation for an instability with a wavelength $\lambda = 400$ km, assuming an elastic thickness of 30 km, a Young's modulus of 70 GPa, a Poisson's ratio of 0.25, a coefficient of friction of 0.2, $w_o = 500$ m, and $\tau_{xy}^o = 20$ MPa (i.e. an horizontally-averaged shear stress of ~ 12 MPa). Fig. 6.17A shows that in areas close to $\lambda/2$ (i.e. above the cold plume), slip can take place along translithospheric reverse faults with orientations $20^\circ < \theta < 35^\circ$ from the horizontal. On the contrary, in regions near $x = 0$ (i.e. above the upwelling), the available shear is always significantly less than the shear resistance (Fig. 6.17D), and slip is precluded. If either the elastic thickness is reduced or the horizontal stresses

increased, the critical state ($F_A/F_R = 1$) is reached for larger fault angles near $x = \lambda/2$. For example, when the elastic thickness is reduced to 25 km, the critical state is reached for a reverse fault dipping $\sim 55^\circ$. Alternatively, a maximum shear stress τ_{xy}° of only ~ 11 MPa (i.e. horizontally-averaged value of ~ 6.6 MPa) is needed to put a fault dipping $\sim 35^\circ$ in the critical state. It is important to note that a highly conservative value for the ridge-push was used in these calculations (1.0×10^{12} N m $^{-1}$). When a value more representative of mature oceanic lithosphere is used ($\sim 2.0 - 3.0 \times 10^{12}$ N m $^{-1}$), faults dipping 35° and 55° reach the critical condition for maximum basal shear stresses of only $\lesssim 10$ MPa in plates with elastic thickness 40 and 30 km, respectively. In this case, increasing the coefficient of friction to 0.3 produces identical results to those for a ridge push of 1.0×10^{12} N m $^{-1}$.

As long as the scenario and stress directions remain the same, the situation depicted in Fig. 6.17 is representative of all possible combinations of parameters. The most favourable regions for the lithosphere to fail are always above the cold plume.

As a further test on the analytical model, a similar experiment to that studied by Hall et al. (2003), where the only driving force is the ridge push, is performed. If the present analytical approximation is valid, it should give comparable results for similar system parameters. Hall et al. (2003) did not provide the width of the weak zone used in their numerical experiments. However, they did include it in their Fig. 2, from which a width of around 10 km can be estimated. Their elastic thickness, estimated from the thermal structure of the plate, is between 30 - 40 km. This means that an initial fault plane dipping $\sim 76^\circ$ from the horizontal is appropriate for the present purpose. Hall et al. (2003) estimated that an average ridge push of $\sim 1.0 \times 10^{12}$ N m $^{-1}$ and a coefficient of friction of around 0.02 are necessary to overcome the shear resistance of a translithospheric fault. When these parameters are included in the analytical model for a fault dipping 76° , and neglecting other stresses, the predicted F_A/F_R ratios are 1.1

and 0.66 for elastic thicknesses of 30 and 40 km, respectively. The former value is greater than the critical case, suggesting that slip along the fault is possible, in agreement with the results of Hall et al. (2003). Despite the simplicity of this comparison, the above experiment indicates that predictions from the present model are comparable to those from more complex numerical models.

6.4.7 Available negative buoyancy: the sinking of the lithosphere at the onset of subduction

Once the conditions for failure are satisfied, the whole lithosphere can begin to founder only if the available negative buoyancy generated by the gravitational instability is enough to bend the lithosphere and pull it into the mantle. It is reasonable to assume that before subduction can evolve into a self-sustained system, the decoupled oceanic lithosphere above the instability has to be bent at least until it reaches a shape comparable to that of actual oceanic trenches (i.e. the tip of the incipient slab has to reach a depth of 3 to 4 km below the level of the surrounding oceanic floor (e.g. Schubert et al., 2001; Watts, 2001)). The required average force to accomplish this is given by Eq. (6.59) divided by two (i.e. the strength of a decoupled lithosphere is reduced by $\gtrsim 50\%$; see Section 6.4.4). This equation can be rewritten in a more useful form by substituting Eqs. (6.36) and (6.58) into it, giving

$$\overline{F_e} = \frac{\lambda}{16} w_o \left[D \left(\frac{2\pi}{\lambda} \right)^4 + \Delta\rho g \right] \quad (6.83)$$

Assuming a wavelength $\lambda = 400$ km, Eq. (6.83) predicts that minimum forces of 2.45×10^{12} and 3.27×10^{12} N m⁻¹ are needed to bend a broken lithosphere with an elastic thickness of 30 km down to depths of 3 and 4 km, respectively. If the elastic thickness is changed to 40 km, minimum forces of 3.51×10^{12} and 4.68×10^{12} N m⁻¹ are required.

To estimate the negative buoyancy resulting from a R-T instability, two temperature snapshots representative of the initial stages in the development of the instability are generated with LitMod (Fig. 6.18A and 6.18C). Then, the resulting densities are compared with those from a reference model with an identical set-up, but with no instability. Finally, once the density difference $\Delta\rho$ between these models is obtained (Fig. 6.18B and 6.18D), the negative buoyancy can be calculated with Eq. (5.4). These density anomalies do not include any previous anomalies arising from the thermal structure of the lithosphere with respect to the adiabatic mantle, and therefore they represent lower bound limits.

The case shown in Fig. 6.18A-B results in a total negative buoyancy of $8.75 \times 10^{12} \text{ N m}^{-1}$ for the region between $x = 600$ and 900 km . In the case shown in Fig. 6.18C-D, a value of $1.04 \times 10^{13} \text{ N m}^{-1}$ is obtained for the same region. These figures are very close to the estimations presented in Section 6.3.1 for the minimum negative buoyancy needed to generate a self-sustained system ($\sim 8.8 \times 10^{12} \text{ N m}^{-1}$; Fig. 6.3). Since these estimations include the elastic resistance, it can be anticipated that an instability such as the one shown in Fig. 6.18 can produce self-sustained subduction. However, according to the discussion in Section 6.4.4, only a certain amount of the total buoyancy is spent in bending the elastic lithosphere. A lower bound estimation of the force available for bending can be obtained by considering only the negative buoyancy originating above the deflected $700 - 800^\circ \text{C}$ isotherm, since material above this isotherm deforms slowly enough to be approximately considered a static load for the elastic plate at all times. When this condition is applied to the calculation of the negative buoyancy, the case shown in Fig. 6.18A-B gives a value of $2.2 \times 10^{12} \text{ N m}^{-1}$, while the case shown in Fig. 6.18C-D gives $4.1 \times 10^{12} \text{ N m}^{-1}$. These values cover $> 85\%$ of the range for minimum forces calculated with Eq. (6.83). Bearing in mind that these estimates are lower bounds for the maximum attainable negative buoyancy, it is concluded that lithospheric bending and foundering by a gravitational instability is a viable process.

6.5 Discussion

A number of potential criticisms to the proposed scenario for subduction initiation are discussed here. The more general implications in terms of geophysical observables and potential sites favourable to subduction initiation will be discussed in Chapter 7.

(a) One of the most important simplifications which have been made to study the initiation of subduction driven by a R-T-type instability is the assumption of a representative constant Newtonian viscosity for the viscous part of the lithosphere. If the non-Newtonian component is dominant, this assumption overestimates the viscous shear stresses that can be transferred to the elastic upper part of the lithosphere. On the other hand, as Korenaga and Jordan (2003) pointed out, the transition from an infinitesimal perturbation to a finite amplitude instability cannot be controlled by a purely non-Newtonian viscosity, since this results in a virtually infinite effective viscosity (i.e. without a predefined background stress field non-Newtonian viscosity cannot be defined). Only when the cold downwelling is fully developed the Newtonian component is more likely to control the effective viscosity. An inspection of thermal fields and velocity gradients predicted by numerical simulations of convection with temperature-dependent non-Newtonian rheology highlights some differences with their Newtonian counterparts (cf. Schubert et al., 2001). Foremost among these is the positive feedback in localized regions of high shear, whereby rapid deformation and reduced viscosities couple to produce small-scale high-velocity downwellings and upwellings. This situation would enhance the decoupling of the convective flow from the rigid upper part of the lithosphere and preclude the development of larger instabilities necessary to initiate subduction. However, the development of larger and slower instabilities (where the Newtonian component of viscosity would be dominant) is likely to take place simultaneously with small-scale convection, since these two mechanisms operate at different scales (see e.g. Solomatov & Moresi, 2000; Schubert et al., 2001; Korenaga & Jordan, 2003; Huang

& Zhong, 2005, and references therein). If this is the case, the shear stresses on the top of the viscous layer near the descending cold plume should be approximately of the same order than the normal stresses within it, and the present analytical theory applies.

(b) Throughout this chapter the viscous flow between $0 < x < \lambda/4$ was assumed to be the specular image of the flow between $\lambda/4 < x < \lambda/2$ for the region $0 < y < q$ (Fig. 6.11C). Although this assumption is in qualitative agreement with predictions from numerical simulations, it is expected to overestimate the magnitude of the forced upwellings (i.e. return flow). Cold plumes typically exhibit 5 - 20 % higher vertical velocities than surrounding upwellings. The effect that this asymmetric flow pattern would have on the calculations presented in this chapter can be approximated by introducing a positive constant in Eq. (6.21) that takes into account the asymmetry of the flow. The inclusion of this constant implies that the loading function (Eq.(6.34)) has to be modified accordingly, which in turn affects the calculation of the function $f(y)$. However, for typical vertical velocities from numerical experiments, the final effect of including this constant is to facilitate the failure of the lithosphere above the downwelling, and to produce greater (negative) deflections of the trench (4 - 5 km below the level of the surrounding oceanic floor). Therefore the main conclusions presented in this chapter remain unchanged.

(c) Results from numerical simulations of convection suggest that the negative buoyancy of an instability increases continuously until it reaches a quasi steady-state, when the instability is fully developed (e.g. King et al., 2002; Lowman et al., 2003; Pysklywec & Shahnas, 2003). Eventually, the large thermal perturbation from the instability tends to disappear as other sources of negative buoyancy (i.e. cold plumes) are generated in the mantle (e.g. King et al., 2002; Lowman et al., 2003). This suggests that a temporal offset could exist between the failure of the lithosphere and the initiation of lithospheric foundering, as estimated in sections 6.4.6 and 6.4.7. This depends basically

on the evolution of the viscous stresses (i.e. velocities) with time, which typically exhibit a marked increase when the instability is starting its accelerating phase, a short-lived peak, and a steep decrease when the instability is fully developed (e.g. Marotta et al., 1998; Korenaga & Jordan, 2003). Whole lithosphere failure occurs when the instability is sufficiently developed to provide the necessary stresses (Section 6.4.6). If by the time this condition is fulfilled the negative buoyancy has become large enough to trigger the bending and foundering of the plate, no temporal offset exists, and subduction would start. However, if lithospheric failure occurs when the velocities reach a peak, or shortly before, and prior to the attainment of the minimum negative buoyancy necessary for subduction, the foundering of the plate would be precluded. This is because the velocities, and therefore the stresses, decrease significantly after they have reached the peak. If they decrease below the threshold to produce slip along a translithospheric fault by the time the negative buoyancy is enough to cause bending and foundering, subduction would not start. Unfortunately, this cannot be evaluated with the present analytical theory, and more rigorous numerical experiments are needed to test the validity of this hypothesis.

(d) An uncertain factor in the present model is the effect of the third dimension. Most relevant is the question of whether quasi-cylindrical plumes or sheets are more likely to develop in the mantle. This cannot be analyzed within the scope of the analytical theory. However, 3-D numerical experiments for Earth-like planets show that the convection pattern is characterized by sheet-like cold downwellings and quasi-cylindrical hot upwellings (e.g. Bercovici et al., 2000; Schubert et al., 2001; Lowman et al., 2003). The former behaviour resembles present-day subduction zones. It also supports the present 2-D modelling of instabilities, since variability along the third dimension is reduced. While this seems to be the case for fully developed instabilities, it does not mean that lateral variability of buoyancy forces does not play a role. Indeed, buoyancy forces exhibit significant lateral variability in the first stages of a sheet-like downwelling

development (e.g. King et al., 2002; Lowman et al., 2003). This along-strike variation in the buoyancy force creates a strike-slip component in the stress field of the elastic lithosphere that cannot be accounted for in a 2-D geometry.

Another important factor that is introduced in 3-D geometries, that would not otherwise exist, is the toroidal component of the viscous flow (cf. Bercovici et al., 2000). While this toroidal field could account for as much as 50 % of the total kinetic energy of the Earth's plate motion, its origin and relation with plate dynamics are still poorly understood (cf. Bercovici et al., 2000). It is generally believed that horizontal variations in viscosity (or plate strength) are needed to obtain a toroidal component. When put into the present context, this means that if the force provided by a sheet-like downwelling pulls the lithosphere, and part of this lithosphere is weaker in some areas than in others, the differential motion that results can lead to strike-slip type shear and toroidal motion. Alternatively, a toroidal field could be also generated from convective motion only (i.e. from within the medium) (cf. Bercovici et al., 2000). Due to the lack of detailed information on this processes, no unambiguous statement can be given regarding its effect on the initiation of subduction.

Table 6.1: Parameters used in the energy balance estimation (Fig. 6.10)

g [m s ⁻²]	ρ [kg m ⁻³]	ΔT	α [K ⁻¹]	v_o [m s ⁻¹]	η_c [Pa s]	η_l [Pa s]
9.81	3300	300	3.0×10^{-5}	3.0×10^{-9}	2.0×10^{20}	1.0×10^{22}
η_f [Pa s]	l_{fv} [km]	l_{ff} [km]	v_r [m s ⁻¹]	w_f [km]	$\tau_{friction}$ [MPa]	$\dot{\epsilon}$ [s ⁻¹]
1.0×10^{20}	50	50	$v_o/3$	5.0	30	1.5×10^{-15}

Table 6.2: Parameters assumed in the calculation of viscous shear stresses and plate deflection (Fig. 6.13).

	λ [km]	y [km]	q_o [MPa]	η [Pa s ⁻¹]	v_o [m s ⁻¹]	T_e [km]	D [N m]
SVF1	350	50	50	10^{23}	10^{-12}	20	4.98×10^{22}
SVF2	350	50	50	10^{23}	10^{-11}	20	4.98×10^{22}
SVF3	350	50	50	10^{24}	10^{-12}	20	4.98×10^{22}
SVF4	350	50	50	10^{24}	10^{-11}	20	4.98×10^{22}
WVF1	350	50	20	10^{24}	10^{-11}	20-40	$4.98-3.98 \times 10^{22}$
WVF2	350	50	30	10^{24}	10^{-12}	20-40	$4.98-3.98 \times 10^{22}$
WVF2	350	50	50	10^{23}	10^{-12}	20-40	$4.98-3.98 \times 10^{22}$

Figure 6.1: Profiles of density contrast ($\Delta\rho$) with depth between oceanic lithosphere and adiabatic reference models RM-SI and RM-SO. The vertical thin line marks the value $\Delta\rho = 50 \text{ kg m}^{-3}$. The profile for a plate with an undepleted PUM composition (i.e. no depletion) is included in D (thin lines). Values of depth-averaged $\Delta\rho$ in kg m^{-3} are shown for the lithospheric mantle only (numbers within brackets) and for the whole plate.

Figure 6.2: Temperature field used to calculate the negative buoyancy of a subducting oceanic plate. A) tip of the slab at 150 km depth; B) tip of the slab at 180 km depth; C) tip of the slab at 250 km depth.

Figure 6.3: Negative buoyancy of a 120 km thick oceanic slab plunging vertically into the upper mantle. The grey rectangle indicates the minimum force for initiating a self-sustained system as estimated by McKenzie (1977). The solid black lines enclose values predicted by SLSM1 for an oceanic plate with a crust ranging from 6 to 10 km thick. The intersection of these lines with the grey rectangle give the minimum depth that the tip of the slab has to reach in order to overcome resistance forces. The dashed line is the estimation of Mahatsente and Ranalli (2004) for a plate plunging at a constant velocity of 5 cm a^{-1} at a dip angle of 45° .

Figure 6.4: Sketch of the geometry used to compute the ridge-push force. (Figure based on Fig. 1 of Parsons & Richter, 1980).

Figure 6.5: Ridge push force as a function of plate age. Dashed line = Half-space cooling model; solid line = plate model of Parsons & Richter (1980); Black dots = this study. (Figure based on Fig. 3 of Parsons & Richter, 1980).

Figure 6.6: Average stresses and fault shear resistance (solid lines) arising from the ridge push force as a function of fault orientation. Fault angles are measured from the horizontal. The coefficients of friction used to calculate fault shear resistance are shown next to the respective lines. σ_A = average normal stress for a ridge push = 2.95×10^{12} N m⁻¹; σ_B = average normal stress for a ridge push = 2.0×10^{12} N m⁻¹; τ_A = average shear stress for a ridge push = 2.95×10^{12} N m⁻¹; τ_B = average shear stress for a ridge push = 2.0×10^{12} N m⁻¹.

Figure 6.7: Sketch of the proposed scenario for the initiation of subduction driven by a R-T instability. The black thin layer represents the elastic part of the lithosphere. Idealized stream lines and flow directions generated by the instability are schematically shown. The system evolves from A to E.

Figure 6.8: Geometry and boundary conditions used to derive the governing equations of the model. Initial undeformed state (top), final deformed state (middle), and Cartesian space used to analyze the viscous flow, elastic deformation, and stress transfer (bottom).

Figure 6.9: Degree of isostatic compensation as a function of instability wavelength. T_e = elastic thickness, N = horizontal force.

Figure 6.10: Total dissipation as a function of plume length (l_p) for different wavelengths (λ). The case of a sinusoidal plume with an initial $\lambda_{in} = 450$ km and a final $\lambda_{qs} = 260$ km is also shown.

Figure 6.11: Comparison between the flow pattern predicted by the analytical theory with that from more rigorous numerical simulations. A) and B) are two snapshots of temperature and velocity at for the onset of an instability (From Korenaga & Jordan, 2003). The dashed boxes represent approximately the region where the present analytical theory applies. C) Flow pattern predicted by the analytical theory.

Figure 6.12: Diagrams of vertical velocity component versus plume length (depth) measured from the top of the viscous layer for several combinations of q_0 , η , and v . The shaded area indicates the range of realistic velocity profiles from different numerical experiments cited in the text.

Figure 6.13: A) Shear stresses in the viscous layer at $y = 0$. The symmetry axis of the cold plume is at $\lambda/2$. B) Maximum deflection in the elastic plate as function of its elastic thickness for three different vertical loads (q_o). Parameters used in SVF and WVF models are listed in Table 6.2.

Figure 6.14: Stresses acting on the elastic/brittle part of the lithosphere. σ_R = compressive ridge-push stress, σ_U = tensile stress arising from the undulation of the plate, σ_B = bending (fibre) stresses due to flexure, σ_V = tensile/compressive stresses arising from the vertical gradient in the shear stress, σ_N = vertical stress causing the deflection, τ_v = basal shear stress, τ_s = vertical shear stress due to flexure.

Figure 6.15: Plot of σ_{xx}^T for an elastic plate 30 km thick. A) $w_o = 0$ m; $\tau_{xy}^o = 30$ MPa; Ridge push = 30 MPa. B) $w_o = 1000$ m; $\tau_{xy}^o = 0$ MPa; Ridge push = 30 MPa. C) $w_o = 500$ m; $\tau_{xy}^o = 30$ MPa; Ridge push = 30 MPa. D) $w_o = 1000$ m; $\tau_{xy}^o = 60$ MPa; Ridge push = 30 MPa. In all cases the 0 and 100 MPa contour lines are shown. The colour scale saturates at 0 and 200 MPa.

Figure 6.16: A) Orientations of σ_1 (solid thin lines) and σ_2 (dashed thin lines) for the case of an elastic plate 30 km thick, an instability wavelength $\lambda = 400$ km, $w_o = 500$ m, and $\tau_{xy}^o = 20$ MPa (no vertical exaggeration). The orientation of potential shear faults (thick solid lines) at both ends are indicated. B) Magnitude of the principal stress difference resulting from the combination of ridge push (σ_R), basal shear stress (τ_V) and normal vertical stress (σ_N). C) Same as in (B) but for bending stresses only ($\sigma_B + \sigma_U + \tau_S$). The colour scale is the same for the three panels and represents the principal stress difference ($\sigma_1 - \sigma_2$) in MPa.

Figure 6.17: Ratio between total available shear force and total fault shear resistance (F_A/F_R) plotted as a function of fault orientation θ . The insets are diagrams indicating how θ is measured in each case. A) $x = \frac{1}{2}\lambda$. B) $x = \frac{3}{8}\lambda$. C) $x = \frac{2}{16}\lambda$. D) $x = 0$.

Figure 6.18: Snapshots of temperature (A and C) for the initial stages of a developing R-T instability. B) and D) are the respective density anomalies $\Delta\rho$ in kg m^{-3} resulting from the thermal fields. The elongated horizontal anomalies at ~ 50 km depth are caused by the displacement of the spinel-garnet transition.

CHAPTER 7

Summary and Discussion

This chapter summarizes the main results of this thesis and briefly discusses the general implications of the model for subduction initiation presented in Chapter 6 in terms of predicted geophysical observables and potential sites at which a new subduction zone may be initiated.

7.1 Main results

- (a) A new combined geophysical-petrological methodology to model the thermophysical properties of the lithospheric-sublithospheric mantle has been presented. This approach integrates the latest data on mineral physics, geochemistry, petrology, and geophysical information relevant to the first 300 km of depth. It permits to model two-dimensional vertical transects in a self-consistent manner, giving constraints on possible compositional fields and attainable lithospheric buoyancy for any lithospheric-sublithospheric model.
- (b) The methodology has been applied to a number of synthetic and real transects in both oceanic and continental domains to study their density, thermal, and seismological structure, and to evaluate the effects that compositional heterogeneities have on their relative stability with respect to the convective sublithospheric mantle. Predicted geophysical observables (SHF, elevation, gravity and geoid anomalies, and seismic velocities) have been used as constraints to the models. The results can be summarized as follows:
 - (i) The highly depleted composition typically assumed for Archean lithosphere cannot be representative of the whole lithospheric (thermal or seismological) thickness. A model in which the cratonic keel is composed of at least two

boundary layers (i.e. a thick thermal boundary layer including a chemical boundary layer in its upper part) has been shown to be a necessary condition for reconciling petrological and geophysical data. The bottom of the highly depleted chemical boundary layer is located in the depth range of 150 - 185 km. Allowance for a slightly depleted composition, intermediate between typical Phanerozoic and typical Archean, down to the bottom of the thermal boundary layer is consistent with geophysical observables and can explain the observed S-wave anomalies at depths of 350 - 400 km beneath cratons. Archean keels can be positively/neutrally buoyant with respect to the sublithospheric mantle down to depths of 300 - 350 km, making them more resistant to convective thinning.

- (ii) The inclusion of compositional and compressibility effects in Phanerozoic continental domains suggest that mechanisms other than pure thickening are necessary to destabilize the root of a thickened lithosphere. Processes such as eclogitization of injected asthenospheric melts and/or metasomatism by asthenospheric fluids may be necessary to drive the development of a gravitational instability.
- (iii) For the oceanic lithosphere, a plate model with an asymptotic thermal thickness (depth to the 1300 °C isotherm) of 110 ± 5 km is consistent with all the available geophysical and petrological data. Plates with basal temperatures in excess of ~ 1430 °C at depths < 100 km are difficult to reconcile with geophysical evidence. The resultant density structure of mature oceanic lithosphere makes it gravitationally unstable with respect to the sublithospheric mantle after $\gtrsim 30 - 80$ Ma, depending on the adopted adiabatic reference model. However, density contrasts $\Delta\rho$ attained by mature oceanic plates with respect to the sublithospheric mantle never exceed $\sim 40 \text{ kg m}^{-3}$. These values are significantly lower than the typical $70 - 100 \text{ kg m}^{-3}$ assumed in lithospheric

modelling. In order to reach such large density contrasts a source of negative buoyancy other than its normal thermal structure must be invoked.

- (c) A new model for the initiation of subduction triggered (or assisted) by a Rayleigh-Taylor instability has been presented. This model is more consistent with the evidence presented in this thesis than other models. An analytical theory has been developed and applied to show that the initiation of a new subduction zone by a Rayleigh-Taylor instability with a minimum wavelength of ~ 400 km is feasible. The finite growth of the instability provides: (i) the necessary forces to produce whole lithospheric failure, and (ii) the necessary negative buoyancy to bend the elastic part of the plate and to initiate its foundering.

7.2 Discussion

The model presented in Chapter 6 predicts that subduction can take place when a gravitational instability with a certain minimum size develops in the lower part of mature oceanic lithosphere and uppermost sublithospheric mantle. This model accounts for the observation that mature oceanic plates that follow a “normal” evolution trend cannot produce enough negative buoyancy by thermal cooling to trigger subduction initiation. It can explain both the existence of old (> 90 Ma) oceanic lithosphere in ocean basins and the absence of subduction in mature passive margins affected by considerable sedimentary loads. It is also consistent with realistic values of frictional strength along translithospheric discontinuities, as well as with evidence from numerical experiments on mantle convection. However, the present analytical theory cannot predict the precise location at which subduction may be initiated.

Numerical simulations of mantle convection show that large cold downwellings in a convecting fluid develop preferentially either at places where the upper horizontal flow

of a convective cell is totally or partially blocked (e.g. where the thermal thickness of the lithosphere changes abruptly, such as in a transform margin or across a fracture zone, Cooper et al., 2004; O'Neill et al., 2004), at plate boundaries (e.g. King et al., 2002; Lowman et al., 2003), or where the cold upper thermal boundary layer becomes too thick (e.g. Korenaga & Jordan, 2003; Zaranek & Parmentier, 2004). As previously recognized by many authors, all of the above point towards passive or transform margins, large and old oceanic basins, and large fracture zones as potential places for subduction incitation. These models give important insights into the problem of identifying the sites more prone to nucleate a new subduction zone, but they cannot predict the precise location at which it will take place. An attempt to accomplish this can be done by comparing the predictions of geophysical observables by the model in Chapter 6 with the real observables on a global scale.

Fig. 7.1 shows the relative predictions of SHF, geoid anomalies, elevation (considering a single plate with an elastic thickness $T_e = 35$ km), and P-wave seismic anomalies for the two thermal fields depicted in Fig. 6.18. The SHF anomaly changes only by 5 - 7 mW m⁻² with respect to the surrounding values. Since this variation is well within the uncertainties of most SHF measurements, SHF surveys are not appropriate to locate such thermal perturbations. On the other hand, elevation and geoid anomalies caused by the instability are $\Delta E \sim -550$ to -950 m and $\Delta N \sim -5.5$ to -10.0 m with respect to the surrounding values, respectively. Although these anomalies are large enough to be recognizable in geophysical surveys, they have to be taken with caution. Since elevation and geoid anomalies calculated with LitMod are strictly isostatic anomalies (see Chapter 4), and consequently they do not consider dynamic components, the resulting anomalies are expected to be upper bound values.

The resulting P-wave seismic anomaly for the case in Fig. 6.18A (as percentage variation with respect to the background velocity structure) indicates maximum variations

of $\gtrsim 1.75$ % in the core of the instability. An identical result is obtained for the thermal field in Fig. 6.18B (not shown here because differences between the two thermal fields are unimportant). Given the size of the anomaly, seismic studies with horizontal grid resolution $> 2^\circ$ would only “see” an averaged value. Representative averaged values of ~ 1.4 and 0.4 % are obtained at depth intervals of 100 - 200 km and 200 - 300 km, respectively. Assuming a typical $d\ln V_S/d\ln V_P \sim 1.5$ in the upper mantle, the above P-wave anomalies translate into S-wave anomalies of ~ 2.1 and 0.6 %. Again, these values are large enough to be identified by seismic tomography studies.

When comparing the predicted observables with global databases, it is found that five main sites exhibit all of the above features with comparable (but still smaller) magnitudes (Fig. 7.2):

- (a) Sohm Abyssal Plain (Grand banks transform margin): negative elevation > 5300 m; geoid low $\gtrsim 5$ m; S-wave anomaly at 100 - 200 km ~ 2 %.
- (b) Gulf of Guinea (The Côte d’Ivoire-Ghana transform margin): negative elevation > 5000 m; geoid low > 4 m; S-wave anomaly at 100 - 200 km ~ 2 %.
- (c) Pernambuco Abyssal Plain (offshore Brazil, south of Romanche Fracture zone): negative elevation $\gtrsim 5500$ m; geoid low > 6 m; S-wave anomaly at 100 - 200 km ~ 1.5 %.
- (d) Argentine Abyssal Plain (north of Malvinas Fracture zone): negative elevation $\gtrsim 6000$ m; geoid low > 6 m; S-wave anomaly at 100 - 200 km ~ 1.5 %.
- (e) Western Enderby Abyssal Plain (The Antarctic passive margin): negative elevation > 5300 m; geoid low > 6 m; S-wave anomaly at 100 - 200 km ~ 2 %.

Of these sites, the Argentine Abyssal Plain exhibits anomalies closest to the predictions from the theoretical model, suggesting that a gravitational instability may be

developing beneath the ocean basin. This is consistent with estimations of stresses and dynamic topography from mantle circulation models, which locate an anomalous high-stress, low-topography area in the Argentine Abyssal Plain (Steinberger et al., 2001). However, no seismic activity has been reported in this area. Future work including detailed lithospheric-sublithospheric modelling, seismic studies, and ocean drilling in the five identified regions is needed to test the present hypothesis.

Figure 7.1: Predictions of surface heat flow anomalies (ΔSHF), geoid anomalies (ΔN), and elevation anomalies (ΔE) for the two thermal fields shown in Fig. 6.18. The gray areas depicts the range of variation between the case in Fig. 6.18A and Fig. 6.18B. The lower panel shows the P-wave anomaly resulting from the thermal field in Fig. 6.18A. All anomalies are estimated with respect to surrounding values.

Figure 7.2: Location map of potential sites where a new subduction zone may be initiated. 1) Sohm Abyssal Plain; 2) Gulf of Guinea; 3) Pernambuco Abyssal Plain; 4) Argentine Abyssal Plain; 5) Western Enderby Abyssal Plain. SWIR = Southwestern Indian Ridge.

APPENDIX A

Analytical solution for the elastic bending of the lithosphere

Eq. (4.15) (or 6.33) is a linear fourth-order, non-homogeneous differential equation, and therefore its general solution is of the form $w(x) = w_H(x) + w_P(x)$, where $w_H(x)$ is the solution of the homogeneous part and $w_P(x)$ is the solution of the non-homogeneous part (Kreyszig, 1988). The solution of the homogenous part is well known in the literature (e.g. Hetényi, 1979)

$$w_H(x) = e^{(Gx)} \{c_1 [\cos(Fx)] + c_2 [\sin(Fx)]\} + e^{(-Gx)} \{c_3 [\cos(Fx)] + c_4 [\sin(Fx)]\} \quad (\text{A.1})$$

where

$$F = \sqrt{\xi + \frac{N}{4D}} \quad (\text{A.2})$$

$$G = \sqrt{\xi - \frac{N}{4D}} \quad (\text{A.3})$$

$$\xi = \frac{1}{2} \sqrt{\frac{\Delta \rho g}{D}} \quad (\text{A.4})$$

and c_1 , c_2 , c_3 , and c_4 are constants that need to be determined from boundary conditions.

The solution of the non-homogeneous part is (Eq. (6.35))

$$w_P(x) = w_o \cos\left(\frac{2\pi x}{\lambda}\right) \quad (\text{A.5})$$

Boundary conditions for the case of an infinite plate under the action of finite distributed load $q(x)$ are

$$w = 0 \quad \text{when} \quad x \rightarrow \infty \quad (\text{A.6})$$

$$\frac{dw}{dx} = 0 \quad \text{when} \quad x = 0 \quad (\text{A.7})$$

These boundary conditions imply $c_1 = c_2 = 0$, $c_3 = c_4 = c$, and the deflection is therefore given by

$$w(x) = e^{(-Gx)} \{c[\cos(Fx)] + c[\sin(Fx)]\} + w_o \cos\left(\frac{2\pi x}{\lambda}\right) \quad (\text{A.8})$$

Since the load pattern is a sinusoid with constant wavelength and peak load (q_o), it is expected that the deflection will essentially follow the same pattern. This implies that the deflection should be zero at $x = \pm \lambda/2$, which is satisfied when setting the remaining constant $c = 0$. Accordingly, the deflection of the elastic lithosphere above the instability is estimated as [Eq.(6.37) in the text]

$$w(x) = w_o \cos\left(\frac{2\pi x}{\lambda}\right) = w_P(x) \quad (\text{A.9})$$

Although this assumption is consistent with the assumed physical model in Chapter 6, it is recognized that it may overestimate the magnitude of the deflection above the return upwellings by $\sim 5 - 20 \%$ (see item (b) in Section 6.5, Chapter 6). As shown in Fig. 6.9, the effect of the horizontal force N on the final deflection is negligible, and therefore it can be ignored in all relevant equations.

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