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**An Analytical Model for
Computing Weld Microstructures**

by

© Cynthia E. Henwood
B. Eng. (Mechanical)

A thesis submitted to the Faculty of Graduate
Studies and Research in partial fulfillment
of the requirements for the Degree of

Master of Engineering

Department of
Mechanical and Aeronautical Engineering
Carleton University
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The undersigned recommends to the Faculty of Graduate Studies and Research, acceptance of the thesis: *An Analytical Model for Computing Weld Microstructures*, submitted by Cynthia E. Henwood, in partial fulfillment of the Degree of Master of Engineering.

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Abstract

An analytical model for computing weld microstructures is developed in this thesis. The model tracks microstructural changes in the weld fusion and heat-affected zones throughout a thermal cycle. The Ashby grain growth relationship is used to determine the austenite grain size. Kirkaldy decomposition kinetics is used to predict the decomposition of austenite. These are Avrami type equations, which determine the amount of ferrite, pearlite, and bainite formed during cooling of a weld. The Rosenthal equations and a 2D transient finite element thermal analysis are used to model the heat flow, and provide the necessary thermal histories to the microstructure algorithm. Microstructure predictions of grain size, phase fractions, and heat-affected zone hardness are compared with experimentally measured values for a bead-on-thick plate weld.

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Microstructure Program

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Nomenclature

A	- property of the precipitate
Ae_1	- ferrite-pearlite phase boundary temperature ($^{\circ}\text{C}$)
Ae_3	- austenite-ferrite phase boundary temperature ($^{\circ}\text{C}$)
Al	- aluminum (wt. %)
As	- arsenic (wt. %)
B	- property of the precipitate
B_s	- bainite start temperature ($^{\circ}\text{C}$)
C	- carbon (wt. %)
C_a	- carbon content of ferrite (wt. %)
C_c	- carbon content of carbide or nitride (wt. %)
C_{eut}	- carbon content of the eutectic (wt. %)
C_{γ}	- carbon content of austenite (wt. %)
C_m	- carbon content of metal used to form precipitate (wt. %)
Cr	- chromium (wt. %)
Cu	- copper (wt. %)
FEA	- finite element analysis
g	- grain size (μm)
g_0	- initial grain size (μm)
G	- ASTM grain size index
GMA	- gas metal arc welding
h_s	- saturation thickness (mm)
H	- hardness (VPN)
H_b	- hardness of bainite (VPN)
H_{fp}	- hardness of ferrite and pearlite mixture (VPN)
H_m	- hardness of martensite (VPN)
HAZ	- heat-affected zone
k_1	- grain growth constant

M_s	- martensite start temperature ($^{\circ}\text{C}$)
Mn	- manganese (wt. %)
Mo	- molybdenum (wt. %)
N	- nitrogen (wt. %)
Ni	- nickel (wt. %)
P	- phosphorus (wt. %)
q/v	- heat input (J/m)
Q	- activation energy for grain growth (cals/mole)
r	- radial distance from heat source (m)
R	- universal gas constant (cals/mole K)
S	- sulphur (wt. %)
Si	- silicon (wt. %)
T	- temperature ($^{\circ}\text{C}$)
T_{diss}	- precipitate dissolution temperature ($^{\circ}\text{C}$)
T_l	- liquidus temperature ($^{\circ}\text{C}$)
T_m	- melting point temperature ($^{\circ}\text{C}$)
T_0	- ambient temperature ($^{\circ}\text{C}$)
T_p	- peak temperature ($^{\circ}\text{C}$)
T_s	- solidus temperature ($^{\circ}\text{C}$)
Ti	- titanium (wt. %)
t	- time (s)
V	- vanadium (wt. %)
V'	- cooling rate at 700°C ($^{\circ}\text{C/hr}$)
v	- welding velocity (mm/s)
W	- tungsten (wt. %)
X	- phantom phase fraction
X_A	- fraction of austenite
X_B	- fraction of bainite
X_F	- fraction of ferrite
X_{FE}	- equilibrium fraction of ferrite
X_{FP}	- total fraction of ferrite and pearlite
X_L	- fraction of liquid

X_M	- fraction of martensite
X_P	- fraction of pearlite
X_{PE}	- equilibrium fraction of pearlite
X_S	- fraction of solid
α	- thermal diffusivity (m^2/s)
λ	- thermal conductivity ($J/m\ s\ ^\circ C$)
η	- arc efficiency
ρ	- density (g/cm^3)
τ	- time of transformation to ferrite (s)
$\tau_{8/5}$	- 800-500 $^\circ C$ cooling time (s)
ξ	- direction (m)

Chapter 1

Introduction

In engineering practice, the most important structural material is steel. By far the most common method of joining steel is welding. During welding the base material is subject to a thermal cycle, and as a result the internal structure, and therefore the mechanical properties of the workpiece in this area change. These structural changes can lead to problems with the joint. The most serious difficulty is the formation of cracks that occur as the weld cools. Cracks can appear at high temperatures (so-called hot cracking) or at low temperatures (cold cracking). A typical heat-affected zone crack is shown in Figure 1. In addition a part may also develop cracks in service from the combined effects of stress and corrosion. The weld is the most sensitive area of a structure for stress corrosion cracking. Along with cracking problems are low fracture toughness and fatigue resistance in the weld region.

Figure 1

Illustration of weld cracking in the heat-affected zone.

The most sensitive area of the weld is usually the heat-affected zone. Shown in Figure 2 is a photograph of a weld, with a sketch showing the base metal, heat-affected zone (HAZ), and the weld metal. The heat-affected zone is that part of the base metal, which, even though it does not melt, undergoes structural changes due to the thermal cycle that occurs as the heat source passes. The least reliable area of the weld is the coarse grained region close to the weld metal.

Figure 2 Weld showing fusion zone, heat-affected zone, and base metal.

The structure of the fusion and heat-affected zones depends primarily on the thermal cycle (especially cooling), the grain size, and the carbon and alloy content of the steel. The effect of increasing carbon and alloy content is, in general, to increase strength and hardness. Carbon especially has a strong effect on these properties. A high heat input rate leads to a relatively coarse grained material because the material spends more time above

the precipitate dissolution temperature, thereby allowing more time for uninhibited grain growth. A large grain size increases the susceptibility to cracking, and lowers the toughness and fatigue resistance.

At relatively high temperatures a structure called austenite is formed. As the material cools austenite decomposes into any of several alternative structures, namely ferrite, pearlite, bainite, and martensite. The mechanical properties (hardness, toughness, wear resistance, etc.) of these transformation products are very different, and therefore the performance of a part can vary widely due to the microstructure. Over and above the effect of structure is thermal shrinkage, which causes severe biaxial and triaxial residual stresses in the neighborhood of the weld. If the material has insufficient plasticity, cracks may form in the HAZ as the weld cools, even before a part is put into service. In addition, very hard materials tend to be brittle, and possibly dangerous in service. As a general guideline, a HAZ hardness of 350 VPN is considered to be the upper limit, below which cracking will not be a problem. In general, the structure must be known to determine the properties of the material. Since cracks often form dynamically as the weld cools it is necessary to trace transient structural changes as well as the residual values if the mechanism is to be understood.

As previously mentioned, the reason for structural changes in the HAZ is the short time, high temperature heat treatment that is the result of the weld thermal cycle. A typical thermal cycle is illustrated in Figure 3 a. The cooling rate of the weld is heat input sensitive. A high heat input gives rise to slow cooling and austenite decomposes to proeutectoid ferrite, and then pearlite. However, as the cooling rate increases, the distance over which carbon atoms can diffuse is reduced, and there is a tendency to form structures involving shorter movements of atoms. These structures are bainite and martensite. A CCT (continuous cooling transformation) diagram of a low carbon steel is shown on Figure 3 b. This further illustrates the fact that pearlite formation requires a slow cooling rate. Ferrite will form at higher cooling rates than pearlite. Martensite is formed under very fast cooling conditions, it is the hardest of all of the transformation products. In addition to cooling rate, the higher the carbon content, the harder and more brittle the bainite/martensite transformation products. Figure 3 c traces the structure of a typical weld. The initial phases that may be formed (on heating) are ferrite and pearlite, then ferrite and austenite as the temperature increases. Austenite grains grow once the precipitates have dissolved.

Figure 3

a) Typical thermal cycle during a welding heat treatment, b) pictorial representation of transient microstructure during a thermal cycle and, c) continuous cooling transformation (CCT) diagram for a steel of composition of 0.16 C, 1.12 Mn, 0.22 Si, 0.12 Ni, 0.99 Cr.

On tooling, austenite decomposes to a combination of ferrite, pearlite, bainite, and/or martensite.

There are perhaps three models available which can be used to predict the austenite transformation products in the neighborhood of a weld. Two of the early methods are those of Bastien [1, 2] and Alberry [3]. These are not considered appropriate for this investigation since they are not very comprehensive, and are, therefore, difficult to implement in a computer system. The most recent relatively comprehensive model is based on the work of Ashby et al [4, 5]. This method uses comparative kinetic models for grain growth and carbide dissolution, which are integrated over the weld thermal cycle to obtain the final grain size. Semi-empirical equations, based on carbon equivalence concepts, are used to predict the microstructure (% of martensite, bainite, and ferrite/pearlite) of the HAZ, as well as hardness (based on a rule of mixtures relationship). The Ashby approach gives only the final grain size and structure; transient microstructural changes during a thermal cycle are not included in the model.

The Rosenthal heat flow theory [7] was combined with the Ashby relationships to test the applicability of this method for computing weld microstructure. However, this method was difficult to interpret from the Ashby publications. An attempt was made to reproduce a so-called welding diagram contained in the original publication [5], showing the grain size and hardness profiles throughout the HAZ of a small weld. A comparison of the published diagram and that computed by this author is shown in Figures 4 a and b. The original thesis work was consulted and still the interpretation problems were not solved. There were inconsistencies between the published papers and the thesis, and while this author is convinced that the work constitutes a valuable contribution to the literature, interpretation difficulties prohibited further investigation.

One of the most fundamental austenite decomposition models available is that of Kirkaldy and Venugopalan [6]. Relationships are established for the formation of bainite, pearlite, and ferrite from austenite. The model is based on austenite grain size, composition, temperature, and time. Up to this point the theory has been applied to CCT diagrams, Jominy bar tests, and other relatively long time heat treatments. Welding is a short time, high temperature process, and is therefore a very different application. In the model developed during this investigation, the theory is applied in incremental form to

Figure 4 Welding Diagrams – hardness and grain size profiles: a) calculated curves and b) published curves [5] for a Nb microalloyed steel. GMA welding, $V = 18$ volts, $I = 100$ amps, and $v = 2.1$ mm/s.

the weld thermal cycle. At the start of the thermal cycle, (i.e. on heating), the structure is assumed to be close to equilibrium. Above the precipitate dissolution temperature grain growth takes place (governed by Ashby grain growth kinetics), and as the material cools the austenite decomposes, governed by the Kirkaldy relationships.

The objective, and contribution, of this thesis is to predict the final structure, and indeed the transient microstructural changes using the Kirkaldy reaction kinetics. This is based on the welding parameters and the chemistry of the base material. This is part of a comprehensive finite element based system for predicting weld thermal changes - thermal stress, structure, properties; and defects.

The theory is presented in Chapter 2, and the computer implementation and testing is in Chapter 3. Computer results are compared to experimental values in Chapter 4, and the capability of the system is analyzed in the same chapter. A general discussion is presented in Chapter 5. This chapter also looks at the need for future work in this area, and the role of this microstructure algorithm as part of an overall simulation package. Final conclusions are given in Chapter 6

Chapter 2

Microstructural Model Description

2.1 Overview

As identified in the previous chapter, the objective of this research is to predict the final microstructure, and transient microstructural changes, in the fusion and heat-affected zones of a weld. The first step in this process is to generate the thermal cycle. The heat transfer theory used for this purpose is from two sources. One is the classical approach, based on the theory of Rosenthal, and the other is the more recent finite element technique. In general, the welding parameters are submitted to a heat transfer model, and time - temperature thermal histories throughout the fusion and heat-affected zones are generated. Thermal cycles provide the basis for computing microstructural changes. On heating, the material is assumed to be in equilibrium until austenite grain growth begins. The structure in this region can be calculated from the equilibrium phase diagram. Austenite grain growth is governed by Ashby's kinetic equations. On cooling, austenite decomposition occurs and this is governed by the Kirkaldy kinetic relationships. Implementing the above into a complete microstructural model allows prediction of transient and residual microstructures.

2.2 Thermal Cycle Computation

There are basically two theoretical approaches available for computing weld thermal cycles. The classical method is based on the theory of moving heat sources originated by Rosenthal in 1945 [7]. While it is a convenient way of computing the thermal history throughout the weld metal and heat-affected zones, the accuracy of the calculations can be called into question due to many assumptions contained in the method. Recently finite element analysis has been applied to this problem with considerable success. This is primarily because the finite element method has considerable capacity for incorporating model details and less assumptions are necessary.

2.2.1 The Classical Method

Figure 5 . Bead-on-plate welding situation used to illustrate the Rosenthal solution to the Fourier equation.

The basic bead-on-plate welding situation, such as that shown above, is used to illustrate the Rosenthal solution to the Fourier equation [7]. The heat flow is characterized as either 2D (two dimensional) or 3D (three dimensional). The heat flow is said to be 3D for relatively shallow penetration welds on 'thick' plate. To simplify this investigation all heat flow situations investigated are 3D, and only 3D theory is documented. The heat source is assumed to be a point travelling at constant speed along a semi-infinite plate. The solution to the Fourier equation is based on the concept of a quasi-stationary temperature distribution. The term 'quasi-stationary' means that the temperature field does not change in time with respect to the moving heat source. Two coordinate systems are usually defined, a fixed system (x, y, z) with respect to the workpiece, and another that moves with the heat source (ξ, y, z) (see Figure 5). When the heat flow is 3D the temperature field is given by:

$$T(r, \xi) = T_0 + \frac{q/v}{2\pi\lambda r} \exp - \left[\frac{r}{2\alpha} (\xi + r) \right] \quad (2.1)$$

$$r = \sqrt{\xi^2 + y^2 + z^2} \quad (2.2)$$

$$\xi = x - vt \quad (2.3)$$

where:

- T_0 - is the initial temperature of the workpiece
- r - is the distance measured from the moving heat source
- λ - is the thermal conductivity (J/m s K)
- α - is the thermal diffusivity (m^2/s)
- q/v - is the heat input (J/m)

Note that the above thick plate equation is used only if the plate thickness is greater than the saturation thickness, given by Graville [8]:

$$h_s = \sqrt{\frac{q/v}{\rho c(T - T_0)}} \quad (2.4)$$

where:

- ρ - is the density (kg/m^3)
- T - is the current temperature ($^{\circ}C$)

The principal disadvantage of the Rosenthal model is that it assumes that the thermal conductivity (λ) and thermal diffusivity (α) are constant over the entire thermal cycle, whereas in reality they are functions of temperature. In addition, a point source representation is assumed and this results in an infinite temperature at the centre of the heat source - clearly unrealistic. Due to this fact, the spatial thermal distribution is not accurate, especially close to the heat source. This accuracy improves as the distance from the heat source increases. At the same time, it has been shown by Ion [9] that if measured and calculated peak temperatures are matched, the thermal cycle generated by Equation 2.3 is a good approximation to the actual thermal cycle. The principal advantage of the method is that it is easy to implement and is, therefore, used by many engineers in practice. For this reason it was considered necessary to research the Rosenthal model.

2.2.2 Finite Element Method

The finite element computational method can also be used to generate thermal cycles throughout a weld. It gives an excellent representation of the thermal history in both the fusion and heat-affected zones. The spatial accuracy of the temperature distribution is excellent - considerably better than that of the Rosenthal method. The transient non-linear finite element program ASGARD, developed at Carleton University, was used for this part of the analysis. A two-dimensional cross-sectional analysis was selected for this investigation. It is recognized that a full 3D analysis is the preferred method of calculation. The difference is that the 3D analysis includes longitudinal heat flow whereas the 2D cross-sectional model assumes that this is insignificant. However, this author opted for the simplicity of the 2D configuration to begin with, because of the complexity of the microstructure routine. Integrating the microstructure routine with the full 3D analysis is a problem that is recommended for future work. In the 2D analysis, the heat source travels with velocity v in the z direction of a plate (as shown in Figure 6). A reference plane is established in the $x - y$ coordinate direction. As shown in Figure 6 b, the heat source is represented by a double ellipsoid configuration that is roughly the shape of the weld puddle. A Gaussian energy distribution is imposed on the ellipsoid in all three dimensions. It is a maximum immediately under the heat source and decays exponentially to the ellipsoid boundaries. The double ellipsoid heat source is arbitrarily set to a size that is 5 to 10 % smaller than the weld pool.

The size of the heat source is estimated by the weld pool dimensions which can be determined for any general welding situation by the methods of Christensen [10]. The figure used to predict the ellipsoid depth in this investigation is reproduced from Christensen's work. This is given in Figure 7. The abscissa is an operating parameter n , based on the net heat input to the plate.

$$n = \frac{qv}{4\pi\alpha\lambda(T_L - T_0)} \quad (2.5)$$

where:

q - is the net heat input (J/sec)

v - is the welding speed (mm/sec)

Figure 6

Finite Element Analysis: a) schematic of welding configuration, b) double-ellipsoid with superimposed Gaussian energy distribution used to model a welding heat source and, c) 2D cross-sectional finite element mesh for analysing the welding situation.

Upper Scale: Depth plus weld reinforcement

Lower Scale: Depth without reinforcement (required depth).

Solid line is the average of the fusion zone depth (h_w) and the HAZ depth (h_f). Ellipsoid calculations require the HAZ depth. Therefore a value of h is taken from below the solid line.

Figure 7 Christensen's diagram for determination of weld pool depth.

T_L - is the liquidus temperature ($^{\circ}\text{C}$) (Equation 2.37)

On the ordinate the so-called reduced depth is plotted:

$$\xi = \frac{h_w v}{2\alpha} \quad (2.6)$$

where:

h_w - is the depth of the ellipsoid

Using these parameters the depth of the ellipsoid is determined. Similar procedures were used to determine the width and length of the ellipsoid. This method provides an excellent representation of the weld pool, and, therefore, a good estimate of the heat source. A detailed description of the double ellipsoid heat source can be found in references [11], and [12].

The finite element mesh used to model the problem situation is shown in Figure 6 c. By using symmetry, only one half of the reference plane is analysed. The elements used are two-dimensional grading elements developed and implemented into the ASGAR finite element system by McDill [13] at Carleton University. These elements allow for faster computations than are possible with conventional arrangements because the mesh is less complicated. However, accuracy is not sacrificed with these elements. Along with the advantages previously mentioned the finite element approach uses variable thermal properties throughout the analysis.

2.3 Microstructural Modelling

The thermal cycle is necessary for the overall analysis, but the principle focus of this research is to model the microstructural changes that take place in and around a weld on heating and cooling. The technique employed in developing the complete model is to use a stepwise approach over a thermal cycle, and to determine the changes in microstructure after each step. An Fe-C phase diagram is given in Figure 8 a to indicate the transformation regions that must be considered on heating and cooling. In addition, a typical thermal cycle is shown in Figure 8 b, indicating the various transformation regions and the transformation temperatures (which can also be referenced to the Fe-C phase diagram).

Figure 8

Microstructure Modelling: a) weld indicating a position in the HAZ that reaches a temperature of T_p , b) Fe/C phase diagram identifying the cooling path and critical temperatures and c) thermal cycle identifying regions that must be considered when implementing the microstructure algorithm.

2.3.1 Transformations on Heating

1) Initialization of Ferrite and Pearlite (Region i)

On heating the steel is assumed to be in equilibrium. If the initial temperature is between ambient and A_{e1} (A_{e1} is shown on the phase diagram as the 727 °C isotherm), the initial structure is a mixture of ferrite and pearlite (as indicated on Figure 8 a).

An empirical relationship for the A_{e1} temperature is taken from the work of Leslie [14] as follows:

$$A_{e1} = 723 - 10.7Mn - 16.9Ni + 29.0Si + 16.9Cr + 290As + 6.4W \quad (2.7)$$

The amount (volume fraction) of ferrite is calculated using a lever law relationship:

$$X_F = \frac{C - C_{eut}}{C_\alpha - C_{eut}} \quad (2.8)$$

$$X_P = 1 - X_F \quad (2.9)$$

where:

- X_F - is the fraction of ferrite
- X_P - is the fraction of pearlite
- C - the carbon content of the steel
- C_{eut} - the carbon content of the eutectic
- C_α - the carbon content of the ferrite

The carbon content of the eutectic is given by another empirical relationship from the United States Steel Bain Laboratories, and also published by Leslie [14]:

$$C_{eut} = (910 - 15.2Ni + 44.7Si + 104V + 315Mo + 13.1W - (30Mn + 11Cr + 20Cu - 700P - 400Al - 120As - 400Ti) - A_{e1})^2 / 203^2 \quad (2.10)$$

The carbon content of the ferrite below A_{e1} is given by Equation 2.11, assuming a linear decrease from the eutectic value to a value of 0. at 20 °C (ambient temperature). The empirical relationship is given as:

$$X_F = \frac{T - 20}{A_{e1} - 20} (0.105 - 115.3 \cdot 10^{-6} A_{e1}) \quad (2.11)$$

2) Ferrite and Austenite Formation (Region ii)

When the temperature of the steel exceeds A_{e1} it is assumed that the pearlite transforms immediately to austenite. Between the A_{e1} and A_{e3} temperatures the steel is a mixture of ferrite and austenite. The A_{e3} temperature is given by yet another empirical relationship based on the work of Leslie [14]:

$$A_{e3} = 910 - 203C^2 - 15.2Ni + 44.7Si + 104V + 315Mo + 13.1W - (30Mn + 11Cr + 20Cu - 700P - 400Al - 120As - 400Ti) \quad (2.12)$$

Since the structure is assumed to be in equilibrium, the amount of ferrite (and austenite) can be determined using the lever law:

$$X_F = \frac{C - C_\gamma}{C_\alpha - C_\gamma} \quad (2.13)$$

$$X_A = 1 - X_F \quad (2.14)$$

where :

- X_A - is the fraction of austenite
- C_γ - is the carbon content of the austenite
- C_α - is the carbon content of the ferrite

The carbon content of the austenite is found by rearranging Equation 2.12 to give C_γ instead of the A_{e3} temperature:

$$C_\gamma = (910 - 15.2Ni + 44.7Si + 104V + 315Mo + 13.1W - (30Mn + 11Cr + 20Cu - 700P - 400Al - 120As - 400Ti) - T)^2 / 203^2 \quad (2.15)$$

Above A_{e1} the carbon content of the ferrite is given by the following equation (as derived from the Fe-C phase diagram):

$$C_\alpha = 0.105 - 115. \cdot 10^{-6} T \quad (2.16)$$

As the temperature increases the amount of ferrite decreases, and above A_{e3} the material is completely austenite. The intercritical area (between A_{e1} and A_{e3}) is a region that requires some additional explanation. In actual fact, it is well known that equilibrium is not achieved on heating in this region because of limited carbon diffusion in a short time weld cycle. However, superheating kinetics for the steel system are not well known, and in any event the consequences of assuming equilibrium are not that important. If anything the properties of the intercritical region are better than those of the base region. In addition, for those regions where the temperature passes completely through the intercritical, subsequent transformations wipe out the history of the region.

2.3.2 Austenite Grain Growth (Region iii)

As the temperature increases the austenite grains are assumed pinned until the precipitate dissolution temperature is reached. Refer to Figure 8 for the location of the grain growth region on a typical thermal cycle. The temperature required for complete dissolution is taken from Ashby et al [5]:

$$T_{DISS} = \frac{B}{A - \log[C_m^a C_c^b]} \quad (2.17)$$

where A and B are the constants of the solubility product, and C_m^a and C_c^b refer to the concentration of metal (eg. Nb or Ti) and non-metal (eg. C or N) species in the material being used to form the precipitates, indexed by their respective precipitate stoichiometries a and b . For example if the precipitate is NbC then $a = 1$ and $b = 1$. However, if the precipitate is V_4C_3 then $a = 4$ and $b = 3$. The concentrations are in wt. %, and the temperature is in Kelvin. NbC and V_4C_3 are the two most common precipitates used to control grain size in modern HSLA steels. The steel considered in this investigation is a NbC microalloyed steel.

The governing equation for austenite grain growth above the precipitate dissolution temperature is based on recent work by Ashby [5]. It is assumed by Ashby that grain growth is diffusion controlled, driven by surface energy. The grain growth equation can be expressed as follows:

$$\frac{dg}{dt} = \frac{k_1}{2g} \exp - \frac{Q}{RT} \quad (2.18)$$

In a weld thermal cycle the grain size is a function of both temperature and time. In view of this Equation 2.18 is rearranged to the following form:

$$g^2 = g_0^2 + k_1 \int_0^\infty \exp \frac{Q}{RT(t)} dt \quad (2.19)$$

where

- g - is the grain size (μm)
- g_0 - is the initial grain size (μm)
- k_1 - is a kinetic constant
- Q - is the activation energy for grain growth (cals/mole)
- R - is the universal gas constant (cals/mole K)

Both k_1 and Q are properties of the precipitate, and are therefore input parameters. Computer implementation of this relationship is detailed in Chapter 3. Grain growth continues until the temperature falls below Ae_3 , at which point the decomposition of austenite begins.

2.3.3 Ferrite Formation from Austenite Above Ae_1 (Region iv)

As the temperature goes below Ae_3 the austenite starts to decompose into alpha (or pro-eutectoid) ferrite. The location of this region on the phase diagram and a typical thermal cycle is shown in Figure 8. Ferrite is a body-centred crystal structure. In the welding process it usually occurs as a network or in parallel laths. It is a fairly soft and ductile structure. The austenite-ferrite transformation is a nucleation and growth transformation. Nucleation frequently occurs at grain boundaries of the austenite. As the ferrite, containing relatively small amounts of carbon, (< 0.25 wt %), is precipitated, it leaves austenite grains that are progressively enriched in carbon as the temperature falls.

The austenite decomposition theory is based on work by Kirkaldy [6]. As mentioned previously, these equations, prior to this research, have not yet been applied to the transformations occurring in relatively short time welding heat treatments. This is a new, and very different, application since it involves a thermal cycle which takes place over a short time period. The time of transformation for ferrite formation is as follows

$$\tau(X, T) = \frac{59.6Mn + 1.45Ni + 67.7Cr + 24.4Mo}{2^{\frac{(G-1)}{2}} (\Delta T)^3 \exp \frac{23500}{RT}} \cdot t \quad (2.20)$$

$$I = \int_0^X \frac{dX}{X^{\frac{2(1-X)}{3}} (1-X)^{\frac{2X}{3}}} \quad (2.21)$$

where

X - is the ratio of the amount of ferrite formed to the equilibrium amount

G - is the ASTM grain size index

ΔT - is the undercooling ($A_{e3} - T$)

The undercooling is a measure of how much the current temperature is below the transformation start temperature, in this case A_{e3} for ferrite formation. Of interest in this research is how much ferrite is formed during a given time interval Δt . The above equation can't be integrated in closed form for a welding thermal cycle because many of the parameters are functions of both temperature and time. Therefore Equation 2.21 is rearranged and the rate of ferrite formation is given by:

$$\frac{dX}{dt} = \frac{2^{\frac{(G-1)}{3}} (\Delta T)^3 \exp - \frac{23500}{RT}}{59.6Mn + 1.45Ni + 67.7Cr + 24.4Mo} X^{\frac{2(1-X)}{3}} (1-X)^{\frac{2X}{3}} \quad (2.22)$$

and

$$X = \frac{X_F}{X_{FE}} \quad (2.23)$$

where

X_F - is the volume fraction of ferrite formed ($0 < X_F < X_{FE}$)

X_{FE} - is the equilibrium amount of ferrite, given by the lever law, equation (2.4)

The above form of the Kirkaldy relationship is appropriate for determining the amount of ferrite formed in a weld thermal cycle. Programming considerations are detailed in Chapter 3 for all of the austenite decomposition relationships.

2.3.4 Pearlite Formation from Austenite (Region v)

As the temperature falls below A_{e1} , ferrite formation continues, governed by the equations of the previous section. However, in this temperature range, pearlite also begins to form (see Figure 8). Pearlite consists of alternate plates of Fe_3C and ferrite, with ferrite being the continuous phase. Pearlite is not a phase, but a mixture of two phases. However, it is easily identifiable under the microscope. The decomposition of austenite to form

pearlite occurs by nucleation and growth. Most theories assume the nucleus is Fe_3C [15]. Once an Fe_3C platelet forms, diffusion depletes the carbon on either side (Figure 9) which favours the nucleation of ferrite. As well, the spacing of the pearlite lamellae affects the hardness of the final structure. At a given transformation temperature for a particular steel, the spacing between Fe_3C laminae is very nearly constant. At lower transformation temperatures this spacing is reduced [16]. This is important because reducing the spacing increases the strength and hardness. Due to the higher carbon content of the pearlite, it is a harder and stronger structure than pure ferrite, but it is less ductile.

As with the ferrite formation, the austenite decomposition is governed by Kirkaldy's equations. An equation similar to the ferrite decomposition relationship (Equation 2.18) exists for the time of transformation to pearlite. This can again be rearranged to give the rate of pearlite formation:

$$\frac{dX}{dt} = \frac{2^{\frac{(Q-1)}{2}} (\Delta T)^3 * D}{1.79 + 5.42(Cr + Mo + 4MoNi)} X^{\frac{2(1-X)}{3}} (1 - X)^{\frac{2X}{3}} \quad (2.24)$$

where:

X - is the ratio of pearlite formed to the equilibrium amount

ΔT - is the undercooling ($A_{e1} - T$)

D is evaluated as:

$$\frac{1}{D} = \frac{1}{\exp - \frac{27500}{RT}} + \frac{0.01Cr + 0.52Mo}{\exp - \frac{37000}{RT}} \quad (2.25)$$

and:

$$X = \frac{X_P}{X_{PE}} = \frac{X_P}{1 - X_{FE}} \quad (2.26)$$

where :

X_P - is the volume fraction of pearlite formed

X_{PE} - is the equilibrium amount of pearlite

The fact that $X_{PE} = 1 - X_{FE}$ follows from the condition that if the maximum amount of ferrite that can be formed is X_{FE} , then the remainder is available to become pearlite. In this temperature range both ferrite and pearlite are formed. However, if the fraction of

pearlite reaches 0.01 (1 %) then the austenite no longer decomposes to ferrite. This follows directly from the CCT diagram of Figure 3.

2.3.5 Bainite Formation from Austenite (Region vi)

Austenite continues to decompose to pearlite, and possibly ferrite, until the temperature reaches the starting temperature for bainite transformation. At this point ferrite and pearlite no longer form. Region vi is shown on the phase diagram (Figure 8) between B_s and M_s . Like pearlite, the reaction product of the bainite transformation is not a phase but a mixture of ferrite and carbide. It forms at lower temperatures than pearlite, and is also a nucleation and growth type reaction. The mechanism of bainite formation differs from that of pearlite, in that bainite grows as plates. Under a microscope, bainite has a characteristic acicular (needlelike) appearance. Bainite does not form until the temperature falls below B_s (the bainite start temperature), which is given by [6]:

$$B_s = 656 - 58C - 35Mn - 75Si - 15Ni - 34Cr - 41Mo \quad (2.27)$$

The amount of bainite formed increases as the temperature is lowered. A rapid cooling rate favors bainite formation over pearlite because the material does not have time to form the separate lamellae of ferrite and carbide. In upper bainite the ferrite is in lath form with elongated carbide particles between them. [15] Lower bainite is composed of large plates, i.e. the carbides form within the ferrite plates. Lower bainite forms just above the start of the martensite transformation temperature and is harder than upper bainite which forms at higher temperatures. The difference in structure is shown schematically in Figure 10. In lower bainite the carbides form within the ferrite plates, rather than between the plates as in upper bainite. The carbides act as pinning points to the mobile dislocations, thereby increasing the hardness of the material. Due to differences in size, shape, and distribution of the iron carbide, bainite is harder, stronger, and tougher than fine pearlite of the same chemical composition. As an example, consider a eutectoid carbon steel, i.e. a steel with 0.8 carbon. Hardness increases from about 15 R_c for coarse pearlite to 38 R_c for fine pearlite, and then to about 40 R_c for upper bainite, to about 55 R_c for the hardest lower bainite [17].

Figure 9

Mechanism of pearlite formation from austenite where the Fe_3C acts as the nucleus.

Figure 10

Schematic of structure of upper and lower bainite illustrating the difference in the location of the carbides.

The equation governing the decomposition of austenite to bainite is again a kinetic equation originated by Kirkaldy, similar to the ferrite relationship (Equation 2.18). The original Kirkaldy relationship is arranged to give the rate of growth of the bainite phase.

$$\frac{dX}{dt} = \frac{2^{\frac{(n-1)}{3}} (\Delta T)^2 \left(\exp - \frac{27500}{RT} \right)}{0.0001(2.34 + 10.1C + 3.8Cr + 19Mo) * Z} X^{\frac{2(1-X)}{3}} (1-X)^{\frac{2X}{3}} \quad (2.28)$$

$$Z = \exp[X^2(1.9C + 2.5Mn + 9Ni + 1.7Cr + 4Mo - 2.6)] \quad (2.29)$$

where:

ΔT - is the undercooling ($B_s - T$)

X - is the amount of bainite

and Z is set to one (1) if $(1.9C + 2.5Mn + 9Ni + 1.7Cr + 4Mo - 2.6) < 0$.

Note that the same governing relationship can be used for both upper and lower bainite. Bainite continues to form until the temperature reaches the transformation start temperature for martensite.

2.3.6 Martensite Formation from Austenite (Region vii)

The decomposition of austenite to martensite begins at a critical temperature called martensite start, M_s , (see Figure 8). Unlike pearlite and bainite decomposition, it is not a nucleation and growth type mechanism. The formation of martensite occurs the instant that the critical temperature, (M_s), is reached. It is produced by a shear movement of the austenite lattice, producing a body-centred tetragonal lattice [18]. Since no diffusion occurs, the martensite must be identical in composition to the austenite from which it formed. Martensite is the hardest of all of the transformation products, and also the most brittle. Except in some special cases, it is usually a structure which is to be avoided. The martensite start temperature is given by [6]:

$$M_s = 561 - 474C - 35Mn - 17Ni - 17Cr - 21Mo \quad (2.30)$$

If, at the martensite start temperature, there is any austenite left, it decomposes to martensite ($X_m = X_\gamma$). For the purposes of this research it was assumed that the austenite

transformed immediately at M_s , even though it actually does not completely change until the martensite finish temperature (M_f) is reached. An equation for M_f could not be located, and therefore all martensite is assumed to form at M_s . This is justified for low carbon structural steels but could be a problem for higher carbon, higher alloy, materials where retained austenite is a possibility. M_f considerations are suggested for future work.

2.4 Hardness of the Heat-Affected Zone

As mentioned previously, hardness can be a good indicator of the susceptibility of a structure to cracking and other problems. The hardness at any point can be calculated using a rule of mixtures relationship, since the volume fractions of ferrite, pearlite, bainite, and martensite are known. The mixtures relationship for hardness is as follows [5]:

$$H = H_m X_m + H_b X_b + H_{fp} X_{fp} \quad (2.31)$$

where H_m , H_b , and H_{fp} refer to the Vickers hardness (VPN) of martensite, bainite, and a ferrite/pearlite mixture respectively:

$$H_m = 127 + 949C + 27Si + 11Mn + 8Ni + 16Cr + 21\log V' \quad (2.32)$$

$$H_b = -323 + 185C + 330Si + 153Mn + 65Ni + 144Cr + 191Mo \\ + (89 + 53C - 55Si - 22Mn - 10Ni - 20Cr - 33Mo)\log V' \quad (2.33)$$

$$H_{fp} = 42 + 223C + 53Si + 30Mn + 12.6Ni + 7Cr + 19Mo \\ + (10 - 19Si + 4Ni + 8Cr + 13QV)\log V' \quad (2.34)$$

$$X_{fp} = X_F + X_P \quad (2.35)$$

The compositions refer to the overall steel composition in wt.%, and V' is the cooling rate at 700 °C (in °C/h). This is related to the 800-500 °C cooling time, ($\tau_{8/5}$), as follows:

$$V' = \left(\frac{800 - 500}{\tau_{8/5}} \right) \left(\frac{1}{3600} \right) \quad (2.36)$$

The value of $\tau_{8/5}$ can be found from the Adams simplified relationship for thick plate [19] as

$$\tau_{8/5} = \frac{q/v}{2\pi\lambda} \left(\frac{1}{500 - T_0} - \frac{1}{800 - T_0} \right) \quad (2.37)$$

where

T_0 - is the ambient (or preheat) temperature ($^{\circ}\text{C}$)

λ - is the thermal conductivity ($= 25 \text{ J/m sec } ^{\circ}\text{C}$)

q/v - is the heat input (J/m)

The above equations provide a method of determining the variation in hardness due to the variations in structure throughout the heat-affected zone.

2.5 Melting and Solidification

In the previous sections, the transformations that take place over a complete thermal cycle are described. The peak temperatures of these thermal cycles have all been less than the melting point temperature. Additional considerations are necessary for the weld metal, i.e. that part of a weld which undergoes melting.

Once the temperature passes the solidus melting begins. Melting is complete when the temperature exceeds the liquidus - the point at which the material is completely liquid. For low alloy compositions, the liquidus and solidus lines can be regarded as functions of carbon content only. These temperatures are given as follows [20]:

$$T_s = 1527 - 181.356C \quad (2.38)$$

$$T_l = 1538 - 80.581C \quad (2.39)$$

If the temperature is between T_s and T_l then part of the material has melted. This is illustrated in Figure 11 which shows the two phase (solid-liquid) region. The fraction of liquid is given by:

$$X_L = \frac{C - C_s}{C_l - C_s} \quad (2.40)$$

Figure 11 Schematic two-phase region (phase diagram) to show how the solid and liquid fractions are computed.

$$X_A = 1 - X_L \quad (2.41)$$

where

C is the carbon content of the steel

C_s is the carbon content of the solid (or austenite)

C_l is the carbon content of the liquid

The fraction of solid is X_A because the solid phase is austenite. The values of C_s and C_l at a given temperature T (refer to Figure 11) are obtained by rearranging Equations 2.38 and 2.39 as follows—

$$C_s = \frac{1527 - T}{181.356} \quad (2.42)$$

$$C_l = \frac{1538 - T}{80.581} \quad (2.43)$$

If the peak temperature at a point is between T_s and T_l then some of the material at this point does not melt, (i.e. part is liquid and part is solid at the peak temperature). The fraction which is liquid becomes part of the weld metal upon cooling. The fraction that does not melt remains as part of the heat-affected zone. During the decomposition of the austenite, the two regions (weld metal and heat-affected zone plus base metal) are separated. The region that partially transforms is called the mushy region. In practice this region is very small, but it has practical importance in that this is the region where hot cracking often occurs.

If the temperature exceeds the liquidus then the material at that particular location has melted. On cooling it becomes part of the weld metal. In principle the composition of the fusion zone is that of the filler wire. However, some base metal is generally fused into the zone together with the filler metal. Dilution values (fraction base metal melted into the fusion zone) are available for most welding procedures. Dilution of the weld metal is accounted for by using the following simple relationship. If D is the dilution, then the composition of the weld metal depends on the composition of the base metal and of the electrode. For example, if C is the weight percent of carbon, the carbon content in the weld metal can be determined from

$$C_{weldmetal} = D * C_{basemetal} + (1 - D) * C_{electrode} \quad (2.44)$$

In this way a realistic composition of the weld metal is determined. In addition, it is not yet known how to calculate grain size in the fusion zone. It is known, however, that the grain size is large - at least as large as the coarse grained region of the HAZ immediately adjacent to the FZ. For the purposes of this investigation the grain size is set to a large value, an ASTM number of 2 (or about 175 microns). It would possibly be better to assign it the value of the maximum HAZ grain size - but this introduces considerable programming complications. This is recommended for future work.

Decomposition computations for the weld metal and heat-affected zone are carried out separately. This is necessary because all of the transformation temperatures are dependent on the composition, and since the weld metal and heat-affected zone have different compositions, the transformations will start and finish at different temperatures. By separating the weld metal and base metal the analysis is simplified, and the user has a straightforward method of investigating either region. While melting and solidification are not difficult in principle they do complicate the coding somewhat.

Chapter 3

Computer Implementation

The goal of this chapter is to provide a description of the program for predicting the final structure, and indeed the transient microstructural changes of a weld from the welding parameters, kinetic parameters, and the material composition. The program is structured so that the development of the code is as straightforward as possible. This chapter deals with key programming considerations for computer implementation of the theory and principles of microstructural modelling.

3.1 Equilibrium Conditions (Regions i and ii)

Implementation of the algorithms in regions i and ii (Figure 12) are straightforward. In region i, below A_{e1} , the equilibrium lever law relationships of Equations 2.7 to 2.11 are used to calculate ferrite and pearlite formation. In region ii the ferrite and austenite formation between A_{e1} and A_{e3} is governed by Equations 2.12 to 2.16.

3.2 Austenite Grain Growth (Region iii)

3.2.1 Implementation of Governing Equations

When the temperature during a thermal cycle exceeds A_{e3} the structure is completely austenite. When the temperature exceeds T_{DISS} , (region iii of Figure 12) the carbides dissolve and austenite grain growth begins. The austenite grain growth relationship is given in Equation 2.19. Since the program calculates the changes in microstructure in a stepwise manner, the equation is arranged to an incremental form and the change in grain size is calculated according to the following:

$$\Delta g = \frac{1}{2g} k_1 \exp - \frac{Q}{RT} \Delta t \quad (3.1)$$

The grain size (g) is determined after every time step using:

Figure 12

Thermal cycle showing the transformation regions and the governing equations as found in Chapters 2 and 3.

$$g = g + \Delta g \quad (3.2)$$

Q is the activation energy for grain growth. The steel in this investigation is a Nb microalloyed steel. The activation energy is determined from a fundamental relationship suggested by Ashby [5].

$$\frac{Q}{RT_m} = 16 \quad (3.3)$$

$$T_m = 1810 - 90C \quad (3.4)$$

where

T_m - is the melting point temperature (K)

One other programming consideration is the incremental approximation of Δg and Δt . Small time steps are required in order to accurately solve the given equation. This was accomplished by controlling the rate of change of grain size in a given time step. For the experimental weld of Chapter 4, at a peak temperature of 1600 K, the effect of controlling the grain growth rate is shown below.

Effect of Grain Growth Rate on Final Grain Size

$\Delta g/g$	g_{final}
%	μm
0.1	53.9
1.0	54.0
5.0	56.4
10.0	63.1

A constraint value of:

$$\frac{\Delta g}{g} < 0.01(1\%) \quad (3.5)$$

was therefore chosen, and is sufficient for proper convergence of the equation. Currently work is being carried out at Carleton in the application of higher order methods to the solution of the grain growth equation [21]

3.2.2 Determination of Grain Growth Constant k_1

Implementation of Equation 3.1 into a computer model requires that the initial grain size (g_0), grain growth constant (k_1), and activation energy (Q) are known. The activation energy can be determined using Equation 3.2. The initial grain size is assumed to be small, about 5-10 microns for the Nb microalloyed steel considered in this investigation. However, the constant k_1 contains uncertain kinetic parameters. In the original presentation of this theory [5] Ashby avoided k_1 by using comparative kinetics, i.e. an experimental measurement of the grain size produced by a certain thermal cycle. In order to keep this program independent of experimental input, k_1 must be determined. Although k_1 is a physical parameter it could not be located in the literature. It was decided that k_1 for the steel used in this investigation would be determined. The original thesis work of Ion [9] contains a set of experimental grain size measurements under various welding conditions at different locations throughout the heat-affected zone. See Chapter 4 for experimental details. Data pertaining to four different welds were used in determining k_1 . These welds cover a wide range of heat input (0.2 to 1.1 kJ/mm) and experimental grain size measurements (11 to 312 μm). Using Equation 3.2, with welding conditions and all known parameters taken from the thesis work, tables of grain size for different values of k_1 were generated. A typical result is shown in Figure 13, for a submerged arc bead-on-plate weld with a heat input of 1.1 kJ/mm. As Figure 13 illustrates, difficulties were encountered in matching both the maximum grain size and the overall variation in grain size. The maximum value is consistently less than the measured value. However, the agreement between the overall distribution of grain size throughout the HAZ is excellent. An exact statistical determination of k_1 was not possible due to the small amount of data. A value of $k_1 = 7 \times 10^{11}$ was chosen after careful examination of the results. The value chosen does not give the best fit for the weld of Figure 13, but it was the best fit for the four welds studied, under a wide range of heat inputs.

Figure 13 Grain size vs peak temperature curves used to determine the kinetic parameter k_1 . Steel composition given in Table 4 and welding parameters in [9]

Figure 14 Schematic illustrating method of calculating 'start' time for grain growth.

3.2.3 Determination of Start and Finish Times for Grain Growth

Austenite grain growth begins when the precipitate dissolution temperature is reached on heating, and is terminated at the A_{c3} temperature on cooling (as indicated on Figure 12). The microstructure program is structured to accept time and temperature information from a thermal cycle at the beginning and end of a series of time steps. However, the program should initiate grain growth at exactly the precipitate dissolution temperature. Due to the piecewise nature of the time and temperature information, a given time step will not usually be exactly at these critical temperatures - and this must be taken into account.

A method was developed to predict when the thermal cycle passes through these critical temperatures (T_{DISS} and A_{c3}). The following approach is developed for the specific case of determining the start time for the grain growth of austenite. A similar approach is applicable to the finish time for grain growth, as well as start and finish times for all of the austenite decomposition reactions. As illustrated in Figure 14, austenite grain growth begins when the temperature exceeds T_{DISS} . T_3 is the temperature at the end of the current time step. T_1 was the temperature at the beginning of the time step. It is necessary to determine the 'start' time - i.e. the time at which the temperature was T_{DISS} . If t_3 and t_1 are the times at the end and beginning of the current time step, respectively, then the start time for grain growth is:

$$t_{start} = t_1 + \left(\frac{T_{DISS} - T_1}{T_3 - T_1} \right) (t_3 - t_1) \quad (3.6)$$

This method is a simple linear interpolation between the beginning and end times for a given time step. A similar approach was used to determine all of the start and finish times. Experimental confirmation of results convinced the author that there was no need for a higher order (cubic, etc.) interpolation technique.

3.3 Austenite Decomposition to Ferrite on Cooling (Region iv)

3.3.1 Implementation of Theory into the Computer Model

As the temperature drops below A_{c3} (Figure 8) the austenite starts to decompose to ferrite. Region iv is shown on the thermal cycle of Figure 12. The governing equation for this transformation is Equation 2.22. The incremental form of Equation 2.22 is

$$\Delta X = \frac{2^{\frac{(G-1)}{3}} (\Delta T)^3 \exp - \frac{23500}{RT}}{59.6Mn + 1.45Ni + 67.7Cr + 24.4Mo} X^{\frac{2(1-X)}{3}} (1 - X)^{\frac{2X}{3}} \Delta t \quad (3.7)$$

The definition of X is given in Equation 2.23. It is called a phantom fraction (i.e. $X = \frac{X_F}{X_{FE}}$) because X_F is the required quantity but the reaction is driven towards X_{FE} . The grain size (g), in microns, is the value determined from the austenite grain growth relationships of the previous section. This number must be converted to the equivalent ASTM grain size index (G) for the above calculation. This is carried out using the relationship:

$$N = 2^{G-1} \quad (3.8)$$

where N is the number of grains/in² at 100X magnification. The final relationship used in the algorithm is:

$$G = 1 + 1.44 \left[\ln \left(\left(\frac{25.4}{g} \right)^2 + 100 \right) \right] \quad (3.9)$$

An initial fraction of ferrite (X_{F0}) of approximately 10^{-12} is chosen, due to the fact that (X_{F0}) must be small in order for Equation 3.7 to converge properly. Small time steps are used in a piecewise continuous approach in order to determine the amount of ferrite formed in any time step. After any time step:

$$\Delta X_F = \Delta X * X_{FE} \quad (3.10)$$

$$X_{F(new)} = X_{F(old)} + \Delta X_F \quad (3.11)$$

For the next time step, the new value of X is given by:

$$X = \frac{X_{F(new)}}{X_{FE(new)}} \quad (3.12)$$

The equilibrium fraction of ferrite (X_{FE}) changes in every time step. It is computed using the lever law relationship of Equation 2.13. As the temperature decreases the equilibrium (or maximum) amount of ferrite that can be formed increases to a maximum at Ae_1 .

Below A_{c1} the equilibrium amount of ferrite is considered constant (the value at the A_{c1} temperature), and is given by Equation 2.8.

The approximation of the integral for ΔX with incremental time steps is a first order (or simple Euler) method which gives accurate, stable, results when used with small (0.1 ms) time steps. This is shown in the following sections.

3.3.2 Convergence of the Decomposition Relationships

As the temperature drops below A_{c3} the austenite starts to decompose, initially to ferrite, then to pearlite, bainite, and finally martensite. Each of the ferrite, pearlite, and bainite transformations are governed by equations of a similar form (Equations 3.7, 3.14, and 3.18). In a general sense these equations are known as the Avrami type relationships. They can be written, for purposes of clarity, in a simplified form:

$$\Delta X = C * X^{\frac{2(1-X)}{3}} (1 - X)^{\frac{2X}{3}} \Delta t \quad (3.13)$$

where

C - function(Grain size, Temperature, Composition, etc.)

If X is plotted as a function of time, the curve has the general shape as given below in Figure 15.

Figure 15 - Schematic representation of isothermal phase transformation kinetics.

Due to the sharp change in the slope of the curve (at some unknown time), careful control over the solution procedure is necessary in order to solve the equation correctly. Initially, control over the equation was structured in a similar manner to that of the grain growth equation, i.e. limits were imposed on the maximum amount of any phase that could be formed in a time period. Limit constraints ranging from 1% to as low as 0.001% were investigated. If, in a given time step, the amount of a given phase formed was greater than the specified upper limit, the time step was reduced. This had the effect of decreasing the amount of ferrite formed in a time step. However, problems were encountered due to the instability of results based on this technique. By varying ΔX , from 1% down to 0.001%, the results (i.e. fractions of ferrite, martensite, etc.) varied as well, and convergence was not assured. In order to solve the stability problem of the transformation equation the approach had to be changed. In a testing procedure it is simpler to look at one equation at a time. The ferrite equation was selected for study. It has the same form as all of the transformation equations, and therefore the conclusions should apply quite generally. To facilitate this the appropriate code was separated from the rest of the program and tested as detailed in the following sections.

3.3.3 Convergence for Isothermal Decomposition

During testing procedures, the more parameters that remain constant, the better the chance of solving the problem. With this philosophy in mind, it was decided to analyze the ferrite formation in an isothermal situation. For testing purposes, a heat treatment at a constant temperature of 650 C for 0.5 seconds gives sufficient time to form ferrite. In these decomposition relationships, another parameter that has a significant effect on the final fraction of austenite that decomposes to ferrite is the initial amount of ferrite, X_{F0} , that is used to begin the transformation. The effect of both the size of the time step, Δt , and the initial amount of ferrite, X_{F0} , was investigated.

If the initial fraction of ferrite remains constant at a very small number then the effect of the size of the time step, Δt , can be investigated as an independent variable. With the initial ferrite fraction, X_{F0} , set at 10^{-12} the time step was varied from 10^{-2} to 10^{-5} seconds. The results are shown in Table 1.

The table clearly shows that by using successively smaller time steps the correct answer is not obtained, (i.e. Equation 3.7 is not solved properly) until Δt reaches 10^{-4} seconds.

Table 1
Effect of Time Step Size on Ferrite Formation^(A)

Δt sec	X_F (B)	Run Time (C)
10^{-2}	.2849	0.2 sec
10^{-3}	.4218	2.5 sec
10^{-4}	.4417	25.0 sec
10^{-5}	.4436	250. sec

(A) - $X_{F0} = 10^{-12}$

(B) - X_F obtained using Equation 3.7

(C) - Run time on an Apollo DN320

As the size of the time step decreases (for a given total time interval) the solution becomes stable. However, the number of steps required to solve the equation increases as well, leading to more intensive computer usage. With 50000 steps required, at a time step of 10^{-5} seconds, the computation takes approximately four minutes. Since the calculation at $\Delta t = 10^{-4}$ sec gives almost the same answer, in one tenth of the time, this value of Δt is used in the balance of the investigation. For ease of comparison, the effect of the initial fraction of ferrite is investigated with, as before, a heat treatment at a constant temperature of 650 C for .5 seconds.

Table 2 indicates that for an isothermal situation with small time steps (10^{-4} sec) the results converge and accurately predict the amount of ferrite formed, if a small initial fraction of ferrite ($X_{F0} < 10^{-10}$) is assumed. Other isothermal tests (not reproduced here) verify this fact.

Table 2
Effect of Initial Fraction of Ferrite on Ferrite Formation^(A)

X_{F0}	X_F (B)
10^{-4}	.5227
10^{-6}	.4600
10^{-8}	.4460
10^{-12}	.4417
10^{-14}	.4413

(A) - $\Delta t = 10^{-4}$ seconds

(B) - X_F obtained using Equation 3.7

3.3.4 Convergence for Variable Temperature Decomposition

The previous test case indicated that small time steps are required in an isothermal situation. However, the main focus of this research is on continuous cooling in a welding situation. Therefore, the second test is to subject the transformation equation to a typical thermal cycle - i.e. through the ferrite transformation range of A_{e3} to B_s . Actual times and temperatures in this temperature range, from a thermal cycle generated using Rosenthal's equations, are used in order to have a realistic test case. The thermal cycle used was generated for the weld that is used for all comparisons in Chapter 4, at a location in the HAZ with a peak temperature of 1300 K. An initial fraction of ferrite at A_{e3} of $X_{F0} = 10^{-12}$ is used, and the time step is varied as summarized in Table 3.

The amount of ferrite at the bainite start temperature (the end of the ferrite transformation) approaches a constant value as the time step is decreased. This confirms the need for small (10^{-4} sec) time steps in order to obtain accurate results. In addition, this solution

Table 3
Effect of Time Step Size on Ferrite Formation

Δt	X_F
sec	at. B_s
10^{-3}	0.6280
10^{-4}	0.7020
10^{-5}	0.7036

technique, as opposed to initial attempts to control ΔX , has the desired effect of keeping ΔX very small, much smaller (10^{-5} times smaller) than in the phase fraction technique. The method of time step control for austenite decomposition to ferrite is equally applicable to all of the related equations - i.e. those for ferrite, pearlite, and bainite. This method was implemented in the microstructure program and has effectively solved the consistency and stability problems, at the expense of a more time-intensive computer program. Currently, work is being carried out at Carleton in the application of higher order methods to the solution of the austenite decomposition equations [21]. So-called 'stiff' ODE (ordinary differential equation) solvers are being tested with the decomposition kinetic equations. Based on the welds investigated in this analysis, the Adams-Bashforth adaptive method is recommended for the solution of the Kirkaldy equations. These solvers will provide a more accurate and faster solution technique than is possible with the simple Euler method.

3.4 Austenite Decomposition to Pearlite (Region v)

As the temperature during a thermal cycle drops below A_{c1} the austenite starts to decompose to pearlite. Region v is shown on Figure 12, between A_{c1} and B_s . The governing equation, which gives the rate of formation of pearlite, is Equation 2.24. This is rearranged in incremental form to give the amount of pearlite formed in a given time step:

$$\Delta X = \frac{2^{\frac{(G-1)}{3}} (\Delta T)^3 * D}{1.79 + 5.42(Cr + Mo + 4MoNi)} X^{\frac{2(1-X)}{3}} (1 - X)^{\frac{2X}{3}} \Delta t \quad (3.14)$$

D is evaluated as in Equation 2.25. As in the case of ferrite formation, the grain size (G)

is the ASTM grain size index, given by Equation 3.9. In addition, the initial fraction of pearlite (X_{P0}) must be small, of the order of 10^{-12} . The testing of the ferrite transformation equation (as explained in the previous section) also applies to the pearlite equation, and the equation converges if time steps of 0.1 ms are used. After any time step, the amount of pearlite which has been formed is given by:

$$\Delta X_P = \Delta X * X_{PE} \quad (3.15)$$

The total amount of pearlite is now:

$$X_{P(new)} = X_{P(old)} + \Delta X_P \quad (3.16)$$

For the next time step, the new value of X is given by:

$$X = \frac{X_{P(new)}}{X_{PE(new)}} \quad (3.17)$$

Pearlite formation continues until the temperature reaches the bainite start temperature, or until $X_P = X_{PE}$.

3.5 Austenite Decomposition to Bainite (Region vi)

As the temperature drops below B_s , conditions favour the formation of bainite over ferrite and pearlite. This is region vi of Figure 12. The governing equation, Equation 2.28, can be rearranged and written in incremental form, to give the amount of bainite formed in a given time period:

$$\Delta X = \frac{2^{\frac{(Q-1)}{3}} (\Delta T)^2 \left(\exp - \frac{27500}{RT} \right)}{0.0001(2.34 + 10.1C + 3.8Cr + 19Mo) * Z} X^{\frac{2(1-X)}{3}} (1-X)^{\frac{2X}{3}} * \Delta t \quad (3.18)$$

Z is evaluated as in Equation 2.29. The initial value of X , (i.e. X_0), is set equal to the value of X_P at B_s . This is because the bainite nucleates on the pearlite, and for the purposes of bainite growth the pearlite is assumed to be 'ghost' bainite. For iterations after the initial, the value of X in Equation 3.18 is given by:

$$X = X_0 + \Sigma \Delta X \quad (3.19)$$

However, the total amount of bainite is:

$$X_B = \Sigma \Delta X \quad (3.20)$$

Bainite formation continues until the martensite start temperature is reached. At this point any remaining austenite immediately transforms to martensite (region vii on Figure 12).

3.6 Determination of Critical Times for Austenite Decomposition

Each of the decomposition reactions starts and finishes at certain critical temperatures. The times at which these temperatures are reached can be determined using an approach similar to that outlined for the grain growth reaction.

3.7 Hardness of the Heat-Affected Zone

The implementation of hardness predictions into the microstructure program involves a straightforward application of Equations 2.31 to 2.37. These calculations are performed once the temperature has gone below the martensite start temperature (M_s), and there is no austenite left to decompose. If, as in the case of higher carbon, higher alloy steels, there was retained austenite at room temperature, some modifications would have to be made to account for the hardness of the austenite phase.

Chapter 4

Results

In the previous chapters the theoretical background to microstructural modelling is presented, along with a discussion of the implementation of the theory in the computer program. In this chapter predicted grain sizes are compared to experimental results. In addition, the correlation between HAZ hardness and the presence of martensite is presented. The transient capabilities of the model are illustrated by observing the different structures present throughout a typical thermal cycle. In general, the results are presented with a goal in mind of demonstrating the capacity of the system for predicting the residual and transient microstructure of a weld. Computer generated results are compared to experimental data in order to further illustrate the accuracy of the method.

4.1 Weld to be Analysed

To assess the validity of applying Kirkaldy reaction kinetics to the weld HAZ experimental results were obtained from the original thesis work of Ion [9], performed at the University of Lulea, Sweden. The steel under investigation is a niobium microalloyed steel, a high strength low alloy structural steel. The composition is shown in Table 4.

Table 4
Chemical Composition of Nb Microalloyed Steel (wt.%)

C	Si	Mn	P	S	Al	Nb	N
0.12	0.16	0.91	0.002	0.005	0.04	0.021	0.011

The properties of this steel depend on small amounts of Nb, which in combination with carbon, forms a fine dispersion of carbides which impedes grain growth, and improve strength

and toughness. The experimental welds are bead-on-plate, some with the submerged arc process and some with the gas metal arc process. Results from four different welds were used in determining k_1 in Chapter 3. The heat inputs range from 0.2 to 1.1 kJ/mm. In this chapter only one of the experimental welds was selected for study. The weld chosen for this investigation had the following welding conditions:

Table 5
Welding Parameters for Test Weld

Process	GMA
Efficiency	0.75
Welding Speed	6.7 mm/s
Current	71 amps
Voltage	20 volts
Bead Depth	1.0 mm
A_{c1} Depth	1.74 mm
Plate Thickness	12.7 mm

The net heat input for this small gas metal arc weld is 0.2 kJ/mm. The bead depth is the depth of the weld bead - i.e. the fusion zone depth.² The A_{c1} depth is the heat-affected zone depth. These two parameters are important when assessing the validity of thermal predictions.

4.2 Thermal Analysis

4.2.1 Modelling of the Heat Source in FEA

In order to compute the weld microstructure a thermal cycle must be generated. In the finite element approach, the weld pool is modelled using an ellipsoidal temperature shape (Figure 6). Using Christensen's method, as outlined in Chapter 2, the dimensions in Table 6 were obtained for the double ellipsoid.

Table 6
Comparison of Weld Pool Parameters

METHOD	a	b	c_1	c_2	Peak Temp	FZ Depth	HAZ Depth	$\tau_{8/5}$
	mm	mm	mm	mm	C	mm	mm	sec
Christensen	1.8	1.8	2.7	4.5	2800	1.75	3.00	0.80
Christensen for Depth of 1 mm	1.0	1.0	1.5	2.5	5600	1.65	3.05	0.80
Experimental	1.0					1.00	1.74	1.00

As indicated in Table 6 the program predicts a fusion zone depth of approximately 1.75 mm. This is to be expected since the depth of the ellipsoid is 1.8 mm. The experimental depth is only 1.0 mm. In addition, the computed Ae_1 depth is about 3mm, giving a heat-affected zone width of 1.25 mm compared to 0.74 mm as reported for the experimental weld. Because this does not compare well it was decided that a second attempt should be made to reproduce the experimental results. The analysis was redone for an ellipsoid depth of 1.0 mm, which is the experimental depth of the fusion zone. The other parameters are given in Table 6. This did not prove to be the solution due to the fact that the fusion zone depth with this ellipsoid was 1.65 mm, and the Ae_1 depth was 3.05 mm, giving a heat-affected zone width of 1.4 mm. These results do not compare as well as those obtained from the Christensen parameters. The reason that the location of the HAZ is this far away from the heat source is excessive superheating in the weld pool that is obtained with the smaller ellipsoid. A maximum temperature of 5600 °C at the centreline of the plate is reached in this case, compared to only 2800 °C previously. (A weld pool temperature of 2800 °C has been shown to be acceptable). Therefore Christensen's predictions for ellipsoid size are chosen since they rationalize the superheat and heat-affected zone better. The other set of data, based on the measured depth, approximate the Rosenthal model which is known to be inaccurate near the heat source. In addition, the Christensen method has been used with considerable success at Carleton [22]. The location of the HAZ of this weld is shown

in Figure 16. Longitudinal heat flow was neglected in the two dimensional analysis. If it had been included then the weld would cool faster, making the fusion and heat-affected zones smaller, and therefore closer to the experimental values. However, this would also increase the cooling rate, and therefore decrease the 800-500 °C cooling time ($\tau_{8/5}$). $\tau_{8/5}$ is already less than the experimental measurement. Therefore a 3D analysis would not likely reproduce the experimental results. One other point to mention in relation to $\tau_{8/5}$ is that the measurement of temperatures in the HAZ is probably not very accurate. In the original thesis work Ion used thermocouples, spot welded to the plate, to take measurements. The spot welding may have had an effect on the measurements, and with a thermocouple width of .2 or .3 mm in a heat-affected zone with a width of less than 1.5 mm, spatial sensitivity could easily lead to a temperature error of 50 or 75 degrees. This would make a considerable difference in $\tau_{8/5}$.

4.2.2 Temperature Contours

An illustrative means of graphically presenting results is by contouring. Temperature contours can be used at any time to show the location of important boundaries such as the solid-liquid interface, etc. At the end of thermal cycle it is important from a microstructural as well as a heat treatment point of view, to know the location of the fusion and heat-affected zones of the weld. This is shown in Figure 16. The fusion zone boundary is marked by the T_f isotherm. The HAZ boundary is marked by the A_{c1} boundary - since below this temperature the phases present in the base metal are not affected by the weld.

4.3 Residual Microstructure

One of the main advantages of this model is that it tracks transient microstructural changes throughout a thermal cycle. Therefore both transient and residual microstructural information can be obtained. The residual microstructure is shown as contours, and compared with experimental results. The transient capability is used to illustrate how the amount of any given phase changes with time.

Figure 16 Finite element mesh showing location of the heat-affected zone and the positions of two nodes in the HAZ used to demonstrate the capacity of the model to predict transient microstructure.

4.3.1 Austenite Grain Growth

The thermal cycle data generated using the 2D finite element analysis is used to predict the microstructure. On heating, the NbC precipitates pin the grains until the dissolution temperature is reached. An initial austenite as-recrystallized grain size of $10\text{ }\mu\text{m}$ is assumed, which is typical of most modern microalloyed steels. Predicted values of the maximum austenite grain size at various locations throughout the HAZ of the test weld are plotted in Figure 17. Also shown are the experimental data points. Grain growth is initiated at T_{DISS} (approximately 1320 K), begins slowly, and becomes more rapid at higher temperatures. There is considerable grain growth near the FZ boundary where the peak temperatures are high. The agreement between the predicted values and the experimental data points is excellent.

4.3.2 Austenite Decomposition to Ferrite

1) Ferrite Contours in the HAZ

The microstructure contours are produced using TAURUS, a graphics package available on the APOLLO network at Carleton University. The ferrite contours in the heat-affected zone at the end of the welding procedure are presented in Figure 18. The ferrite is at a minimum near the fusion zone boundary because the structure at this location is almost completely martensitic. As the distance from the fusion zone increases, conditions favour the formation of ferrite. The ferrite fraction increases, and reaches the equilibrium value of 87 % at the heat-affected zone/base metal (HAZ/BM) boundary.

4.3.3 Austenite Decomposition to Bainite

1) Bainite Contours in the HAZ

The bainite contours in the HAZ of this weld are presented in Figure 19. These contours illustrate the unique intermediate position of bainite in the heat-affected zone of a weld. At the fusion zone, the structure is pure martensite. As the amount of martensite begins to decrease, conditions favour the formation of bainite. Note that the bainite increases more rapidly than ferrite close to the weld. This is because the fast cooling and shorter thermal cycle favours bainite formation over ferrite. However, towards the edge of the heat-affected zone the fraction of bainite decreases, as the conditions for ferrite formation take over.

Figure 17

Grain size vs. peak temperature: experimental results and predictions based on FEA generated thermal cycles. Steel composition and welding parameters are given in Tables 4 and 5.

Ferrite

CONTOUR VALUES

A = 2.00E-01

B = 4.00E-01

C = 6.00E-01

D = 8.00E-01

Figure 18

Ferrite contours in the heat-affected zone of a small bead-on-plate weld of a Nb microalloyed steel. Composition and welding parameters are given in Tables 4 and 5.

Bainite

CONTOUR VALUES

- A = 0.00E+00
- B = 2.50E-01
- C = 5.00E-01
- D = 7.50E-01

Figure 19

Bainite contours in the heat-affected zone of a small bead-on-plate weld of a Nb microalloyed steel. Composition and welding parameters are given in Tables 4 and 5.

4.3.4 Austenite Decomposition to Martensite

1) Martensite, Ferrite, and Bainite in the HAZ

At the end of the welding process the distribution of martensite throughout the heat-affected zone is often of considerable significance. Figure 20 shows the distribution of the ferrite, bainite, and martensite contents throughout the HAZ. At the fusion zone boundary the structure is almost completely martensitic. This is expected due to the higher cooling rates and large grain size (relative to the rest of the HAZ) at the FZ/HAZ boundary. As the distance from the fusion zone increases, the fraction of martensite present in the weld decreases rapidly. However, the next phase to form is bainite. Conditions (cooling rate, etc.) favour the formation of the bainite phase. The bainite reaches a maximum of 77 % at a peak temperature of about 1350 K. Note that while bainite and martensite can reach levels of 100 % in the weld, ferrite and pearlite are limited by equilibrium considerations. Towards the outer edge of the heat-affected zone (the 1000-1200 K range) the amount of ferrite increases towards its equilibrium value. The structure at the HAZ/BM boundary is 87 % ferrite (at this point $X_F = X_{FE}$), and 13 % bainite. Pearlite does not form in the heat-affected zone (or weld metal) of this weld. This is likely due to the relatively rapid cooling rates throughout the weld and HAZ. The 800-500 °C ($\tau_{8/5}$) cooling time is only .8 seconds, and this is the temperature range where pearlite formation takes place. The steel does not have sufficient time to form the separate lamellae of ferrite and carbide. The CCT (continuous cooling transformation) diagram of Figure 3 indicates that the pearlite transformation region will only be reached if the cooling takes place over a longer period of time. The CCT diagram also reinforces the fact that ferrite and bainite will form at faster cooling rates than pearlite. As the cooling rate decreases, ferrite formation is preferred over bainite formation, and the formation of bainite is in turn more likely than martensite.

2) Comparisons with Experimental Results

In the original thesis work Ion measures grain size, martensite volume fraction, and hardness, at several locations in the heat-affected zone. The experimental results for martensite are compared with predicted values in Figure 21. There is an obvious difference in the curves, as the experimental results show a gradual decrease in the fraction of martensite, and the predicted trend shows a 'collapse' in the amount of martensite at

Figure 20

Volume fractions of ferrite, bainite, and martensite throughout the heat-affected zone. Steel composition and welding parameters are given in Tables 4 and 5.

Figure 21

Volume fraction of martensite vs. peak temperature: experimental results and predictions based on FEA generated thermal cycles. Steel composition and welding parameters are given in Tables 4 and 5.

about 1400 K. This structural behavior in the HAZ has been observed before, as shown in [23] and [24]. Therefore, at this point, it is not clear that the measurements are entirely consistent.

4.3.5 Heat-Affected Zone Hardness

The hardness computations are based on a rule of mixtures relationship. A comparison of the computed and measured hardnesses is shown in Figure 22. There is a rapid decrease in both the measured and computed hardness values. The sharp change in the hardness occurs at a peak temperature of about 1450 K. Hardness is very sensitive to the martensite fraction and this would imply that there should be a comparable change in the martensite distribution (Figure 21). This change is shown in the computed curve. If the microstructure relationships are examined it is evident that this occurs because the decomposition relationships are very sensitive to grain size. In the temperature range from 1400-1500 K the grain size is changing quite rapidly (Figure 17). Therefore the martensite fraction (and hardness) should be decreasing rapidly in this region as well. This is supported by the predicted values of martensite and hardness, as well as the hardness measurements. In light of this analysis, the measured martensite fractions may be considered as being somewhat suspect.

The hardness of the heat-affected zone next to the weld metal, i.e. the maximum HAZ hardness, is often of particular interest. This is due to the fact that the maximum hardness can give an idea of whether cracking will be a problem. There are several models available to predict the maximum HAZ hardness in a weld. These models are based on composition and welding parameters (cooling behavior). There is no attempt made to determine the structure at the fusion line. The best of these methods is either that of Yurioka [25] or Suzuki [26]. In addition, the hardness obtained by the method of Arata [27] is reported, along with approaches by Cottrell [28], Terasaki [29], Beckert [30], and Duren [31]. Several of these methods have been previously implemented by this author on a small pocket computer at Carleton University [32]. The findings are summarized in Table 7.

Figure 22

HAZ hardness vs. peak temperature: experimental results and predictions based on FEA generated thermal cycles. Steel composition and welding parameters are given in Tables 4 and 5.

Table 7
Maximum HAZ Hardness Comparison

Hardness Model	VPN
Ion (Exp't)	343-364
Rule of Mixtures	387
Yurioka	376
Suzuki	370
Arata	373
Cottrell	369
Terasaki	378
Beckert	350
Duren	401

These empirical methods tend to support the predicted maximum hardness value of 387. The Yurioka and Suzuki approaches are considered to be reliable for predicting the maximum HAZ hardness for a wide range of steels under a variety of welding conditions [33]. All methods suggest a maximum of value of approximately 370 VPN, with the exception of the Beckert and Duren methods.

4.4 Microstructure Computations based on Classical Theory

In the initial stages of this research two different approaches were used to model the heat flow. The previous results have all been based on using thermal cycles generated using a 2D transient finite element thermal analysis. However, as previously discussed, the classical (Rosenthal) model can give a good approximation to the actual thermal cycle if peak temperatures are matched with measured values. In addition, it is advantageous in practice to have a method that is not dependent on having a computer intensive finite element package available in order to provide useful results. Comparisons can be made between the experimental measurements and predictions based on the two heat flow models. In figures 23, 24, and 25, grain size, martensite, and hardness, respectively, are plotted

Figure 23

Grain size vs. peak temperature: A comparison of experimental measurements and predicted values based on thermal cycles generated using the Rosenthal equations and finite element analysis.

Figure 24

Martensite fraction vs. peak temperature: A comparison of experimental measurements and predicted values based on thermal cycles generated using the Rosenthal equations and finite element analysis.

Figure 25

HAZ hardness vs. peak temperature: A comparison of experimental measurements and predicted values based on thermal cycles generated using the Rosenthal equations and finite element analysis.

versus the peak temperature of the thermal cycle at various locations in the HAZ. The grain size plots show excellent agreement between the measurements and the two predicted curves. The difference in maximum grain size between the two predicted curves is likely due to a small difference in the shape of the two thermal cycles. Both predicted curves of martensite show a similar collapse in the amount of martensite. This is to be expected. In Figure 25, the hardness plot, predictions based on the finite element generated thermal cycle are closer to the measurements than the predictions based on the Rosenthal heat flow computations. In general, the agreement between the Rosenthal and finite element analysis results indicates that the basic thermal cycles, and the important cooling range from 800 to 500 are quite similar. It is evident from this set of results that, providing peak temperatures are matched, the simple classical model can be used with reasonable confidence as a means of providing thermal histories for the microstructure algorithm.

4.5 Transient Microstructure

One of the principle advantages of the model developed during this research is that microstructural changes are tracked throughout a thermal cycle. It is possible to investigate how the amount of any given structure changes with time. A position in the heat-affected zone of this weld that undergoes a thermal cycle with a peak temperature of 1200 K is chosen to illustrate the potential of the system. Refer to Figure 16 for the location of this position (node 98) in the HAZ. On heating the structure is given by the equilibrium relationships. Initially the material is 87 % ferrite and 13 % pearlite. Figure 26 is a plot of phase fraction as a function of time. Pearlite is not shown as it is not part of the HAZ structure after .4 seconds. The temperature exceeds A_{c1} after about 0.4 seconds. The material is now ferrite and austenite. The amount of ferrite continues to decrease, and it disappears completely when the A_{c3} temperature is reached (after about 0.5 seconds). The material is completely austenite during the next 0.55 seconds, while the temperature remains above A_{c3} . On cooling, the temperature drops below A_{c3} after about 1.1 seconds, and the austenite begins to decompose to ferrite. When the bainite start temperature is reached the ferrite formation stops, and the bainite reaction takes over. The final structure at this location is 57 % ferrite and 43 % bainite. A position in the HAZ which reaches a peak temperature of 1600 K is shown as node 102 on Figure 16. The initial structure is the equilibrium mixture of ferrite and pearlite.

Figure 26

Illustration of transient microstructure prediction capability of the model: ferrite, bainite, and austenite volume fractions as a function of time for a location in the HAZ (node 98 of Figure 16) with a peak temperature of 1200 K.

Austenite appears after the temperature exceeds A_{e1} , and ferrite disappears when the temperature exceeds A_{e3} . However, the decomposition of austenite at this location in the HAZ is very different than at node 98. Austenite remains in the material until M_s is reached, and the material becomes completely martensitic. This is shown on Figure 27. The ability to trace the transient microstructure allows for considerable insight as to when during the thermal cycle various reactions are taking place.

Figure 27

Illustration of transient microstructure prediction capability of the model: ferrite, austenite, and martensite volume fractions as a function of time for a location in the HAZ (node 102 of Figure 16) with a peak temperature of 1600 K.

Chapter 5

General Discussion and Future Work

In the previous chapters the theory behind the microstructure algorithm has been discussed, and various results presented. It has been shown that the algorithm provides an excellent approach for predicting the transient and residual microstructures that occur during welding. In this chapter a general discussion of several aspects of the research is presented, along with recommendations for future work in this area.

5.1 Thermal Analysis

Thermal histories are a necessary input to the microstructure model. These are generated using two alternative approaches (see Chapter 2). One is the classical method of Rosenthal, the other a 2D transient finite element thermal analysis. As previously discussed, the spatial accuracy of the Rosenthal model is questionable, and peak temperatures must be matched with measured values if the Rosenthal model is to be used with any degree of accuracy. Computationally, the method is less expensive than performing a finite element analysis. However, FEA provides a more accurate representation of the heat flow in an actual welding situation. The double ellipsoid heat source has been shown to give an accurate representation of the size and shape of the fusion zone.

In this investigation, a 2D cross-sectional analysis has been performed. A complete 3D analysis would be more accurate since it would incorporate longitudinal heat flow. With a 3D analysis, it would likely mean that the actual cooling rate, and the 800-500 cooling time, would be more closely approximated. However, a 3D analysis is considerably more expensive than a 2D analysis. The availability of special grading elements in the ASGARD package was incorporated in the investigation (see Figures 6 and 16). The McDill mesh grading algorithm considerably decreases computer costs compared to standard mesh techniques, and similar grading elements are available in 3D [13]. In addition, as computing costs fall, the costs of complete 3D analyses becomes less prohibitive.

5.2 Microstructure Modelling

A complete model for predicting transient and residual microstructure has been developed during this investigation. The austenite decomposition equations have been shown to be quite accurate in predicting the transformation products. However, these equations require very small time steps in order to accurately solve the transformation equations. One particular small bead-on-plate weld was chosen to study. When this weld is modelled using finite element analysis, thermal histories are input at each time step to each node of the mesh. The time required to determine the complete microstructure throughout the thermal cycle added 30 minutes of computer time to the time taken for just a thermal analysis. This is mainly due to the time intensive solution of the austenite decomposition equations in the heat-affected and fusion zones. Note that the base material, which is the greater part of the mesh (Figure 17), remains at its equilibrium composition. All of the changes occur in the fusion and heat-affected zones. With the current solution technique (a simple Euler method), it takes each node in the HAZ approximately 20 seconds (on an Apollo DN320) to traverse the temperature range from A_{e3} (where ferrite formation begins) to M_s (where bainite formation ends).

Currently, work is being carried out at Carleton in the application of higher order methods to the solution of the austenite decomposition equations [21]. So-called 'stiff' ODE (ordinary differential equation) solvers are tested with the decomposition equations. Based on the welds investigated in this analysis, the Adams-Bashforth adaptive method is recommended for the solution of the Kirkaldy equations. These solvers will provide a more accurate and faster solution technique. For the case of ferrite formation under isothermal conditions (section 3.3.3) the Adams-Bashforth method can obtain convergence of the equation using a step size of 10 ms, as compared to a step size of .1 ms for the simple Euler method.

Another area of special interest is the fusion zone. The microstructure algorithm is relatively complete, but decomposition in the fusion zone has not been examined. The focus of this investigation was directed towards the heat-affected zone. In addition, if a method for predicting fusion zone grain size became available, it could easily be added to the algorithm.

The mushy region is another area that could be given considerable attention since this is the region of a weld where hot cracking may occur. Even though this region falls within a narrow temperature range for the steel in this investigation, the region becomes wider, and therefore more critical, for higher carbon steels.

5.3 Coupling of the Microstructure Algorithm to FEA

Currently, the thermal histories generated from the finite element analysis are used as input to the microstructure program. There is no feedback from the microstructural model to the thermal model. However, it is known that there is heat released when a phase change occurs. Heats of transformation are available for the austenite-ferrite reaction and the austenite-liquid reaction. Ideally, if the thermal analysis was more strongly coupled to the microstructure algorithm, the microstructure routine would determine the heat released (and therefore the temperature change) due to a phase change, and send the information back to the thermal analysis. The thermal model would then recompute temperatures in the region of the phase change. In addition, it would be advantageous if a set of thermal properties for each of the various phases (austenite, ferrite, etc.) was available. This would improve the modelling of the heat flow.

5.4 Applications

The microstructure model developed in this investigation is part of an overall project at Carleton to simulate a variety of manufacturing processes [34]. To this date, most of the research has been focused on welding. Algorithms are being developed which analyze the transient temperature, displacement, stress, and microstructural changes that take place during welding. In addition, an understanding of the microstructure is also important to other manufacturing processes such as forging and casting. During this research a basis has been established for microstructure prediction, which can be expanded to other such processes as research in this area develops.

Chapter 6

Conclusions

Several conclusions can be drawn on the basis of this investigation:

- 1) A complete model for predicting microstructure changes during welding has been successfully developed and tested. The method incorporates the Ashby grain growth relationship, and the Kirkaldy kinetic equations for austenite decomposition to ferrite, pearlite, and bainite. Both residual and transient microstructures throughout the thermal cycle can be predicted.
- 2) The microstructure model has been successfully tested against experimental measurements of grain size, martensite volume fraction, and HAZ hardness for a bead-on-plate Nb microalloyed steel weld. The agreement between the calculated and measured results is excellent.
- 3) Thermal histories required as input to the microstructure algorithm can be generated using the classical method of Rosenthal, or by the more recent finite element method. Due to limitations in the classical model, peak temperatures must be matched with measured values in order for the model to accurately predict the location of the heat-affected zone. If this is done the classical method is a viable alternative to the more computer intensive finite element method. However, if a finite element program is available, a finite element analysis (such as that described in this investigation) provides a significantly more accurate representation of the welding situation.
- 4) The modelling of the microstructural changes that occur during welding is an important addition to the overall package that is being developed at Carleton University to model manufacturing processes. Future applications could include other processes such as casting and forging.

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```

*****
*                               SECTION 11                               *
*   FERRITE & PEARLITE FORMATION FROM AUSTENITE                       *
*****
BAINSTART = 656.0 - 58.0*C(I) - 35.0*MN(I) - 75.0*SI(I) -
& 15.0*NI(I) - 34.0*CR(I) - 41.0*MO(I)
PEARLSTART = 723.0 - 10.7*MN(I) - 16.9*NI(I) + 29.0*SI(I) + 16.9*CR(I) +
& 290.0*AS(I) + 6.4*W(I)
IF ((COOLING .AND. ((PEARLSTART-T3) .GT. FUZ1)) .AND.
& ((AUSTX(I) .GT. 0.) .AND. ((T1-BAINSTART) .GT. FUZ1))) THEN
CALL STARTSTOPC(T3,T1,TIME3,TIME1,BAINSTART,PEARLSTART,
& TEMP,DELTATEMP,DELTATIME)

TIMEINC = 0.0001
TEMP1 = TEMP + DELTATEMP - DELTATEMP*(TIMEINC/DELTATIME)
TEMPINCP = PEARLSTART - TEMP1
TEMPINCF = AE3 - TEMP1
NTSTEPS = DELTATIME/TIMEINC
DO 80 J = 1,NTSTEPS
  IF (JUSTPEARL(I)) THEN
20    CALL PEARLITE (EQFERX,EQPEARLX,FIRSTPEARL(I),
&    PEARLX0,GRAINSIZE(I),TEMP1,TEMPINCP,TIMEINC,C(I),
&    R,CR(I),MO(I),NI(I),XP,AUSTX(I),PEARLX(I),DELTAXP,
&    WMX,BMX,MN(I),SI(I),V(I),W(I),CU(I),P(I),AL(I),AS(I),
&    TI(I),PEARLSTART,I,EQPEARLXT)
75    IF (PEARLX(I) .LT. EQPEARLXT) THEN
      IF (I.EQ.1) THEN
        DELTAPEARLX = DELTAXP * EQPEARLX * BMX
      ELSE
        DELTAPEARLX = DELTAXP * EQPEARLX * WMX
      ENDIF
      DHP = DELTAPEARLX * HFAP (-HFAF ?)
      PEARLX(I) = PEARLX(I) + DELTAPEARLX
      IF (I .EQ. 1) THEN
        IF ((PEARLX(I) + FERX(I)) .GE. BMX) THEN
          PEARLX(I) = BMX - FERX(I)
          AUSTX(I) = 0.0
          GOTO 60
        ELSE
          AUSTX(I) = BMX - (FERX(I) + PEARLX(I))
        ENDIF
      ELSE
        IF ((PEARLX(I) + FERX(I)) .GE. WMX) THEN
          PEARLX(I) = WMX - FERX(I)
          AUSTX(I) = 0.0
          GOTO 60
        ELSE
          AUSTX(I) = WMX - (FERX(I) + PEARLX(I))
        ENDIF
      ENDIF
      TEMP1 = TEMP1 - DELTATEMP*(TIMEINC/DELTATIME)
      TEMPINCP = PEARLSTART - TEMP1
      IF (PEARLX(I) .GT. 0.01) THEN
        JUSTPEARL(I) = .TRUE.
      ENDIF
    ELSE
      GOTO 80
    ENDIF
  ELSE
    CALL FERRITE(EQFERX,FIRSTFER(I),R,
&    NI(I),SI(I),V(I),MO(I),W(I),MN(I),CR(I),CU(I),
&    P(I),AL(I),AS(I),TI(I),C(I),TEMP1,TEMPINCF,TIMEINC,FERX0,
&    FERX(I),GRAINSIZE(I),DELTAXF,XF,PEARLSTART,I,WMX,BMX,G0)
    CALL PEARLITE (EQFERX,EQPEARLX,FIRSTPEARL(I),
&    PEARLX0,GRAINSIZE(I),TEMP1,TEMPINCP,TIMEINC,C(I),
&    R,CR(I),MO(I),NI(I),XP,AUSTX(I),PEARLX(I),DELTAXP,
&    WMX,BMX,MN(I),SI(I),V(I),W(I),CU(I),P(I),AL(I),AS(I),
&    TI(I),PEARLSTART,I,EQPEARLXT)
    IF (I .EQ. 1) THEN
      EQFERXT = EQFERX * BMX
    ELSE
      EQFERXT = EQFERX * WMX
    ENDIF
    IF (FERX(I) .GE. EQFERXT) THEN

```


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Appendix A

This appendix contains a listing of the FORTRAN program developed during this research which predicts the microstructure of a weld.

SUBROUTINE MICROSTRUC (T1,T3,TIME1,TIME3)

```
*****
*  PURPOSE: This program determines, at any given temperature *
*            and time, the volume phases of ferrite, pearlite, *
*            bainite, austenite, or martensite that are present, *
*            as well as determine the grain size and hardness. *
*            It also accounts for weld metal dilution. *
*****
```

```
*  INPUT:  1) The temperatures and times at the beginning (T1 and *
*            TIME1) and end (T3 and TIME3) of the interval. *
*            2) An input data file, containing the composition of *
*            the steel (and of the electrode), material data, *
*            grain growth parameters, and the welding conditions *
*            (the last is necessary in order to calculate the *
*            hardness based on R.O.M.). *
*****
```

```
LOGICAL COOLING, HEATING, FIRSTFER(2), FIRSTPEARL(2),
6 FIRSTGROW(2), JUSTPEARL(2), FIRSTBAIN(2)
```

```
INTEGER I, J
REAL
```

```
1 HFAF, HFAL, C(2), MN(2), SI(2), NI(2), CR(2), MO(2), CU(2),
2 S(2), P(2), AL(2), AS(2), W(2), V(2), FE(2), FUZ1, FUZ2,
3 PEARLSTART, A, B, AEXP, BEXP, CC, CM, GO, CARBAUST, CARBFER,
4 QOVRTT, DELTAG, DELTATIME, EQFERX, X, K1, DELTAX, BAINSTART,
5 MARSTART, AE3, EQPEARLX, FERX(2), PEARLX(2), BAINX(2), MARX(2),
6 AUSTX(2), GRAINSIZE(2), TI(2), XL, FERX0, PEARLX0, T1, T3, TIME1,
7 TIME3, DELTATEMP, TEMP, XP, XF, DELTAXP, DELTAXF, DELTAXE(2),
8 BMX, WMX, EQFERXT, TL, TS, XB(2), HV10(2), VFP, ENERGYIN
```

```
PARAMETER(FUZ1=1.0E-6, FUZ2=1.0E-6, R=1.987)
```

```
* DATA HFAF, HFAL/ 3.3E+08, 2.1E+09 /
```

```
* DATA MW / 12.01115, 54.939, 28.086, 51.996, 58.71, 95.94, 63.54,
* 1 32.064, 30.9738, 26.9815, 74.9216, 183.85, 50.942,
* 2 55.847/
```

```
* DATA / CARBON, MANGANESE, SILICON, NICKEL, CHROMIUM,
* 1 MOLYBDENUM, COPPER, SULFUR, PHOSPHORUS, ALUMINUM,
* 2 ARSENIC, TUNGSTEN, VANADIUM, IRON/
```

***** Dictionary

```
* ALL TEMPERATURES ARE IN DEGREES Celcius
* ALL FRACTIONS ARE WEIGHT FRACTIONS
*****
```

```
* A: precipitation parameter
* AE3: Temp. boundary between austenite+ferrite and aust. region
* AEXP: precipitation coefficient for metal
* AL: weight % of aluminum
* AS: weight % of Arsenic
* AUSTX: fraction of austenite
* B: precipitation parameter
* BAINSTART: bainite start temperature
* BAINX: fraction of bainite
* BEXP: precipitation coefficient for carbide or nitride
* BMX: fraction of material that is base metal (or HAZ)
* C: weight % of carbon
* CARBAUST: carbon content of austenite
* CARBFER: carbon content of ferrite
* CC: wt. % of carbide or nitride (calc of precip. temp.)
* CM: wt. % of metal (used in calc of precip. temp.)
* COOLING: logical, true if T3 > T1
* CR: wt. % of chromium
* CU: wt. % of copper
* DELTAG: change in grain size
```

```

* DELTATEMP: change of temperature
* DELTAX: change in fraction of given phase
* ENERGYIN: heat input = nVI/v, used in hardness calculation
* EQFERX: equilibrium fraction of ferrite
* EQPEARLX: equilibrium fraction of pearlite
* FE: weight % of Iron
* FERX: fraction of ferrite
* FERX0: initial fraction of ferrite (=1.0E-12)
* FIRSTBAIN: logical, true if no bainite has yet been formed
* FIRSTFER: logical, true if no ferrite has yet been formed
* FIRSTGROW: logical, true if no grain growth has occurred yet
* FIRSTPEARL: logical, true if no pearlite has yet been formed
* FUZ1: tolerance of zero 1
* FUZ2: tolerance of zero 2
* FERX0: initial fraction of ferrite
* G: ASTM grain size number
* G0: initial grain size (microns)
* GRAINSIZE: austenitic grain size (microns)
* HEATING: logical, true if T1 > T3
* HFAF: heat of formation from austenite to ferrite
* HFAL: heat of formation from austenite to liquid
* HV10: hardness, VPN, 10 kg load
* I: counter, I=1 refers to Base Metal, 2 to weld metal
* JUSTPEARL: logical, true if pearlite (no ferr.) is being formed
* K1: grain growth kinetic constant
* MARSTART: martensite start temperature
* MARX: fraction of martensite
* MN: weight % of magnesium
* MO: weight % of molybdenum
* NI: weight % of nickel
* PEARLSTART: pearlite start temperature
* PEARLX: fraction of pearlite
* PEARLX0: initial fraction of pearlite
* QOVERRT: Q/RT activation energy for grain growth
* R: gas constant, 1.987 cal/mol K
* T1: temperature at time 1 (degrees C) (last time step)
* T3: temperature at time 3 (degrees C) (this time step)
* TIME1: time at temp 1
* TIME3: time at temp 3
* TL: liquidus temperature
* TS: solidus temperature
* VFP: volume fraction of (ferrite + pearlite)
* W: weight % of tungsten
* WMX: fraction of material that is weld metal
* X: ratio of given phase to equil.fraction of same phase
* XL: fraction of liquid
*****

```

```

      OPEN(UNIT=20,ACCESS='DIRECT',FORM='UNFORMATTED',
&        STATUS='UNKNOWN',FILE='MICRO DATA',RECL=512)

```

```

      READ(UNIT=20,REC=1)C,MN,SI,NI,CR,MO,CU,S,P,AL,AS,W,V,TI,A,B,AEXP,
&        BEXP,G0,QOVERRT,K1,CC,CM,FERX0,PEARLX0,ENERGYIN
      READ(UNIT=20,REC=2)FERX,PEARLX,BAINX,MARX,XL,AUSTX,GRAINSIZE,
&        HV10,WMX,BMX,XB,DELTAXB, FIRSTFER,
&        FIRSTPEARL,JUSTPEARL,FIRSTGROW,FIRSTBAIN

```

```

      R is the gas constant

```

```

      HEATING = .FALSE.
      COOLING = .FALSE.
      IF (T3 .GT. T1) THEN
        HEATING = .TRUE.
      ELSE
        COOLING = .TRUE.
      ENDIF

```

```

      DO 500 I = 1,2

```

```

*****
      SECTION 4
      INITIALIZE STRUCTURE
*****

```

* The structure is initialized to ferrite and pearlite - *

* note that an initial temperature for any run (at any *

* node) must be less than PEARLSTART or else the program *

* will not run properly *

```

      IF (I.EQ. 1) THEN
        PEARLSTART=723.0-10.7*MN(I)-16.9*NI(I)+29.0*SI(I)+16.9*CR(I)+
&        290.0*AS(I)+6.4*W(I)
        IF (HEATING .AND. (PEARLSTART - T3).GT.FUZ1) THEN
          CALL INITIAL(C(I),FERX(I),PEARLX(I),PEARLSTART,
&          NI(I),SI(I),V(I),MO(I),W(I),MN(I),CR(I),
&          CU(I),P(I),AL(I),AS(I),TI(I))
        ENDIF
      ENDIF

```

SECTION 5

FORMATION OF AUSTENITE ON HEATING

```

      IF (I.EQ. 1) THEN
        AE3 = 910.0 - 203.0 * (C(I)**0.5) - 15.2*NI(I) + 44.7*SI(I) +
&        104.0*V(I) + 31.5*MO(I) + 13.1*W(I) - (30.0*MN(I) +11.0*CR(I)+
&        20.0*CU(I)-700.0*P(I)- 400.0*AL(I) - 120.0*AS(I)-400.0*TI(I))
        IF (HEATING .AND. ((T3-PEARLSTART).GT.FUZ1) .AND.
+        ((MARX(I)+FERX(I)+BAINX(I)).GT.FUZ2)) THEN
          PEARLX(I) = 0.0
          CALL FORMAUST(T3,AE3,NI(I),SI(I),V(I),MO(I),W(I),MN(I),CR(I),
+          CU(I),C(I),P(I),AL(I),AS(I),TI(I),FERX(I),AUSTX(I))
        ENDIF
      ENDIF

```

SECTION 6

GRAIN GROWTH OF AUSTENITE ON HEATING

```

      IF (I.EQ. 1) THEN
        TS = 1527. - 181.356 * C(I)
        TPRECIP = B/(A-LOG10( (CM*AEXP) * (CC**BEXP) ))
        TPRECIP = TPRECIP - 273.
        IF (HEATING .AND. ((T3-TPRECIP).GT.FUZ1) .AND.
&        (ABS(1.0-AUSTX(I)) .LT. FUZ2)) THEN
          CALL STARTSTOPH(T3,T1,TIME3,TIME1,TS,TPRECIP,DELTATIME,
&          DELTATEMP,TEMP)

```

* Since we are approximating an integral (for the grain growth

* relationship) with a series of time steps, we decrease the time

* step so that it is independent of T1 and T3, and we control the

* rate of change of grain size in any time step.

```

      TIMEINC = 0.01
      TEMP1 = TEMP - DELTATEMP + DELTATEMP * (TIMEINC/DELTATIME)

```

```

      DO 13 J = 1,100000

```

```

&      CALL GROWAUSTH (TIMEINC,K1,FERX(I),PEARLX(I),AUSTX(I),
&      GO,FIRSTGROW(I),QOVERRT,GRAINSIZE(I),R,TS,
&      TEMP1,DELTAG)

```

```

      IF ((DELTAG/GRAINSIZE(I)) .GT. 0.01) THEN
        TEMP1 = TEMP1 - DELTATEMP*(TIMEINC/DELTATIME) +
&        DELTATEMP*(TIMEINC*0.01/(DELTAG/GRAINSIZE(I)))/DELTATIME
&        TIMEINC = TIMEINC * (.01/(DELTAG/GRAINSIZE(I)))
        GOTO 23

```

```

      ELSE
        GRAINSIZE(I) = GRAINSIZE(I) + DELTAG

```

```

      ENDIF
      IF (TEMP1 .GE. TEMP) THEN
        GOTO 33

```

```

      ELSE
        TEMP1 = TEMP1 + DELTATEMP*(TIMEINC/DELTATIME)
        IF (TEMP1 .GT. TEMP) THEN
          GOTO 33

```

```

      ENDIF
    ENDIF

```

33 ENDIF
 ENDIF

* SECTION 7 *
* MELTING *

IF (I .EQ. 1) THEN
 TL = 1538. - 80.581 * C(I)
 IF (HEATING .AND. ((T3-TS) .GT. FUZ1) .AND.
 & (AUSTX(I) .GT. FUZ2)) THEN
 CALL MELTING(T3,XL,C(I),TL,AUSTX,GRAINSIZE,BMX,WMX)
 ENDIF
ENDIF

* SECTION 8 *
* SOLIDIFICATION *

IF (I .EQ. 1) THEN
*
* This is just a first approximation in order to get the code working
* since it is more exact to use different values of TS for the WM and
* for the HAZ - but it is much simpler to only include dilution after
* the HAZ and WM have completely solidified.
*

 TL = 1538. - 80.581 * C(I)
 IF (COOLING .AND. (XL.GT.FUZ1) .AND.
 & ((TL-T3) .GT. FUZ2)) THEN
 CALL SOLIDIFICATION(T3,TS,FUZ1,C(I),XL,AUSTX,GRAINSIZE,
 + BMX,WMX)
 ENDIF
ENDIF

* SECTION 9 *
* GRAIN GROWTH OF HAZ AUSTENITE ON COOLING *

IF (I .EQ. 1) THEN
 AE3 = 910.0 - 203.0 * (C(I)**0.5) - 15.2*NI(I) + 44.7*SI(I) +
 & 104.0*V(I) + 31.5*MO(I) + 13.1*W(I) - (30.0*MN(I) +11.0*CR(I)+
 & 20.0*CU(I)-700.0*P(I)- 400.0*AL(I) - 120.0*AS(I)-400.0*TI(I))
 TS = 1527. - 181.356 * C(I)
 IF (COOLING .AND. (((T3-AE3) .GT. FUZ1) .OR. ((T1-AE3) .GT.
 & FUZ1)) .AND. (XL .EQ. 0.0) .AND. (GRAINSIZE(I) .GT. FUZ1))
 & THEN
 CALL STARTSTOPC(T3,T1,TIME3,TIME1,AE3,TS,TEMP,DELTATEMP,
 & DELTATIME)
 TIMEINC = 0.01
 TEMP1 = TEMP + DELTATEMP - DELTATEMP * (TIMEINC/DELTATIME)
*
 DO 53 J = 1,100000
73 CALL GROWAUSTC(TIMEINC,K1,QOVERRT,GRAINSIZE(I),
 & TEMP1,DELTAG,R,TS)
 IF ((DELTAG/GRAINSIZE(I)) .GT. 0.01) THEN
 TEMP1 = TEMP1 + DELTATEMP*(TIMEINC/DELTATIME) -
 & DELTATEMP*(TIMEINC*0.01/(DELTAG/GRAINSIZE(I)))/DELTATIME
 TIMEINC = TIMEINC * (0.01/(DELTAG/GRAINSIZE(I)))
 GOTO 73
 ELSE
 GRAINSIZE(I) = GRAINSIZE(I) + DELTAG
 ENDIF
 IF (TEMP1 .LE. TEMP) THEN
 GOTO 63
 ELSE
 - TEMP1 = TEMP1 - DELTATEMP*(TIMEINC/DELTATIME)
 IF (TEMP1 .LT. TEMP) THEN
 GOTO 63
 ENDIF
 ENDIF
53 CONTINUE
63 ENDIF
ENDIF

SECTION 10

FERRITE FORMATION FROM AUSTENITE ABOVE PEARLSTART

```

AE3 = 910.0 - 203.0 * (C(I)**0.5) - 15.2*NI(I) + 44.7*SI(I) +
      104.0*V(I) + 31.5*MO(I) + 13.1*W(I) - (30.0*MN(I) + 11.0*CR(I)
      +20.0*CU(I) -700.0*P(I) -400.0*AL(I) -120.0*AS(I) - 400.0*TI(I))
PEARLSTART=723.0-10.7*MN(I)-16.9*NI(I)+29.0*SI(I)+16.9*CR(I)+
      290.0*AS(I)+6.4*W(I)
IF ( COOLING .AND. ((AE3-T3) .GT. FUZ1) .AND. ((T1-PEARLSTART)
      .GT. FUZ1) .AND. (AUSTX(I) .GT. 0.) ) THEN
      CALL STARTSTOPC(T3,T1,TIME3,TIME1,PEARLSTART,AE3,TEMP,
      DELTATEMP,DELTATIME)

```

```

TIMEINC = 0.0001
TEMP1 = TEMP + DELTATEMP - DELTATEMP*(TIMEINC/DELTATIME)
TEMPINC = AE3 - TEMP1
NTSTEPS = DELTATIME/TIMEINC

```

* Explanation of the following code: even though we use STARTSTOPC
 * to determine the values of DELTATEMP, DELTATIME, and TEMP corres-
 * ponding to this time step, the nature of the equation $\Delta X = \dots$
 * $\dots X(1-X) \dots$ makes it necessary to use smaller time and temperature
 * increments than those that are likely sent by the calling program.
 * This in turn will allow us to predict realistic phase fractions.
 * We control the iteration by placing an upper limit on the size of
 * the time steps (the variable TIMEINC) used during any temperature
 * increment.

```
DO 10 J = 1,NTSTEPS
```

```

22      CALL FERRITE(EQFERX,FIRSTFER(I),R,
      &      NI(I),SI(I),V(I),MO(I),W(I),MN(I),CR(I),CU(I),
      &      P(I),AL(I),AS(I),TI(I),C(I),TEMP1,TEMPINC,TIMEINC,FERX0,
      &      FERX(I),GRAINSIZE(I),DELTAXF,XF,PEARLSTART,I,WMX,BMX,G0)

```

```

      IF (I .EQ. 1) THEN
          EQFERXT = EQFERX * BMX
      ELSE
          EQFERXT = EQFERX * WMX
      ENDIF

```

```

      IF (FERX(I) .LT. EQFERXT) THEN
          IF (I.EQ.1) THEN
              DELTA FERX = DELTAXF * EQFERX * BMX
          ELSE
              DELTA FERX = DELTAXF * EQFERX * WMX
          ENDIF

```

```

      DHF = DELTA FERX * HFAF
      FERX(I) = FERX(I) + DELTA FERX
      IF (I .EQ. 1) THEN
          IF (FERX(I) .GE. BMX) THEN
              FERX(I) = BMX
              AUSTX(I) = 0.0
              GOTO 40

```

```

          ELSE
              AUSTX(I) = BMX - FERX(I)
          ENDIF

```

```

      ELSE
          IF (FERX(I) .GE. WMX) THEN
              FERX(I) = WMX
              AUSTX(I) = 0.0
              GOTO 40

```

```

          ELSE
              AUSTX(I) = WMX - FERX(I)
          ENDIF

```

```

      ENDIF
      TEMP1 = TEMP1 - DELTATEMP*(TIMEINC/DELTATIME)
      TEMPINC = AE3 - TEMP1

```

```

      ELSE
          TEMP1 = TEMP1 - DELTATEMP*(TIMEINC/DELTATIME)
          TEMPINC = AE3 - TEMP1

```

```
      ENDIF
```

```

10      CONTINUE
40      ENDIF

```

```

*****
*                               SECTION 11                               *
*                               FERRITE & PEARLITE FORMATION FROM AUSTENITE *
*****
BAINSTART = 656.0 - 58.0*C(I) - 35.0*MN(I) - 75.0*SI(I) -
& 15.0*NI(I) - 34.0*CR(I) - 41.0*MO(I)
PEARLSTART = 723.0 - 10.7*MN(I) - 16.9*NI(I) + 29.0*SI(I) + 16.9*CR(I) +
& 290.0*AS(I) + 6.4*W(I)
IF ((COOLING .AND. ((PEARLSTART-T3) .GT. FUZ1)) .AND.
& ((AUSTX(I) .GT. 0.) .AND. ((T1-BAINSTART) .GT. FUZ1))) THEN
& CALL STARTSTOPC(T3,T1,TIME3,TIME1,BAINSTART,PEARLSTART,
& TEMP,DELTATEMP,DELTATIME)

TIMEINC = 0.0001
TEMP1 = TEMP + DELTATEMP - DELTATEMP*(TIMEINC/DELTATIME)
TEMPINCP = PEARLSTART - TEMP1
TEMPINCF = AE3 - TEMP1
NTSTEPS = DELTATIME/TIMEINC
DO 80 J = 1,NTSTEPS
  IF (JUSTPEARL(I)) THEN
20 CALL PEARLITE (EQFERX,EQPEARLX,FIRSTPEARL(I),
& PEARLX0,GRAINSIZE(I),TEMP1,TEMPINCP,TIMEINC,C(I),
& R,CR(I),MO(I),NI(I),XP,AUSTX(I),PEARLX(I),DELTAXP,
& WMX,BMX,MN(I),SI(I),V(I),W(I),CU(I),P(I),AL(I),AS(I),
& TI(I),PEARLSTART,I,EQPEARLXT)
75 IF (PEARLX(I) .LT. EQPEARLXT) THEN
  IF (I.EQ.1) THEN
    DELTAPEARLX = DELTAXP * EQPEARLX * BMX
  ELSE
    DELTAPEARLX = DELTAXP * EQPEARLX * WMX
  ENDIF
  DHP = DELTAPEARLX * HFAP (=HFAF ?)
  PEARLX(I) = PEARLX(I) + DELTAPEARLX
  IF (I .EQ. 1) THEN
    IF ((PEARLX(I) + FERX(I)) .GE. BMX) THEN
      PEARLX(I) = BMX - FERX(I)
      AUSTX(I) = 0.0
      GOTO 60
    ELSE
      AUSTX(I) = BMX - (FERX(I) + PEARLX(I))
    ENDIF
  ELSE
    IF ((PEARLX(I) + FERX(I)) .GE. WMX) THEN
      PEARLX(I) = WMX - FERX(I)
      AUSTX(I) = 0.0
      GOTO 60
    ELSE
      AUSTX(I) = WMX - (FERX(I) + PEARLX(I))
    ENDIF
  ENDIF
  TEMP1 = TEMP1 - DELTATEMP*(TIMEINC/DELTATIME)
  TEMPINCP = PEARLSTART - TEMP1
  IF (PEARLX(I) .GT. 0.01) THEN
    JUSTPEARL(I) = .TRUE.
  ENDIF
  ELSE
    GOTO 80
  ENDIF
  ELSE
    CALL FERRITE(EQFERX,FIRSTFER(I),R,
& NI(I),SI(I),V(I),MO(I),W(I),MN(I),CR(I),CU(I),
& P(I),AL(I),AS(I),TI(I),C(I),TEMP1,TEMPINCF,TIMEINC,FERX0,
& FERX(I),GRAINSIZE(I),DELTAXF,XF,PEARLSTART,I,WMX,BMX,G0)
    CALL PEARLITE (EQFERX,EQPEARLX,FIRSTPEARL(I),
& PEARLX0,GRAINSIZE(I),TEMP1,TEMPINCP,TIMEINC,C(I),
& R,CR(I),MO(I),NI(I),XP,AUSTX(I),PEARLX(I),DELTAXP,
& WMX,BMX,MN(I),SI(I),V(I),W(I),CU(I),P(I),AL(I),AS(I),
& TI(I),PEARLSTART,I,EQPEARLXT)
    IF (I .EQ. 1) THEN
      EQFERXT = EQFERX * BMX
    ELSE
      EQFERXT = EQFERX * WMX
    ENDIF
    IF (FERX(I) .GE. EQFERXT) THEN

```



```

GOTO 75
ELSE
  IF (PEARLX(I) .GE. EQPEARLXT) THEN
    GOTO 41
  ELSE
    FERXOLD = FERX(I)
    IF (I.EQ.1) THEN
      DELTAFERX = DELTAXF * EQFERX * BMX
      DELTAPEARLX = DELTAXP * EQPEARLX * BMX
    ELSE
      DELTAFERX = DELTAXF * EQFERX * WMX
      DELTAPEARLX = DELTAXP * EQPEARLX * WMX
    ENDIF
    DHF = DELTAFERX * HFAF
    DHP = DELTAPEARLX * HFAP
    FERX(I) = FERX(I) + DELTAFERX
    PEARLX(I) = PEARLX(I) + DELTAPEARLX

    IF (PEARLX(I) .GT. 0.01) THEN
      calculate ferrite formed up to 0.01 pearlite - note that once
      we have formed 1% (or .01) pearlite than ferrite no longer
      forms ( i.e. JUSTPEARL = .TRUE.)

      FERX(I) = FERXOLD + (FERX(I) - FERXOLD) *
        0.01/PEARLX(I)
      JUSTPEARL(I) = .TRUE.
      IF (I .EQ. 1) THEN
        AUSTX(I) = BMX - (FERX(I) + PEARLX(I))
      ELSE
        AUSTX(I) = WMX - (FERX(I) + PEARLX(I))
      ENDIF
      IF (AUSTX(I) .LT. 0.0) THEN
        AUSTX(I) = 0.0
        GO TO 60
      ENDIF
    ELSE
      IF (I .EQ. 1) THEN
        IF ((FERX(I) + PEARLX(I)) .GE. BMX) THEN
          FERX(I) = BMX * FERX(I) / (FERX(I) + PEARLX(I))
          PEARLX(I) = BMX * PEARLX(I) / (PEARLX(I) +
            FERX(I))
          AUSTX(I) = 0.0
          GOTO 60
        ELSE
          AUSTX(I) = BMX - (FERX(I) + PEARLX(I))
        ENDIF
      ELSE
        IF ((FERX(I) + PEARLX(I)) .GE. WMX) THEN
          FERX(I) = WMX * FERX(I) / (FERX(I) + PEARLX(I))
          PEARLX(I) = WMX * PEARLX(I) / (PEARLX(I) +
            FERX(I))
          AUSTX(I) = 0.0
          GOTO 60
        ELSE
          AUSTX(I) = WMX - (FERX(I) + PEARLX(I))
        ENDIF
      ENDIF
    ENDIF
  ENDIF
  TEMP1 = TEMP1 - DELTATEMP*(TIMEINC/DELTATIME)
  TEMPINCF = AE3 - TEMP1
  TEMPINCP = PEARLSTART - TEMP1
ENDIF
ENDIF
ENDIF
80 CONTINUE
60 ENDIF

```

 * SECTION 12 *
 * BAINITE FORMATION FROM AUSTENITE *

BAINSTART = 656.0 - 58.0*C(I) - 35.0*MN(I) - 75.0*SI(I) -
 15.0*NI(I) - 34.0*CR(I) - 41.0*MO(I)

```

MARSTART = 561.0 - 474.0*C(I) - 35.0*MN(I) - 17.0*NI(I) -
17.0*CR(I) - 21.0*MO(I)
IF (COOLING .AND. (BAINSTART .GT. T3) .AND. (T1 .GT. MARSTART)
.AND. (AUSTX(I) .GT. 0.) .AND. (PEARLX(I) .GT. 0.)) THEN
CALL STARTSTOPC(T3,T1,TIME3,TIME1,MARSTART,BAINSTART,TEMP,
DELTATEMP,DELTATIME)
TIMEINC = 0.0001
TEMP1 = TEMP + DELTATEMP - DELTATEMP*(TIMEINC/DELTATIME)
TEMPINC = BAINSTART - TEMP1
NTSTEPS = DELTATIME/TIMEINC
DO 100 J = 1,NTSTEPS
CALL BAINITE (PEARLX(I),R,TEMP1,TEMPINC,TIMEINC,
GRAINSIZE(I),C(I),CR(I),MO(I),MN(I),NI(I),BAINX(I),
AUSTX(I),DELTAXB(I),FIRSTBAIN(I),XB(I))
IF (I .EQ. 1) THEN
DELTAXB(I) = DELTAXB(I) * BMX
ELSE
DELTAXB(I) = DELTAXB(I) * WMX
ENDIF
DHB = DELTAXB(I) * HFAB (?)
BAINX(I) = BAINX(I) + DELTAXB(I)
IF (I .EQ. 1) THEN
IF ((FERX(I) + PEARLX(I) + BAINX(I)) .GE. BMX) THEN
BAINX(I) = BMX - (FERX(I) + PEARLX(I))
AUSTX(I) = 0.
GOTO 120
ELSE
AUSTX(I) = BMX - (FERX(I) + PEARLX(I) + BAINX(I))
ENDIF
ELSE
IF ((FERX(I) + PEARLX(I) + BAINX(I)) .GE. WMX) THEN
BAINX(I) = WMX - (FERX(I) + PEARLX(I))
AUSTX(I) = 0.
GOTO 120
ELSE
AUSTX(I) = WMX - (FERX(I) + PEARLX(I) + BAINX(I))
ENDIF
ENDIF
TEMP1 = TEMP1 - DELTATEMP*(TIMEINC/DELTATIME)
TEMPINC = BAINSTART - TEMP1
100 CONTINUE
120 ENDIF

```

```

*****
*                               *
*               SECTION 13      *
*   MARTENSITE FORMATION FROM AUSTENITE   *
*****
* This code assumes an instantaneous transformation to marten- *
* site below the Ms (or MARSTART) temperature. If equations *
* are made available to reliably predict the Mf (martensite *
* finish) temperature then it could be easily added to the *
* code. *
*****
IF (COOLING .AND. ((MARSTART-T3) .GT. FUZ1) .AND.
(AUSTX(I) .GT. 0.0)) THEN
CALL MARTENSITE (FERX(I),PEARLX(I),AUSTX(I),
BAINX(I),MARX(I),I,WMX,BMX)
ENDIF

```

```

*****
*                               *
*               SECTION 14      *
*   HARDNESS CALCULATION        *
*****
IF (COOLING .AND. (AUSTX(I) .EQ. 0.0) .AND.
(HV10(I) .EQ. 0.)) THEN
CALL HARDNESS(FERX(I),PEARLX(I),BAINX(I),MARX(I),
HV10(I),C(I),MN(I),NI(I),SI(I),CR(I),
MO(I),V(I),ENERGYIN,BMX,WMX,I)
ENDIF
500 CONTINUE

```

```

*   if (first time doing this calculation for any given node) ,THEN
IF (FIRSTGROW) THEN
    FIRSTGROW = FALSE.
    FERX = 0.
    PEARLX = 0
    AUSTX = 1
    GRAINSIZE = G0
ENDIF
DELTAG = (1.0/(2.0*GRAINSIZE)) * (K1*(EXP(-(Q/(R *
&      (TEMP1+273)))))) * TIMEINC

RETURN
END

```

SUBROUTINE MELTING(T3,XL,C,TL,AUSTX,GRAINSIZE,BMX,WMX)

```

*
* Input Data - T3, XL, C
*
* Output Data - XL, AUSTX, WMX, BMX
*
* Local Variables - CARBS, CARBL

*   global input variables
REAL
1   T3, C, TL
*   global output variables
REAL
1   XL, AUSTX(2), GRAINSIZE(2), BMX, WMX
*   local variables
REAL
1   CARBS, CARBL,XL3

IF (T3 .GE. TL) THEN
*   if the temperature is greater than the liquidus temperature then the
*   node/point is assigned to be completely in the weld metal.

    XL = 1.0
    AUSTX(1) = 0.0
    GRAINSIZE(1) = 0.
    GRAINSIZE(2) = 175.
    WMX = 1.0
    BMX = 0.0
ELSE
*   if the temperature is between the solidus and the liquidus then use
*   the lever law (with the equations of the liquidus and solidus) to
*   determine the fraction of liquid.

    CARBS = (1527.0 - T3)/181.356
    CARBL = (1538.0 - T3)/80.581

    XL3 = (C-CARBS)/(CARBL-CARBS)
    AUSTX(1) = 1.0 - XL3
    DHFAL = (XL3-XL) * HFAL
    XL = XL3
    WMX = XL
    BMX = 1 - XL
    GRAINSIZE(2) = 175.
ENDIF

RETURN
END

```

```

*
* temporary write of data for debugging purpose (this writes the
* data to the screen after every time step)
*

```

```

      WRITE(*,150) TIME3, T3, FERX, PEARLX, BAINX, MARX, XL, AUSTX,
+      GRAINSIZE, HV10, WMX, BMX
150  FORMAT(1X,6F12.6,/,1X,7F12.6)
      PRINT*, '

```

```

*
* save new data in unit 20

```

```

      WRITE(UNIT=20,REC=2) FERX, PEARLX, BAINX, MARX, XL, AUSTX, GRAINSIZE,
&      HV10, WMX, BMX, XB, DELTAXB, FIRSTFER,
&      FIRSTPEARL, JUSTPEARL, FIRSTGROW, FIRSTBAIN

      CLOSE(UNIT=20)
      RETURN
      END

```

```

      SUBROUTINE STARTSTOPH(T3,T1,TIME3,TIME1,T5,T4,DELTATIME,
&      DELTATEMP,TEMP)

```

```

*
* global input variables
*   REAL T1, T3, TIME1, TIME3, T4, T5
* global output variables
*   REAL DELTATIME, DELTATEMP, TEMP
* local variables
*   REAL TIME5, TIME4

      IF (T3 .LE. T5) THEN
        TIME5 = TIME3
      ELSE
        TIME5 = ((T1-T5)/(T1-T3))*(TIME3-TIME1)+TIME1
      ENDIF
      IF (T4 .LE. T1) THEN
        TIME4 = TIME1
      ELSE
        TIME4 = ((T4-T1)/(T3-T1))*(TIME3-TIME1)+TIME1
      ENDIF
      DELTATIME = TIME5-TIME4

*
      IF ((T1.GT.T4) .AND. (T3.LT.T5)) THEN
        DELTATEMP = (T3 - T1)
      ELSE
        IF ((T1.GT.T4) .AND. (T3.GE.T5)) THEN
          DELTATEMP = T5 - T1
        ELSE
          IF ((T1.LE.T4) .AND. (T3.LT.T5)) THEN
            DELTATEMP = T3 - T4
          ELSE
            DELTATEMP = T5 - T4
          ENDIF
        ENDIF
      ENDIF

*
      IF (T3 .LT. T5) THEN
        TEMP = T3
      ELSE
        TEMP = T5
      ENDIF

*
      RETURN
      END

```

```
SUBROUTINE STARTSTOPC(T3,T1,TIME3,TIME1,T5,T4,TEMP,DELTATEMP,
DELTATIME)
```

Purpose: since the phase transformations (and grain growth) start and finish at specific temperatures, it is necessary to have an interpolation routine which determines at what time in a thermal cycle these temperatures are reached.

global input variables

```
REAL T1, T3, TIME1, TIME3, T4, T5
```

global output variables

```
REAL TEMP, DELTATEMP, DELTATIME
```

local variables

```
REAL TIME4, TIME5
```

```
IF (T5 .LE. T3) THEN
```

```
TIME5 = TIME3
```

```
ELSE
```

```
TIME5 = ((T1-T5)/(T1-T3))*(TIME3-TIME1)+TIME1
```

```
ENDIF
```

```
IF (T1 .LE. T4) THEN
```

```
TIME4 = TIME1
```

```
ELSE
```

```
TIME4 = ((T4-T1)/(T3-T1))*(TIME3-TIME1)+TIME1
```

```
ENDIF
```

```
DELTATIME = TIME5-TIME4
```

```
IF ((T1 .LE. T4) .AND. (T3 .GE. T5)) THEN
```

```
DELTATEMP = ABS(T3 - T1)
```

```
ELSE
```

```
IF ((T1 .LE. T4) .AND. (T3 .LT. T5)) THEN
```

```
DELTATEMP = ABS(T5 - T1)
```

```
ELSE
```

```
IF ((T1 .GT. T4) .AND. (T3 .GE. T5)) THEN
```

```
DELTATEMP = ABS(T3 - T4)
```

```
ELSE
```

```
DELTATEMP = ABS(T5 - T4)
```

```
ENDIF
```

```
ENDIF
```

```
ENDIF
```

```
IF (T3 .LT. T5) THEN
```

```
TEMP = T5
```

```
ELSE
```

```
TEMP = T3
```

```
ENDIF
```

```
RETURN
```

```
END
```

```
SUBROUTINE INITIAL(C,FERX,PEARLX,PEARLSTART,
NI,SI,V,MO,W,MN,CR,CU,P,AL,AS,TI)
```

*Determine Initial Structure - as ferrite fraction and pearlite fraction

*Input Data : C

*Output Data: FERX, PEARLX

* global input variables

```
REAL C
```

* global output variables

```
REAL FERX, PEARLX
```

```
CARBAUST =
```

```
+ (910.0-15.2*NI+44.7*SI+104.0*V+315.0*MO+13.1*W -
```

```
+ (30.0*MN+11.0*CR+20.0*CU-700.0*P-400.0*AL-
```

```
+ 120.0*AS-400.0*TI)-PEARLSTART)**2.0/203.0**2.0
```

```
FERX = (CARBAUST - C)/(CARBAUST - 0.022)
```

```
PEARLX = .1.0 - FERX
```

RETURN
END

SUBROUTINE FORMAUST(T3,AE3,NI,SI,V,MO,W,MN,CR,CU,
C,P,AL,AS,TI,FERX,AUSTX)

* Input Data - T3,NI,SI,V,MO,W,MN,CR,CU,P,AL,AS,TI
* Output Data - FERX,AUSTX
* Local Variables - CARBFER,CARBAUST
*
* global input variables
REAL
1 T3, NI, SI, V, MO, W, MN, CR, CU, P, AL, AS, TI, C, AE3
* global output variables
REAL
1 FERX, AUSTX
* local variables
REAL
1 CARBFER, CARBAUST

IF (T3 .GE. AE3) THEN
AUSTX = 1.0
FERX = 0.0
ELSE
CARBAUST=
+ (910.0-15.2*NI+44.7*SI+104.0*V+315.0*MO+13.1*W -
+ (30.0*MN+11.0*CR+20.0*CU-700.0*P-400.0*AL-
+ 120.0*AS-400.0*TI)-T3)**2.0/203.0**2.0
CARBFER = 0.105 - 115.3E-6*T3
FERX=(CARBAUST-C)/(CARBAUST-CARBFER)
AUSTX=1.0-FERX
ENDIF
RETURN
END

SUBROUTINE GROWAUSTH (TIMEINC,K1,FERX,PEARLX,AUSTX,G0,
& FIRSTGROW,QOVERRT,GRAINSIZE,R,TS,
& TEMP1,DELTAG)

* Input Data - DELTATIME, K1, QOVERRT, FERX, PEARLX, G0

* Note: CM is the concentration (wt. %) of metal species, and CC is
* the concentration of non-metal species - i.e. for NbC precipitates
* - CC = C and CM = Nb, and a = AEXP and b = BEXP. Also QOVERRT = Q/RT

* global input variables
LOGICAL FIRSTGROW
REAL
1 TIMEINC,TEMP1, K1, QOVERRT, R, TS, GRAINSIZE
* global output variables
REAL
1 FERX, PEARLX, AUSTX, DELTAG
* local input variables
REAL
1 Q

Q = QOVERRT * R * (TS + 273)

```

*   if (first time doing this calculation for any given node) ,THEN
IF (FIRSTGROW) THEN
  FIRSTGROW = .FALSE.
  FERX = 0.
  PEARLX = 0.
  AUSTX = 1.
  GRAINSIZE = G0
ENDIF
DELTAG = (1.0/(2.0*GRAINSIZE)) * (K1*(EXP(-(Q/(R *
  (TEMP1+273)))))) * TIMEINC

RETURN
END

```

SUBROUTINE MELTING(T3,XL,C,TL,AUSTX,GRAINSIZE,BMX,WMX)

```

*
* Input Data - T3, XL, C
*
* Output Data - XL, AUSTX, WMX, BMX
*
* Local Variables - CARBS, CARBL
*

```

```

* global input variables
  REAL
  1 T3, C, TL
* global output variables
  REAL
  1 XL, AUSTX(2), GRAINSIZE(2), BMX, WMX
* local variables
  REAL
  1 CARBS, CARBL,XL3

```

```

  IF (T3 .GE. TL) THEN

```

```

* if the temperature is greater than the liquidus temperature then the
* node/point is assigned to be completely in the weld metal.

```

```

  XL = 1.0
  AUSTX(1) = 0.0
  GRAINSIZE(1) = 0.
  GRAINSIZE(2) = 175.
  WMX = 1.0
  BMX = 0.0

```

```

ELSE

```

```

* if the temperature is between the solidus and the liquidus then use
* the lever law (with the equations of the liquidus and solidus) to
* determine the fraction of liquid.

```

```

  CARBS = (1527.0 - T3)/181.356
  CARBL = (1538.0 - T3)/80.581

```

```

  XL3 = (C-CARBS)/(CARBL-CARBS)
  AUSTX(1) = 1.0 - XL3
  DHFAL = (XL3-XL) * HFAL
  XL = XL3
  WMX = XL
  BMX = 1 - XL
  GRAINSIZE(2) = 175.

```

```

ENDIF

```

```

RETURN
END

```

SUBROUTINE SOLIDIFICATION(T3,TS,FUZ1,C,XL,AUSTX,GRAINSIZE,
BMX,WMX)

* global input variables

REAL

1 T3, C, FUZ1, TS

* global output variables

REAL

1 AUSTFZX, XL, GRAINSIZE(2), AUSTX(2)

* local variables

REAL

1 CARBS, CARBL, XL3

* At a given point austenite inside the two phase mushy region is of two
* types, weld metal austenite which is associated with the fraction
* that is liquid, and HAZ austenite which is associated with the solid
* phase. As well, points/nodes inside the two phase region will
* have two grain sizes associated with them - an GRAINSIZE which
* is computed IN THE SECTION ON GRAIN GROWTH DURING COOLING and a FZ
* grain size which is SET TO 175 microns (ASTM 2) in the previous section
* since the previous section checks that the fraction of liquid is between
* 0 and 1.

IF ((T3 .GT. TS) .AND. (T3 .LT. TL)) THEN

* when solidifying, if the temperature is between the solidus and the liquidus,
* we determine the amount of liquid using the lever law, and compute the increment
* in the amount of weld metal austenite (AUSTX(2))

CARBS = (1527.0 - T3) / 181.356

CARBL = (1538.0 - T3) / 80.581

XL3 = (C - CARBS) / (CARBL - CARBS)

AUSTX(2) = AUSTX(2) + (XL - XL3)

XL = XL3

ELSE

IF (T3 .LT. TS) THEN

XL3 = 0.

AUSTX(2) = AUSTX(2) + (XL - XL3)

XL = 0.

ENDIF

ENDIF

RETURN

END

SUBROUTINE GROWAUSTC (TIMEINC,K1,QOVERRT,GRAINSIZE,
TEMP1,DELTA G,R,TS)

* Using the above condition AUSTX = 1.0 we assume that even for nodes
* /points in the mushy region - to which we assigned to be fusion zone
* austenite (AUSTX) - the array containing AUSTX for these nodes
* /points was not zeroed when they entered the mushy region since we
* want to do a grain growth calculation which will be associated with
* the 'solid' part of the region.

* global input variables

REAL

1 TIMEINC,TEMP1, K1, QOVERRT, R, TS, GRAINSIZE

* global output variables

REAL

1 DELTAG

* local input variables

REAL

1 Q

Q = QOVERPT * R * (TS + 273)

DELTA G = (1.0/(2.0*GRAINSIZE)) * (K1*(EXP(-(Q/(R * (TEMP1 + 273)))))) * TIMEINC

RETURN
END

SUBROUTINE FERRITE (EQFERX, FIRSTFER, R,
NI, SI, V, MO, W, MN, CR, CU, P, AL, AS, TI, C,
TEMP1, TEMPINC, TIMEINC, FERX0, FERX,
GRAINSIZE, DELTAX, X, PEARLSTART, I, WMX, BMX, G0)

* Note: the grain size has previously been calculated as g in microns
* The equation below needs the ASTM grain size number using the
* following conversion: 1 micron = 1/(1000*25.4) inches. Therefore
* there are 25400/g grains in one inch, or (25400/g)**2 in 1 sq.in.,
* or (25400/g)**2 * 1E-4 grains/sq.in at 100X = N = 2 ** (G-1).

* R is the gas constant = 1.987 cal/kg K

* global input variables

LOGICAL FIRSTFER

INTEGER I

REAL

1 TIMEINC, GRAINSIZE, EQFERX, MN, NI, CR,

2 MO, W, CU, AL, AS, TI, C, V, P, EQFERXT,

3 FERX0, R, TEMPINC, TEMP1, PEARLSTART, WMX, BMX

* global output variables

REAL FERX, X, DELTAX

* local variables

REAL

1 COMPFAC, XFAC, EXPFAC, CARBAUST, CARBFER, G

IF (TEMP1 .LT. PEARLSTART) THEN

* this is using the fact that if the temperature falls below the
* pearlite start temperature, the carbon content of the austenite
* will be the value that it is at pearlite start, and the carbon
* content of the ferrite will decrease linearly (to 0.0 at 20 C).

CARBAUST =

+ (910.0-15.2*NI+44.7*SI+104.0*V+315.0*MO+13.1*W -

+ (30.0*MN+11.0*CR+20.0*CU-700.0*P-400.0*AL-

+ 120.0*AS-400.0*TI)-PEARLSTART)**2.0/203.0**2.0

CARBFER = ((TEMP1-20.)/(PEARLSTART-20.)) * (0.105 -
+ 115.3E-6*PEARLSTART)

ELSE

CARBAUST=

+ (910.0-15.2*NI+44.7*SI+104.0*V+315.0*MO+13.1*W -

+ (30.0*MN+11.0*CR+20.0*CU-700.0*P-400.0*AL-

+ 120.0*AS-400.0*TI)-TEMP1)**2.0/203.0**2.0

CARBFER = 0.105 - 115.3E-6*TEMP1

ENDIF

EQFERX = (CARBAUST - C) / (CARBAUST - CARBFER)

IF (I .EQ. 1) THEN

EQFERXT = EQFERX * BMX

ELSE

EQFERXT = EQFERX * WMX

ENDIF

```
IF (FERX .LT. EQFERXT) THEN
```

```
  IF (FIRSTFER) THEN  
    FIRSTFER = .FALSE.  
    IF (FERX .EQ. 0.0) THEN  
      FERX = FERX0  
    ENDIF  
    IF (GRAINSIZE .EQ. 0.0) THEN
```

```
* this piece of code is necessary since if the temperature does not go above  
* the precipitation temperature then the grain size will still be set to zero -  
* therefore we will use the initial grain size in this case.
```

```
      GRAINSIZE = G0  
    ENDIF  
  ENDIF
```

```
  X = FERX / EQFERXT
```

```
  G = 1.0 + 1.44 * (LOG ((25.4/GRAINSIZE)**2.0 * 100.0))
```

```
  COMPFAC = 59.6*MN + 1.45*NI + 67.7*CR + 244*MO
```

```
  XFAC = X**(2*(1-X)/3) * (1-X)**((2*X)/3)
```

```
  EXPFAC = EXP(-(23500./(R*(TEMP1+273.))))
```

```
  DELTAX = ((2.0**((G-1.0)/2.0) * (TEMPINC)**3.0 *  
    EXPFAC * XFAC) / COMPFAC) * (TIMEINC)
```

```
  ENDIF  
  RETURN  
  END
```

```
* IF (GRAINSIZE .EQ. 0.0) THEN  
* GRAINSIZE = G0
```

```
* this piece of code is necessary since if the temperature does not go above  
* the precipitation temperature then the grain size will still be set to zero -  
* therefore we will use the initial grain size in this case.
```

```
  SUBROUTINE PEARLITE (EQFERX,EQPEARLX,FIRSTPEARL,  
    & PEARLX0,GRAINSIZE,TEMP1,TEMPINC,TIMEINC,C,  
    & R,CR,MO,NI,X,AUSTX,PEARLX,DELTAX,WMX,BMX,  
    & MN,SI,V,W,CU,P,AL,AS,TI,PEARLSTART,I,EQPEARLXT)
```

```
* global input variables  
  LOGICAL FIRSTPEARL  
  INTEGER I
```

```
  REAL
```

```
  1 DELTATEMP, DELTATEMP, CR, MO, NI, R, X, GRAINSIZE,  
  2 EQFERX, EQPEARLX, PEARLX0, TEMP1, MN
```

```
* global output variables
```

```
  REAL AUSTX, PEARLX, AUSTFZX
```

```
* local variables
```

```
  REAL
```

```
  1 G, EXPFAC1, EXPFAC2, DP, COMPFAC, XFAC, DELTAX, CARBAUST,  
  2 CARBFER
```

```
  CARBAUST =
```

```
  + (910.0-15.2*NI+44.7*SI+104.0*V+315.0*MO+13.1*W -
```

```
  + (30.0*MN+11.0*CR+20.0*CU-700.0*P-400.0*AL-
```

```
  + 120.0*AS-400.0*TI)-PEARLSTART)**2.0/203.0**2.0
```

```
  + CARBFER = ((TEMP1-20.)/(PEARLSTART-20.)) * (0.105 -  
  + 115.3E-6*PEARLSTART)
```

EQFERX = (CARBAUST - C) / (CARBAUST - CARBFER)

EQPEARLX = 1.0 - EQFERX

IF (I.EQ. 1) THEN

EQPEARLXT = EQPEARLX * BMX

ELSE

EQPEARLXT = EQPEARLX * WMX

ENDIF

IF (PEARLX.LT. EQPEARLXT) THEN

IF (FIRSTPEARL) THEN

FIRSTPEARL = .FALSE.

PEARLX = PEARLX0

ENDIF

X = PEARLX / EQPEARLXT

* grainsize calculation:

G = 1.0 + 1.44 * (LOG ((25.4/GRAINSIZE)**2.0 * 100.0))

EXPFAC1 = EXP(-(27500.0/(R*(TEMP1+273.))))

EXPFAC2 = EXP(-(37000.0/(R*(TEMP1+273.))))

DP = ((1.0/EXPFAC1) + (.01*CR + 0.52*MO)/EXPFAC2)
** (-1.0)

COMPFAC = 1.79 + 5.42*(CR + MO + 4.0*MO*NI)

XFAC = X**(2.0*(1.0-X)/3.0) * (1.0-X)**((2.0*X)/3.0)

DELTAX = ((2.0**((G-1.0)/2.0) *

(TEMPINC)**3.0 * DP) / COMPFAC) * XFAC * TIMEINC

ENDIF

RETURN

END

SUBROUTINE BAINITE (PEARLX,R,TEMP1,TEMPINC,TIMEINC,
GRAINSIZE,C,CR,MO,MN,NI,BAINX,AUSTX,DELTAX,
FIRSTBAIN,X)

* global input variables

LOGICAL

1 FIRSTBAIN

REAL

1 DELTATIME, DELTATEMP, C, CR, MN, MO, NI, R, GRAINSIZE,

2 PEARLX, TEMP

* global output variables

REAL

1 BAINX, AUSTX, DELTAX

* local variables

REAL

1 X, EXPFAC, G, XFAC, COMPFAC1, COMPFAC2, TEST

IF (FIRSTBAIN) THEN

FIRSTBAIN = .FALSE.

X = PEARLX

ELSE

X = X + DELTAX

ENDIF

EXPFAC = EXP(-(27500/(R*(TEMP1+273.))))

G = 1.0 + 1.44 * (LOG ((25.4/GRAINSIZE)**2.0 * 100.0))

XFAC = X**(2.0*(1.0-X)/3.0) * (1.0-X)**((2.0*X)/3.0)

COMPFAC1 = 2.34 + 10.1*C + 3.8*CR + 19.0*MO

TEST = -1.9*C + 2.5*MN + 0.9*NI + 1.7*C + 4.0*MO - 2.6

IF (TEST.LT. 0.0) THEN

COMPFAC2 = 1

ELSE

COMPFAC2 = EXP((X**2.0) * (1.9*C + 2.5*MN + 0.9*NI
+ 1.7*CR + 4.0*MO - 2.6))

ENDIF

DNUM = 2.0**((G-1.0)/2.0) * (TEMPINC)**2 * EXPFAC * XFAC
DDEN = COMPFAC1 * COMPFAC2 * .0001
DELTAX = (DNUM/DDEN) * TIMEINC

RETURN
END

SUBROUTINE MARTENSITE (FERX, PEARLX, AUSTX,
BAINX, MARX, I, WMX, BMX)

* global input variables

REAL

1 FERX, PEARLX, AUSTX, BAINX, WMX, BMX, MARX

INTEGER I

* Input Data - FERX, BAINX, PEARLX, MARX, WMX, BMX

* Output Data - MARX, AUSTX

AUSTX = 0.000000

IF (I.EQ. 1) THEN

MARX = BMX - (FERX + BAINX + PEARLX)

ELSE

MARX = WMX - (FERX + BAINX + PEARLX)

ENDIF

* other version(new one) - where martensite transformed depends
* on the martensite start and finish temperatures.

SUBROUTINE MARTENSITE(HFAF, AUSTX, MS, MF, T4, T5, MARX)

DMARX = AUSTX * (T5-MS) / (MF-MS)

MARX = MARX + DMARX

AUSTX = AUSTX - DMARX

DHFAF = DMARX * HFAF

RETURN

END

SUBROUTINE HARDNESS(FERX, PEARLX, BAINX, MARX, HV10,
C, MN, NI, SI, CR, MO, V, ENERGYIN, BMX, WMX, I)

* This subroutine uses Ashby's method (ref. Ion, Easterling,
* and Ashby, A Second Report on Diagrams of , Acta Metall.,
* Vol. 32, No. 11, pp. 1949 - 1962, 1984) of calculating the
* hardness of steels based on a rule of mixtures relationship.

* The cooling rate at 700 C (V in K/hr) is approximated by
* VPRIME = (800 - 500)/deltat centreline, (of Rosenthal).

* Note: this is Rosenthal's relationship for thick plate, with
* a thermal conductivity of 25 J/m sec K.

* HV10 is the Vickers hardness number (10 kg load).

* global input parameters

REAL

1 FERX, PEARLX, BAINX, MARX, C, MN, NI, CR, MO,

2 SI, V, ENERGYIN, BMX, WMX

INTEGER

1 I

* global output parameters

REAL

1 HV10

* local variables

REAL

1 VPRIME, HMART, HBAIN, HFP, TAU85, COND

COND = 25.

PI = 3.1415926

TAU85 = ((ENERGYIN * 1000.)/(2. * PI * COND)) * ((1./480.)
- (1./780.))

VPRIME = (800.-500.)/TAU85 * 3600.

HMART = 127. + 949.*C + 27.0*SI + 11.0*MN + 8.0*NI + 16.*CR
+ 21*LOG10(VPRIME)

6 HBAIN = -323. + 185.0*C + 330.0*SI + 153.*MN + 65.*NI + 144.*CR
6 + 191.*MO + (89. + 53.*C - 55.*SI - 22.*MN - 10.*NI
6 - 20.*CR - 33.*MO) * LOG10(VPRIME)

6 HFP = 42. + 223.*C + 53.*SI + 30.*MN + 12.6*NI + 7.*CR
6 + 19.*MO + (10. - 19.*SI + 4.*NI + 8.*CR + 130.*V)
6 * LOG10(VPRIME)

VFP = FERX + PEARLX

HV10 = MARX * HMART + BAINX * HBAIN + VFP * HFP

IF ((I.EQ.1) .AND. (BMX .GT. 0.0)) THEN

HV10 = HV10/BMX

ELSE

IF ((I.EQ.2) .AND. (WMX .GT. 0.0)) THEN

HV10 = HV10/WMX

ENDIF

ENDIF

RETURN

END

END

2/2.06.88

FIN