**An atomistic study of dislocation interactions
with the γ/γ' (Ni/Ni₃Al) interface of a
nickel based single crystal super alloy**

by

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A thesis submitted to
the Faculty of Graduate Studies and Research
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the requirements for the degree of

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The undersigned recommend to
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Abstract

Dislocation interactions are known to be responsible for the ductility and brittleness of materials. A study of how dislocation activities is affected by the interface between two phases of a nickel based single crystal super alloy is presented here.

Atomistic simulations were performed to study the interactions of a $\langle 110 \rangle$ externally introduced dislocations in presence of misfit dislocations on the $\text{Ni}/\text{Ni}_3\text{Al}$ (γ/γ') interface in the super alloy, with the interface between these phases. The Embedded Atom Method (EAM) has been used for the energy simulation and minimization with the Conjugate Gradient Method (CGM).

Dislocations were generated at appropriate spacings in relation to the misfit dislocation in simulation cells relaxed using rigid boundary conditions in two directions and periodicity along the direction of the dislocation line. Shear strains leading to shear stresses were applied in small steps on the computational cell to drive the dislocations across the interface.

Based on the resulting configurations, each $\langle 110 \rangle$ dislocation dissociates into $\langle 121 \rangle$ shockley partials with core spreading of the partial dislocations on the $\{111\}$ slip plane. From the resulting stresses and observation of the relaxed configurations, it was concluded that the interface acts as a barrier to dislocation motion. Also the resistance of the interface is dependent on the dislocation type and the position of the misfit dislocation.

The $\frac{a}{6}[1\bar{1}\bar{2}]$ partial dislocation encounters a significant barrier to its motion across the interface unlike the $\frac{a}{6}[21\bar{1}]$ partial dislocation. Also the interfacial misfit dislocation when directly in the path of a gliding dislocation could either completely stop the motion of the dislocation or allow it to pass through the interface with relative ease depending on the nature of the dislocation.

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List of Symbols

γ	Nickel phase
γ'	Ni_3Al phase
δ	Lattice parameter misfit
τ	Shear stress
G	Shear modulus
$\vec{b}$	Burgers vector of dislocation
τ_{th}	Theoretical shear stress
E_{pp}	Pair potential energy
E_o	Constant reference volumetric energy
r_{ij}	Interatomic distance between atoms
V_2^{eff}	Effective pair potential
E_{tot}	Total energy
F_i	Embedding energy
ρ	Density
ϕ	Interatomic interaction
a	Lattice parameter
E_{coh}	Cohesive energy
C_{11}, C_{12}, C_{44}	Elastic constants
ΔE_v	Vacancy formation energy
H	Thickness
H_a	Anisotropic factor
f_i	Fraction of thickness
s	Dislocation spacing
H_c	Critical thickness

M^*	Average bi axial modulus
ν	Poisson's ratio
μ	Shear modulus
λ	Lame's constant
U_i	Displacement of atom i
X_i	Co-ordinate of the position of atom i
ϵ	Applied strain
N	number of atoms
m_1	Slip plane normal
τ_{res}	Resolved shear stress
σ_{ij}	Atomic level stress tensor
S_j	Slip direction vector
$E_{relaxed}$	Relaxed energy of the atoms
σ_0	Stress to move leading dislocation up to the interface
σ_l	Stress to move leading dislocation across the interface
σ_t	Stress to move trailing dislocation to the interface
σ_b	Barrier strength of the interface
Ω	Volume of inner cell

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Chapter 1

Introduction

1.1 The single crystal nickel based super alloy

Highly-alloyed, precipitate-hardened, nickel-based super alloys have unique properties for use as structural materials at elevated temperatures. Their creep, fatigue, thermal fatigue and corrosion resistance have been significantly improved through chemistry modifications. Many materials which require resistance to high temperatures such as turbine blades are made from these alloys.

Polycrystalline turbine blades with equiaxed grain structures often fail due to creep and environmental induced cracking along the grain boundaries that are aligned perpendicular to the stress axis of the blade [1]. This led to the development of directional solidification processes which eliminate the transverse grain boundaries. Finally a break through was made by completely eliminating the grain boundaries through the use of carefully fabricated single crystal super alloys. These super alloys have superior creep resistance over the polycrystalline and the directional solidified alloys.

Single crystal nickel based super alloys are used in nuclear reactors, submarines, airframes, steam power plants, chemical plants and other applications with the largest portion

being in marine, and aircraft gas turbines due to their high temperature strength, resistance to creep, adequate ductility, and resistance to oxidation and hot corrosion. These alloys consist of two phases, γ and γ' , which in combination produce an alloy of higher strength. A significant factor in this strength increase is the interface between the two phases [2]. The γ phase is nickel rich fcc solid solution matrix, while the γ' phase is an ordered precipitate of Ni_3Al having a $L1_2$ type structure. The volume fraction of the γ' phase in modern nickel based single crystal super alloys (NBSCS) is about 50 - 70 percent [3] which is embedded in the nickel rich solid solution matrix γ .

There exist misfit dislocations at the γ/γ' interface due to the lattice parameter mismatch δ , which is defined from the lattice parameters of the matrix and precipitate γ and γ' respectively as

$$\delta = \frac{a_{\gamma'} - a_{\gamma}}{a_{\gamma'}} \quad (1.1)$$

where a_{γ} and $a_{\gamma'}$ are the lattice parameters of Ni and Ni_3Al respectively. Figure 1.1 shows two blocks of atoms having different lattice constants. Putting the two blocks together leads to subjecting block B to tension (i.e., it is strained) and the block A to compression if a coherent interface with no dislocations is formed. Therefore the lattice misfit introduces a significant internal stress in the crystal. These stresses may be relieved by misfit dislocations at the interface, leading to an incoherent or semicoherent interface [4].

In this research, a computational study using atomic scale modelling is used to study this interface, specifically its resistance to dislocation transmission from γ to γ' and thus its role in the strength of nickel based single crystal super alloys (NBSCS). In the simulations a dislocation is introduced into the softer γ layer, followed by application of shear strain resulting in shear stresses which drives this externally introduced dislocation across this interface in the presence of the interfacial misfit dislocations. This is done along specific

Figure 1.1: Showing two blocks of atoms strained when brought together due to different lattice parameters. A and B shows the configuration before and after being brought together respectively (taken from [4])

planes and at different positions relative to the misfit dislocation. An estimate of the stress required to overcome the interface barrier will serve as a measure of the strength of this interface. Also the interaction between the two dislocations (the misfit and the introduced dislocation) will be studied.

An atomistic approach is used for this study using the embedded atom method (section 3.1.1) to obtain the total energy of the configuration and energy minimization of each structure based on the conjugate gradient method (section 3.2).

1.2 Objective of thesis

This thesis focuses on the Ni/ Ni_3Al super alloy which has found use especially in turbine engines. As the interface between Ni and Ni_3Al has been shown to play an important role in the creep resistance of this alloy, the atomic scale details of this interface and its strength are the focus of this study.

This thesis therefore focuses on this interface with the aim of getting a better understanding of how dislocations interact with it. Since dislocation activities are known to affect whether a material will be ductile or not, a proper understanding of the dislocations interacting with this interface is expected to shed more light on the strength of this alloy.

In getting a detailed understanding of this interface then, the critical stress required to move dislocations across from Ni into the Ni_3Al phase will be determined. Furthermore since the difference in the lattice parameters of the constituents of this alloy has led to misfit dislocations being formed naturally at the interface, the relationship between the introduced dislocation and the misfit dislocations will be studied. That is, we shall find out if the positions of the introduced dislocation relative to the misfit dislocation has any effect on its motion and on the stress to move it across the interface.

1.3 Overview of the thesis

The remainder of chapter 1 include the description of the fcc and the $L1_2$ crystal structures, a brief explanation of plastic deformation and how it is linked with dislocation motion is also explained. Also included in this chapter is the continuum and atomistic approach to computer simulations, the areas where each of these methods has been used and some of the advantages and disadvantages of both methods.

Chapter 2 gives a summary of similar work done in this field and related fields on this alloy and the likes. An in-depth look of how the alloy fails is examined from different perspectives: atomistic simulation, and microscopic analysis using high resolution transmission electron microscopes (microscopy) and diffraction methods. Also, a detailed explanation of dislocations in fcc crystals is explained.

Chapter 3 gives the detailed computational procedure. It showed how the structure was built and the determining parameters. It also gives an explanation of the embedded

atom method and the conjugate gradient method as a means of calculating the energy of the structure and its minimization respectively. Conclusions drawn from the simulations and discussion of results is covered in chapter 4 while the last chapter (chapter 5) gives the final conclusions. Details of calculations not shown in the body of the thesis which are of importance and applicable to future work are given in the appendix.

1.4 The face centered cubic and the $L1_2$ crystal structures

A lot of engineering materials including metals and ceramics are made up of small crystals or grains where atoms are packed in a regular repeating three dimensional pattern. This periodically repeating pattern of arrangement of the atoms is termed crystalline and the actual arrangement of the atoms is called the crystal structure. In visualizing the crystalline structures, atoms are represented as solid spheres having well defined diameters. This is termed the atomic hard sphere model in which spheres representing nearest neighbor atoms touch one another as in Figure 1.2.

Most pure metals have a simple crystal structure usually simple cubic, face centered cubic, body centered cubic or the hexagonal structures, while most alloys and non metallic compounds have a more complex structure. Figures 1.3 and 1.4 show the fcc crystal structure as in Ni and the $L1_2$ structure as in Ni_3Al respectively. Quite a number of engineering materials are however, not pure metals but alloys of two or more metals and solid solutions. The lattice structure of some solid solutions are such that the atoms are arranged randomly on the atomic positions, therefore, for such an arrangement, the two atoms A and B constituting the solid solution can occupy any of the available atomic sites. But in some cases however, each type of the constituting atoms only occupy specific lattice point such that a well defined distribution of the atoms is obtained. Such a situation can

Figure 1.2: Hard sphere model for atomic arrangement

Figure 1.3: The fcc crystal Structure, having atoms at the centre of each face of the cube and at the corners

Figure 1.4: The $L1_2$ crystal structure of Ni_3Al . Similar to the fcc structure in Figure 1.3 but the corner atoms now are the aluminium atoms while the faces of the cube has nickel atoms

be explained as a lattice of crystal A interpenetrating that of crystal B [5] and the result is an ordered solid solution whose lattice structure is now termed a “*super lattice*”. The γ' structure is a typical example of a super lattice. The size of a cube of Ni_3Al is slightly larger than that of Ni and smaller than that of Al due to the difference in the atomic size of the two atoms (Al atoms being bigger than Ni atoms). Therefore since larger Al atoms replace the corner atoms in the fcc structure of Ni there exist an elongation in the length of each side of the cube to accommodate the larger Al atoms and hence the increase in the cube size.

For the face centered cubic (fcc) structure, the atoms are positioned at the corners of a cube referred to as the unit cell and at the centre of each of the six faces of the cube. The atoms touch along the $[011]$ directions and this is termed the closed packed direction.

The (111) planes are the most important in the fcc structure as they are the close packed planes (Figure 1.5) and contain the closed packed directions which are 60° apart.

Figure 1.5: The (111) closed packed planes of atoms in fcc structure

The stacking sequence of the (111) planes is the ABCABCABC arrangement as shown in Figure 1.6. This particular arrangement is one in which the atoms take up the least volume and is called a closed packed structure [6].

It is important to note that there is another alternative for stacking the close packed planes one on another. After the first two layers A and B are obtained there are two possibilities for the third layer, either into the position C as in fcc structure or directly above those atoms in the first layer, thereby generating a ABABAB sequence. This second possibility gives rise to the hexagonal closed packed (hcp) structure. Quite a number of metals belong to either of these structures, for example Ca, Ni, Cu, Ag, Al have the fcc crystal structure while Ti, Mg, Be, Zr, Zn have the hcp structure. The choice of what structure an element takes is a function of that which gives it the lowest energy. Generally then, materials do not necessarily have to be closed packed but take on the structure which

Figure 1.6: The closed pack stacking sequence of fcc crystals

results in the lowest energy configuration [6], as determined by the quantum mechanics of atomic bonding.

1.5 Plastic deformation

Plastic deformation occurs in a perfect crystal when a plane of atoms slides over the atoms on the adjacent plane (Figure 1.7a and b). For this to take place a sufficient amount of stress has to be applied to the structure. The shear stress required for this was first calculated by Frenkel [5]. He assumed that there is a periodic shearing stress to slide one layer over the other given by:

$$\tau = \frac{Gb}{2\pi a} \sin \frac{2\pi x}{b} \quad (1.2)$$

Where G is the shear modulus, b the spacing between atoms in the direction of the shear stress, a , the spacing of the rows of atoms and x , the distance away from the low

Figure 1.7: Illustration of how atoms slide over one another in estimating the stress for slip. (a) atoms at their equilibrium position, (b) the top layer has slipped a distance x relative to the lower layer.

energy equilibrium position. The theoretical critical stress τ_{th} is thus obtained when $\sin \frac{2\pi x}{b}$ is maximum, therefore:

$$\tau_{th} = \frac{Gb}{2\pi a} \quad (1.3)$$

Real crystals however, are not perfect, they have defects which reduces their strength. The calculated resolved shear stresses measured in real crystals, (even in the well annealed ones) are many order of magnitudes smaller than the theoretical critical stress τ_{th} . The wide variation between the predicted value and the experimentally calculated value is attributed to imperfection in the crystal. The dislocation is a defect that has the effect of allowing materials to deform plastically (yield) at stresses much lower than the predicted theoretical stress.

1.6 Continuum models

The branch of mechanics which focuses on the stresses in the three states of matter (solid, liquid and gas) and their deformation is termed mechanics of a continuous medium [7]. The continuum theory is the form of partial differential equations describing the conservation laws and constitutive relations. It is assumed that all mathematical functions based on this theory are continuous and the derivatives also continuous. Further more continuum theories rest on the assumption that the relevant fields that describe the state of the material vary slowly on the atomic scale. Therefore the theory breaks down in the vicinity of lattice defects and cannot model any phenomenon on the atomistic scale such as dislocation nucleation and material fracture [8].

The continuum approach has been successful in quite a number of areas such as solid and fluid mechanics. It is very efficient, simple and often involves very few material parameters, but it becomes inaccurate for problems in which the detailed atomistic processes affect the macroscopic behavior of the material, or when the scale of the medium becomes small enough that the continuum approximations becomes unsuitable [4].

However, despite the lapses, the continuum model has been used in conjunction with continuum field models of dislocations, and finite element methods to solve several dislocation problems [8], such as computing the overall stresses due to dislocations, interactions between dislocations and the stress driven motion of dislocations. Other features such as stress concentration due to dislocation pile up [8], hardening by inclusions impeding dislocation motion and fatigue crack growth have been modelled using the combination of continuum and atomistic models.

1.7 Atomistic simulation

From section 1.6 above, it is clear that to fully understand the behavior and responses of materials, a detailed atomistic modelling may be required. Macroscopic properties of materials are obtained from atomistic observations, especially for small models in the nanometer range. The explanation to why materials are brittle or ductile is linked to bond breaking and the deformation that takes place due to dislocations. Such details cannot be revealed by the continuum approach and hence require atomistic explanations.

The breakthrough by physicists in the 1920's gave the knowledge to describe the behaviour of nature down to the atomistic scale in terms of atoms and electrons [9]. The improved development in the computer world which has led to the production of faster and cheaper computers has also significantly aided this process. This improved knowledge obtained using computers for atomistic simulations has led to it being a major field in physics, chemistry and biology [9].

Several methods exist for performing various calculations using atomistic simulations. In most cases the methods differ from one another in terms of the speed, accuracy and ability to describe specific phenomena. These atomistic simulations give the exact nature of the study being done as the results are obtained from the most fundamental possible approach. However, it must be realized that despite the accuracy and significance of computer simulations, a simulation is not nature [9] and it is therefore essential that which ever simulation method is being used, the result should in as much as possible be compared with experimental values.

1.7.1 Atomistic modelling

The structure to be modelled is built by representing each atom in the structure by their coordinates in three dimensions and placing them in a simulation box. Each atom interacts

with its neighboring atoms according to known forces and the energy associated with each atom is computed. By summing up the energies of the individual atoms the overall energy for the structure is determined. The energy of the configuration is described using inter-atomic potentials, which are function of the position of the atomic nuclei. Also included in the potentials is the electron - nucleus interaction, since the positions of the nuclei affects those of the electrons. Various atomic potentials have been developed for these simulations, with each one having its up side and down side as will be discussed in chapter 3.

Quite a number of methods exist for performing atomistic modelling and the choice depends on the goal and the available method. In molecular dynamics approach an assembly consisting of N atoms for example is governed by $3N$ simultaneous equations of motion which are derived as a function of time for simulating the movement of each atom [10]. Several other methods have been used for these simulations, the quasi-dynamic method, the direct variation method and Monte Carlo methods are a few examples.

The quasi-dynamic method of simulation is employed at zero Kelvin, and the equilibrium (lowest energy) configuration obtained by minimizing the kinetic energy of each atom and allowing them to converge to the minimum energy position [4]. The direct variation method involves adjusting the atomic co-ordinates of each atom until the net force on all atoms reaches the minimal.

For the present work, after building the block of atoms (based on the structure of the alloy considered, such as the lattice type and lattice parameter), the energy of the configuration so obtained is taken as the starting point for the minimization process. The atoms are then moved around using the the conjugate gradient method to minimize the energy. The final configuration is thus the one with the entire structure in the lowest possible energy based on the atomic potentials used and is termed the “*relaxed*” configuration. The difference between the energies of the new position and the previous one is taken and the

process is continued until this difference becomes insignificant. This method of atomistic simulation works well in getting accurate results but requires significant computer memory and time for each simulation (a function of the size and starting configuration).

Chapter 2

Background and Literature Review

2.1 Previous studies on Ni/Ni_3Al and related structures

Despite the high temperature properties of these alloys, it has been found that under the application of uniaxial stress at elevated temperatures the morphology of the precipitate changes, ultimately leading to failure [11]. This change is termed "rafting" of the γ' precipitate which is as a result of coarsening of the precipitates. Previous work done by Kolbe, Dlouhy and Eggeler has shown experimental evidence of a relationship between the susceptibility to coarsening and dislocation interactions with the interface [12]. The study of dislocations in these alloys is therefore necessary to get a better knowledge on this change in morphology, with an eye toward explaining the effect of dislocations on future coarsening. Several approaches has been taken to explain this phenomenon, atomistic simulations, experimental creep test and investigation of effect of other alloying elements among others are examples of the different approaches taken to get a better understanding of these alloys.

2.1.1 Computational approach

Atomistic simulations have been used in great detail to study dislocation emission and motion and to predict strength of materials. The formation and characteristics of misfit dislocation in heterostructures has been done extensively by Nandekar [13]. Using the f.c.c. Au/Ni (15.9% mismatch) as a case study, he concluded that nucleation of misfit dislocations in compressed films begin by formation of vacancies near the film surface. The simulation also demonstrated that the site of nucleation of the dislocation is near the free surfaces and also showed the differences in energies for the 60 degrees and 90 degrees dislocations for the (111) and (110) interfaces. The activation energy barrier for misfit dislocations in his work was then interpreted to be the energy required to generate vacancies leading to the misfit dislocations, and that dislocation types depended on interface orientations.

The interaction of $\frac{1}{2} \langle 110 \rangle$ screw dislocations with symmetric [110] tilt boundaries was investigated by a group of researchers using atomistic simulations [14]. They came up with useful information on the attraction of a lattice Shockley partial dislocation towards grain boundary and transmission through the grain boundary under the influence of a shear stress in Cu_3Au .

The Coupled Atomistic and Discrete Dislocation (CADD) method described by [15] has been used for multiscale modelling of plasticity, combining simultaneously atomistic and continuum degrees of freedom. This method combines atomistic and continuum regions that communicate across a coherent interface. CADD is able to track dislocations as they pass through the atom / continuum boundary. It is specifically useful in the study of problems involving a large number of dislocation which would be too cumbersome for fully atomistic modelling, and is able to produce accurate atomistic details when required.

A fully atomistic simulations of dislocation / interface interactions was done by Rao and Hazzledine [16] using Cu-Ni multilayer as an example. They investigated four parameters

that attribute to the fact that a nanolayered structure of two types of metals possesses increased strength as the layer thickness is reduced. The parameters responsible for this were the elastic moduli, lattice parameter, gamma surface and slip plane mismatches between adjacent layers. The barrier strengths of various interfaces was studied and the strength of misfit dislocations as barriers to glide dislocations investigated.

An atomistic structural study of the mechanism responsible for the improved ductility in polycrystalline Ni_3Al was studied by Da Chen, Min Lu and Lin T. [17]. They concluded that Boron enhances the cohesive strength of the grain boundaries and simultaneously eases the slip transfer across the boundary. This conclusion was based on their results which show that Boron segregation facilitates the Ni rich layer to serve as a source and sink of dislocation, thereby easing the slip transfer across grain boundary. Stress concentration across the boundary by pile up of dislocations is therefore relieved and thus the tendency for intergranular fracture is reduced.

2.1.2 Experimental approach

The microstructure of the single crystal super alloy as obtained by the work of Pierre carron and Tasadduq [18] is shown in Figure 2.1. Previous work done on determining the locally acting loads during service life of a turbine blade by investigation of the microstructure revealed that the γ/γ' precipitates of which the blade is made of are oriented on a cuboid to cuboid bases in same orientation [19]. The picture seen in Figure 2.1 shows the microstructure in 2-D, but in 3-D, each of the flat plate seen is actually a cuboid and the orientation of the cuboid in both phases are same, e.g the $\langle 110 \rangle$ direction in the γ' phase is parallel to that of the γ phase and same to all other directions.

At very high operating temperatures of about 900° centigrade, it has been experimentally found that the γ' cuboidal precipitates become unstable and link together to form plates called "rafts". This process, "*coarsening*" of γ' precipitates leads to the instability

Figure 2.1: The γ/γ' microstructure of a first generation single crystal superalloy. The large whitish blocks are the γ' precipitates and the dark patches in between them is the γ matrix (taken from [18])

of this strengthening phase and therefore a reduction in the creep resistance of the alloy [20].

A study of the coarsening of the strengthening γ' phase was studied by T.M Pollock and S. Argon [21]. Two samples of the super alloy containing about 70 % volume of the γ' was used with one sample containing a higher fraction of Ta and Ti to alter the lattice parameter misfit. Creep tests were performed on the samples and the results were analyzed using the transmission electron microscope. They concluded that the orientation of the rafts formed on application of stress depends on the positive / negative sense of the misfit of the alloy, they also found that the coarsening which is directional does not occur at a significant rate until some amount of creep has occurred introducing dislocations into the microstructure, and that rafting occurs by the coalescence of the γ' phase on well defined planes.

A dislocation based criterion for the raft formation in Nickel based single crystal super

alloys was reported by Buffiere and Ingot [3], and supported by experimental observations. They found that the precipitate face which exhibit dislocations will grow during creep by coarsening of the γ' phase. Also, the mechanism responsible for this relationship can be linked to the effect of these dislocations on coherency stresses.

Aoki and Izumi [22] also did a study on the effect of Boron as an alloying element in Ni_3Al , as it accounts for an improved ductility at ambient temperature. The effect of other alloying elements on the super alloy has also been done by Linruo Zhao [1]. A high temperature strengthening was linked to the addition of Re. This was attributed to the the slow diffusion of Re thereby reducing the γ' coarsening rate at high temperatures. The formation of of Re rich clusters in the γ matrix and Re-induced negative $\gamma - \gamma'$ misfits has been linked to a prolonged stress ruptured life [1].

2.2 Dislocations

Dislocations are the phenomenon used to explain the ductility in metals as it accounts for the plastic deformation. A simple illustration of a dislocation begins with the idea of slip. In an ideal case, a crystal deforms by planes of atoms sliding over one another. There is one unit of slip on a slip plane when all the atoms on one side of the plane moved to a position initially occupied by the nearest neighbor in the direction of slip. Therefore a unit slip does not disturb the crystal perfection as the atoms are left in register across the slip plane [23].

For most real crystals, however, a uniform slip across the slip plane does not occur. An illustration is shown in Figure 2.2 where a unit slip has occurred only over a portion of the crystal, with an unslipped region on the other part of the crystal. The slipped region and the unslipped region are separated by the dislocation. From the figure, line AD (dislocation line) is the boundary within the crystal separating the slipped area ABCD

Figure 2.2: Slip leading to edge dislocation. A unit slip has occurred over the area ABCD and the dislocation line AD separates the slipped and unslipped regions (taken from [23])

from the unslipped area.

Putting the atoms in the structure of Figure 2.2 and looking in along line AD, shows the position of the dislocation (Figure 2.3). This type of dislocation is called edge dislocation. If now the dislocation was able to move across the slip plane from one side of the crystal to the other then the crystal will deform as shown in Figure 2.4. This shows how slip, dislocation and dislocation motion leads to plastic deformation.

This same idea could be more clearly seen from atomistic view by considering Figure 2.5 where the edge dislocation has moved from plane A (a), to plane B (b) and finally to produce a unit step of slip as shown in (c) under the application of shear stress. The plane along which the dislocation line moves is the slip plane and the final result gives a permanent deformation.

Dislocations are linear imperfections (line defects) that occurs at places where the crystal stacking has been disrupted such as to produce an extra half plane as in edge dislocation or a spiral as in screw dislocation. Figure 2.3 shows an edge dislocation with

Figure 2.3: Showing a plane of atoms normal to the dislocation line of Figure 2.2 and the dislocation formed as a result of slip (taken from [23])

an extra half plane of atoms. The dislocation line is defined along the edge of the extra plane of atoms. Atoms above the dislocation lines are compressed while those below are pulled apart as seen in the slight curvature for the vertical planes of atoms which bends around the extra half plane of atoms. The distortion decreases as one move away from the dislocation and far away from it the crystal is in its perfect form. When the extra half plane is above the slip plane as in Figure 2.3 is referred to as positive edge dislocation and when it is below, a negative edge dislocation.

A screw dislocation can be thought of as formed when a shear stress is applied on a block as to produce the distortion shown in Figure 2.6, the upper front region of the crystal has been shifted by one atomic distance to the right relative to the bottom part.

One very important definition of a dislocation is expressed in terms of the Burgers circuit. Any atom to atom path taken in a crystal containing dislocations which forms a closed loop is termed Burgers circuit. An example of a Burgers circuit is shown in Figure

Figure 2.4: Dislocation motion leading to plastic deformation. (a) application of shear stress to deform the crystal. (b) and (c) dislocation has moved a fraction of the offset b . (d) dislocation has moved to the other end of the crystal (taken from [23])

Figure 2.5: Motion of edge dislocation on the slip plane resulting in a step being formed on the surface of the crystal (taken from [24])

Figure 2.6: Illustration of a screw dislocation (taken from [24])

2.7 a i.e path MNOPQ. When the same path is taken in a material without a dislocation, the circuit does not close Figure 2.7 b. This shows that the first case encloses at least one dislocation. The vector required to close the circuit as shown in 2.7 b is termed the Burgers vector $\vec{b}$, also defined as the magnitude and direction of the lattice distortion associated with a dislocation.

When this atom to atom movement is made in two crystals, one having an edge dislocation and the other a screw dislocation, the Burgers vectors are found to have different directions with respect to the dislocation line. The Burgers vector is perpendicular to the dislocation line for edge dislocations and parallel to the dislocation line for screw dislocations.

Most dislocations found in materials are, however, neither pure edge nor pure screw but a combination of both. This condition is termed a mixed dislocation. The Burgers vector and dislocation line in this case are neither parallel nor perpendicular. All the three

Figure 2.7: Burgers circuit of dislocation, (a) Burgers circuit enclosing a dislocation, (b) the same Burgers circuit drawn in a perfect crystal shows the closure failure (taken from [5])

Figure 2.8: Showing the 3 dislocation types. At point A it is pure screw, while at point B it is pure edge, for regions between A and B the character is mixed (taken from [24])

different types of dislocations (edge, screw and mixed) are shown in Figure 2.8, the lattice distortion produced away from the two faces is mixed, with the dislocation having both edge and screw character. It is worthy to note that even though a dislocation changes direction and type (e.g edge to screw or mixed), the Burgers vector will be the same at all points along the dislocation line.

2.2.1 Dislocations in fcc crystals

Many of the important metals used in engineering have the fcc crystal structure. The energetically favoured dislocation in fcc has the $\frac{a}{2}[110]$ Burgers vector of dislocation and the slip plane is the $\{111\}$ plane [5]. The slip plane and the direction of motion of dislocation

Figure 2.9: Thompson's Tetrahedron showing the various slip systems in a fcc structure (taken from [5])

is termed the *slip system*. This depends on the the crystal structure of the given metal and it is that which gives the minimum atomic distortion on the motion of the dislocation [24]. As stated in section 1.4, the slip plane has the most dense atomic packing (see Figure 1.5), i.e the greatest planar density. The direction of slip has the highest linear density. For the FCC crystal structure, the $\{111\}$ planes and $[110]$ directions are the slip planes and directions respectively. There are four (111) type planes and each consists of three possible $[110]$ directions. Each combination of a plane and a direction constitute a slip system thus there are twelve slip systems in the fcc structure as shown in Figure 2.9 (*Thompson's Tetrahedron*). Folding the big triangle DDD (Figure 2.9) along lines AB, BC and AC brings all the points D together to form the tetrahedron. This resulting tetrahedron contains four triangles representing the four (111) type slip planes of the fcc structure. The orientation of each of the planes in the crystal is as seen in Figure 1.5

Heidenreich and Shockley suggested that a unit dislocation would dissociate into two half (*partial*) dislocations [25]. This has been shown to be true and could be explained

using the Thompson tetrahedron. Considering the triangle at about the centre of the Figure for example, it shows the (111) plane and the three possible full dislocations on this plane with their corresponding partial dislocations. The following dissociation takes place:

$$\frac{a}{2}[0\bar{1}1] = \frac{a}{6}[1\bar{2}1] + \frac{a}{6}[\bar{1}\bar{1}2] \quad (2.1)$$

$$\frac{a}{2}[1\bar{1}0] = \frac{a}{6}[1\bar{2}1] + \frac{a}{6}[2\bar{1}\bar{1}] \quad (2.2)$$

$$\frac{a}{2}[\bar{1}01] = \frac{a}{6}[\bar{1}\bar{1}2] + \frac{a}{6}[\bar{2}11] \quad (2.3)$$

The terms on the left hand side are the full Burgers vector of dislocation, while those on the right are the Schockley partials.

As the two partials separate they leave a band of stacking fault between them on the slip plane. Elastic interactions between the partials suggest that the two half dislocations should move further apart but as they do, the area of the fault increases and so does the energy of the crystal. Therefore, an equilibrium configuration is reached with a finite spacing between the dislocations and having a fixed stacking fault width. Crystals with a high stacking fault energy therefore, have closely spaced partials e.g Al and those with a low stacking fault energy (such as Au) have widely spaced partials.

2.2.2 Dislocations in Ni_3Al super lattice

Figure 1.4 is the Ni_3Al super lattice structure, if the aluminium atoms do not occupy well defined positions then the dislocation in the crystal will be similar to that of an fcc structure as described in section 2.2.1. But since the atoms are in an ordered position,

Figure 2.10: Positions of atoms on two adjacent (111) planes of Ni_3Al superlattice (taken from [5])

this introduces a difference in the dislocation of this structure. This $L1_2$ structure is quite similar to that of the fcc but for the different atoms, and so it has the same slip planes and slip directions. Figure 2.10 is the arrangement of atoms on a (111) plane of Ni_3Al superlattice, the shaded circles are the aluminium atoms and the open circles are the nickel atoms.

In a pure metal having an fcc structure, the slip $\frac{a}{2}[\bar{1}10]$ produces a unit dislocation, but in Figure 2.10 above, such motion leads to moving the atom at position X to Y and thus there is a change in the arrangement of atoms across the slip plane mainly due to a Ni atom now occupying the position of an Al atom. Such a distortion in the arrangement of atoms creates an antiphase boundary. However, this distortion is removed when the atoms are further moved by another displacement of $\frac{a}{2}[\bar{1}10]$ which brings the atom initially at X

to Z. Therefore in the Ni_3Al lattice, a full dislocation termed “*superlattice dislocation*” is a combination of two $\frac{a}{2}[\bar{1}10]$ joined by an antiphase boundary. From the energetic point of view, the $\frac{a}{2}[\bar{1}10]$ dislocations will then dissociate into Schockley partial dislocations of type $\frac{a}{6}[1\bar{2}1]$. The dislocation in the $L1_2$ crystal structure is thus termed “*super dislocation*” because of the longer repeat distance in the lattice. Dislocations from Ni cannot easily cross the interface into Ni_3Al because of the super lattice nature of Ni_3Al .

2.2.3 Precipitation hardening

Precipitation hardening is one of the heat treatment method used to increase the strength of metals and alloys. Such metals and alloys have a solid solubility which decreases as the temperature falls, they therefore have the potentials for precipitation hardening [26]. These precipitates are second phases which is not dissolved but dispersed in the matrix and are the source of strength in most Aluminium and Titanium alloys [27]. These precipitates obstructs dislocation motion during deformation by making the dislocation bow between them leaving a dislocation loop around the particle. Alternatively the dislocation could be forced to cut through the precipitate [28] but this is usually though to do as the precipitates are stronger than the matrix. By this restricted motion of the dislocation during deformation, the alloy is thus strengthened.

Precipitation strengthening involves heating the alloy to a temperature where the second phase is completely dissolved such that there exist only one phase as shown in Figure 2.11.

An alloy of composition Co is heated and held at temperature T_o till all the β phase is dissolved. The alloy is then cooled rapidly to room temperature (T_1), usually by quenching in cold water such that the β phase is prevented from being formed, thus in this condition the alloy consist of supper saturated solid solution of α phase. The final step is the formation of the tiny uniformly dispersed precipitates (β phase) which is obtained after leaving the alloy for a sufficiently long time at T_1 (natural aging). Alternately the super saturated solution could the heated to temperature T_2 at which there is increased diffusion and held till the precipitates are formed (artificial aging). Figure 2.12 shows the products obtained during the process of aging the supersaturated solution. In order to achieve a lower energy state, the precipitates are spontaneously formed until the equilibrium phase is obtained and this is accompanied by a reduction in energy of the alloy.

It should be noted that the strength of the final product is a function of the properties

Figure 2.11: A hypothetical Binary Phase diagram for two metals A and B. Note the solid solution α has a decreasing solid solubility in A as the temperature decreases

Figure 2.12: Stages in precipitate formation from the high energy supersaturated phase to the equilibrium position through the spontaneous release of energy [taken from [28]]

Figure 2.13: A schematic curve showing the strength of a precipitation hardened alloy with aging time at a given temperature[taken from [28]]

of the β phase, the precipitation temperature and aging time. Different precipitates will therefore have a different combination of these conditions for optimum strength. Figure 2.13 shows the relationship between the aging time at a given temperature and strength of the alloy.

Chapter 3

Simulation tools and computational procedure

3.1 Atomic potentials

The pair potential method, a two - body inter - atomic potential derived from fundamental considerations or by empirical means [29, 30] has been used by many physicists for atomistic simulation. The Lennard-Jones potentials, Born-Mayer potential, etc. are based on this method [4]. This method gives the total energy of a block of atoms directly but requires the use of an accompanying volume dependent energy to describe the elastic properties of a metal [31]. Any uncertainty therefore in the volume may automatically affect the reliability of the results of a pair potential calculation since the elastic properties of the solid may not be accurately represented. This problem arises in calculations involving surfaces, due to the fact that the exact termination of the volume on an atomic scale at the surface is not well defined.

Finally, the pair potential, though has been very successful in applications to inert elements such as Helium, fails when it comes to application on chemically active metals.

It was shown that the energy of hydrogen atom in a transition metal cluster cannot be represented by pair interactions [32] but that of helium can be represented.

For a given block of atoms the total energy of all atoms using the pair potential method is obtained by summing up the energy of each pair of atom. Each pair of atom has an atomic interaction which contributes to the total energy of the structure. The configuration energy of the structure based on the pair potential is given by equation 3.1 [33, 34].

$$E_{pp} = E_o + \frac{1}{2} \sum \sum V_2^{eff}(r_{ij}) \quad (3.1)$$

E_o is a constant reference energy or volumetric energy, r_{ij} is the interatomic distance between atoms i and j and $V_2^{eff}(r_{ij})$ is the effective pair potential.

A better potential for treating metallic systems is the embedded atom method [35] which can be applied to inert and chemically active metals and also to crystal structures which includes defects. This is made possible since the problem of volume-dependent energy is replaced by the embedding energy which is electron density dependent and the density is always clearly defined. A detailed explanation of the embedded atom method is given next.

3.1.1 Embedded atom method

As stated in chapter 1, the embedded atom method is used for the atomistic computation in this thesis. This method is adequate for treating most metallic systems where dislocations, fractures, surfaces, impurities, etc are important [35]. The embedded atom method was developed on the assumption that each atom in a given configuration can be viewed as an impurity in the host of other atoms, and from the quasiautom concept the total energy of the atoms is given by

$$E_{tot} = \sum F_i(\rho_{h,i}) \quad (3.2)$$

Where F_i is the embedding energy, $\rho_{h,i}$ is the density of the host at the position $\vec{r}_i$ but without atom i, and therefore, the total energy is the sum of the individual contribution from each atom. Equation 3.2 however, neglects the core-core repulsion which is corrected by including an additional term which takes the form of a short range pairwise repulsion between the cores. The total energy now including this term is

$$E_{tot} = \sum F_i(\rho_{h,i}) + \frac{1}{2} \sum \phi_{ij}(r_{ij}), \quad (3.3)$$

where ϕ_{ij} is the pair potential, r_{ij} is the distance between atoms i and j. Comparing equation 3.3 with equation 3.1 for the pair potential method, the volumetric energy E_o has been replaced with the density dependent F_i which helps to overcome the ambiguity associated with defining the volume in the pair potential method. Taking Nickel as an example, a plot showing the relationship between the density and the embedding energy is shown in figure 3.1.

On the assumption that the host density is approximately equal to the sum of the contribution from each neighbor's electron density (ρ) of the constituting atoms, then

$$\rho_{h,i} = \sum \rho_j(r_{ij}) \quad (3.4)$$

The energy is thus a function of only the position of the atoms. ρ_j is the contribution to the total density from atom j, $\rho_{h,i}$ is the total host electron density at atom i. Figure 3.2 shows the relationship between the density and inter - atomic distance in Ni.

Figure 3.3 shows the relationship between the interatomic interaction ϕ_{ij} and the interatomic distance in Ni. It is clear from the figure that the interatomic repulsive force between the atoms are greatest when atoms are closer together.

Figure 3.1: Plot showing the embedding energy $F(\rho)$ against density (ρ) in Nickel

Figure 3.2: Plot showing a reduction in the density as the inter - atomic distance increases

Figure 3.3: Graph showing the interatomic interaction vs atomic distance in Nickel

$F(\rho)$ and $\phi(r)$ are determined from the properties of the pure metal for each element, such as the lattice constants, cohesive energy, vacancy formation energy, heat of sublimation etc. In the case of an alloy the unlike atom pair potential is taken as the geometric mean of the interaction between like atoms $\phi_{(ii)}$ and $\phi_{(jj)}$. The inter atomic pair potential for dissimilar atoms is therefore given by

$$\phi_{ij}(r) = \sqrt{(\phi_{(ii)}\phi_{(jj)})} \quad (3.5)$$

where $\phi_{(ii)}(r)$ and $\phi_{(jj)}(r)$ are the interatomic interactions between like atoms.

Some constraints are imposed on these functions to give satisfactory results. F is linear at higher densities and constrained to zero at zero density. The cut off radius was chosen to be the shortest distance to give an acceptable fit such that beyond this distance atoms are assumed not to interact and $\phi(r)$, $\rho(i)$ and ϕ are all zero at distances greater than the cut off radius.

3.1.2 Interatomic potentials for Ni, Al, and Ni_3Al

Accurate potentials for the NiAl system of alloys using the EAM approach have been produced by [36] and is used for the simulation in this work. These potentials have been fitted to treat Ni, Al and Ni_3Al alloys. Only the essential results from the fit is presented below, a detailed result and procedure is found in article [36].

For the properties shown in tables 3.2, 3.1 and 3.3, a is the lattice parameter, E_{coh} ¹ is the cohesive energy, B is the bulk modulus², C_{11} , C_{12} and C_{44} are the elastic constants. ΔE_{vac} is the vacancy formation energy, SISF and APB are the super intrinsic stacking fault and the antiphase boundary energy respectively. The calculated values are obtained using the potentials and from the tables it can be seen that these values are in reasonable

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¹where 1 eV equals 1.6022×10^{-19} Joules

²where 1 erg/cm³ equals 0.1 Pa

Table 3.1: Metal properties used in fit for *Ni* with the calculated and experimental values.

<i>Ni</i> properties	Experimental values	calculated values
a (Å)	3.52	3.52
E_{coh} (eV)	4.45	4.45
$B(10^{12} \text{ erg/cm}^3)$	1.81	1.81
$C_{11}(10^{12} \text{ erg/cm}^3)$	2.47	2.44
$C_{12}(10^{12} \text{ erg/cm}^3)$	1.47	1.49
$C_{44}(10^{12} \text{ erg/cm}^3)$	1.25	1.26
ΔE_v (eV)	1.6	1.6

Table 3.2: Metal properties used in fit for *Al* with the calculated and experimental values

<i>Al</i> properties	Experimental values	calculated values
a (Å)	4.05	4.05
E_{coh} (eV)	3.36	3.36
$B(10^{12} \text{ erg/cm}^3)$	0.79	0.79
$C_{11}(10^{12} \text{ erg/cm}^3)$	1.14	1.07
$C_{12}(10^{12} \text{ erg/cm}^3)$	0.619	0.652
$C_{44}(10^{12} \text{ erg/cm}^3)$	0.316	0.322
ΔE_v (eV)	0.75	0.73

Table 3.3: Metal properties used in fit for *Ni₃Al* with the calculated and experimental values

<i>Ni₃Al</i> properties	Experimental values	calculated values
a (Å)	3.567	3.53
E_{coh} (eV)	4.57	4.59
$C_{11}(10^{12} \text{ erg/cm}^3)$	2.30	2.46
$C_{12}(10^{12} \text{ erg/cm}^3)$	1.50	1.37
$C_{44}(10^{12} \text{ erg/cm}^3)$	1.31	1.23
ΔE_v (eV)	1.6 ± 0.2	1.64(Ni), 1.87(Al)
SISF (111) (mJ/m^2)	140 ± 14	83
APB (111) (mJ/m^2)	180 ± 30	142

agreement with the experimental values.

3.2 Conjugate gradient method

The conjugate gradient method is one of the techniques used for energy minimization of a set of atoms under a given interaction model. It is used here to obtain the equilibrium state configuration of a group of atoms. This method proceeds by generating vector sequences of iterates (i.e., successive approximations to the solution), residuals corresponding to the iterates, and search directions used in updating the iterates and residuals. It uses the gradient of the function in locating the minimum as the gradient predicts the path and how the function changes. After obtaining the initial gradient, the process continues by searching for a lower value of the function in a direction which is conjugate to the old gradient. A comprehensive explanation of this method is given in [37].

3.3 The computational cell

The computational cell consists of Ni and Ni_3Al constructed on a cuboid to cuboid basis with the same orientation and the boundary plane being the (001) as is known from diffraction pattern results from experimental analysis done on samples by Richard and Fonda [2].

The dimensions of the box (as justified in a section 3.5) is 167 Å by 155 Å by 5 Å in the x, y and z directions respectively and having a total of 11,704 atoms. The axes of the two crystals were oriented such that $x = [1\bar{1}0]$, $y = [001]$ and $z = [110]$. This is obtained by rotating the crystal from the standard xyz [100] orientation to this preferred orientation to aid visualization. The use of periodic boundary conditions means that the cell contains two interfaces, one at the middle and one on the top / bottom as shown schematically in figure 3.4. The rectangle (2-d view of the box containing the atoms) shown in the picture

Figure 3.4: Two interfaces formed in the simulation cell as a result of applying periodic boundary conditions.

represent the simulation cell, periodic copies are made by placing a duplicate copy of one rectangle on the other such that the two lines labelled as interface 1 match each other. With this configuration, two interfaces are thus obtained in our simulation cell. The use of the minimum periodic length (5 Å) in the z direction means that our simulation will only contain straight dislocations with infinite line length along the z direction.

3.4 Determining the right computational cell

From the preliminary understanding of the structures of the γ / γ' interface, the first step in the simulation is to build the appropriate starting structure. With knowledge of the crystal structures, we could simply build a block of Ni atoms and that of Ni_3Al and bring them together to obtain the desired interface. However, due to the difference in lattice parameters of the two materials there arises the difficulty of the size to build such that when brought together they match exactly in length along the interface. This is required so that periodic boundary conditions can be applied to the simulations and the result of this is depicted in Figure 3.4. To obtain the correct structure, and ensure that misfit dislocations are correctly introduced, the number of columns of Ni has to be at least one more than that of Ni_3Al in the x direction. Also, to maintain the correct ratio of 3:1; Ni:Al, in γ' , a minimum of two different layers of atoms is required in the z direction such that the smallest size of simulation box will have a thickness of two atomic distance along this direction.

After obtaining the correct size of the crystals and bringing them together there exist the interface dislocations as expected, but upon relaxation, spacing between the dislocations on the adjacent interfaces in the y direction will vary depending on the initial configuration used for the simulation. Thus we systematically varied the initial configuration until the lowest energy arrangement of the misfits was obtained. This final structure is shown in Figure 3.8, and more detail is given in section 3.7.

Analysis of multilayers [38] show that there exist for every given thickness a correct dislocation spacing along the interface, we were therefore faced with the difficulty of building a structure with the right size and dislocation spacing for our case. For example, by building the same structure as shown in Figure 3.8, but with 10 more Ni and Ni_3Al layers along the x direction, the spacing between dislocations along the interface will increase

by approximately 25Å. This led to reviewing the work done by Shoykhet, Grinfeld and Hazzledine [38] where a detailed study of the correct thickness and dislocation spacing for similar analysis has been done, as shown in the next section.

3.5 The critical thickness and correct dislocation spacing

A detailed study of the internal stresses and strains in coherent multilayers has been performed by [38]. Of interest to us in this study is that of equi-biaxial case in a regular bilayered material as in this study. Considering a bilayered material with thickness H , with one layer f_1H thick and the other f_2H thick, where f_1 and f_2 are the fraction of the total thickness for layers 1 and 2 respectively. The multilayer loses coherency when a grid of edge dislocations with Burgers vector $\vec{b}$ appears on each interface, and the dislocations are spaced at a distance s apart.

By minimizing the sum of the dislocation energy and the uniform elastic energy per unit area with respect to the dislocation spacing s , the dislocation mismatch was found to be :

$$\frac{b}{s} = \delta - \frac{\mu M^* b \ln(f_1 \frac{H}{b})}{2\pi(1-\nu)H M_1 M_2 f_1 f_2} \quad (3.6)$$

$$M_1 = 2\mu_1 \frac{1+\nu_1}{1-\nu_1} \quad (3.7)$$

$$M^* = f_1 M_1 + f_2 M_2 \quad (3.8)$$

Where M^* is the average biaxial modulus for the two layers and subscripts 1 and 2 for

layers 1 and 2 respectively. Equation 3.6 becomes zero and therefore s becomes infinite at a critical value (H_c) of H obtained from:

$$\frac{H_c}{b} = \frac{\mu M^* \ln(f_1 \frac{H_c}{b})}{2\pi(1-\nu)\delta M_1 M_2 f_1 f_2} \quad (3.9)$$

H_c is the largest thickness of the bi layer before the coherent interface becomes unstable and misfit dislocations will occur.

Solving equation 3.9 for H_c as applied to our case we obtained the critical height at which misfit dislocation exists to be 136.16 Å . The corresponding dislocation separation distance s for values of H greater than H_c is obtained by solving equation 3.6. In order to solve equations 3.6 and 3.9, we have used Voigt averages [39] to convert the anisotropic material properties into two isotropic elastic constants λ and μ . Where λ is Lamé constant and μ is the shear modulus. The average value of the elastic constants for the two materials is then used in equations 3.6 and 3.9. The anisotropic factor H_a according to [39] is given by:

$$H_a = 2C_{44} + C_{12} - C_{11} \quad (3.10)$$

The Voigt averages are calculated as shown below

$$\lambda + 2\mu = C_{11} + \frac{2}{5}H_a \quad (3.11)$$

$$\mu = C_{44} - \frac{1}{5}H_a \quad (3.12)$$

$$\lambda = C_{12} - \frac{1}{5}H_a \quad (3.13)$$

In order to verify the accuracy of the results obtained from equations 3.6 and 3.9 (which

are based on continuum elasticity) with atomistic results, we built different structures with a thickness $H = 489.47 \text{ \AA}$, a convenient value that is greater than the critical thickness H_c , and we then varied the dislocation spacing. Figure 3.5 shows the plot of the surface energy per unit area against dislocation spacing s for this simulation. The lowest energy value was obtained at $s = 272.23 \text{ \AA}$. This was in good agreement with equations 3.6 and 3.9 which predict $s = 269.35 \text{ \AA}$ at this value of H . This suggests that the continuum analysis of [38] accurately predicts the equilibrium dislocation spacing as a function of H , but suggest that very large s or very large H are required in atomistic simulations to study an elastically ideal interface.

Therefore using the ideal s will give us a very large computational cell with too many atoms, which will take much longer to simulate than is practical. A compromise was thus reached and a smaller cell was used with a thickness of $1.15H_c$, and spacing $s = 157.92 \text{ \AA}$. This is smaller than the correct spacing, and therefore one limitation of our simulations is the existence of excess elastic strain in the crystal. This gives us the largest reasonable dislocation spacing and ensures that our thickness is above the critical thickness for the material.

3.6 Periodic boundary conditions

A periodic boundary is an important technique used in atomistic simulations. It involves making a simulation that consist of a few hundreds or thousands of atoms behave as if it was infinite. This is done to eliminate the effect of free surfaces which finite samples have. This will ensure that the internal structure of the sample is dominated by internal (bulk) forces rather than surface forces.

Figure 3.6 illustrates this condition. The atoms in the shaded box represents the system being simulated while the surrounding boxes gives the exact copies (in all details) of each

Figure 3.5: Showing the plot of energy per unit area vs dislocation separation

Figure 3.6: Figure showing periodic boundary position of atoms. The shaded square (unit cell) has periodic copies all around it (taken from [40])

atom in the reference cell. The arrows, for example, represent the motion of each atom and it must be same in atoms of all adjacent cells. Therefore, if an atom leaves the simulation cell it is replaced by another with exactly identical properties on the opposite side, and the number of atoms in the cell is always constant. As explained in section 3.1.1 and shown in Figure 3.6, r_{cut} is the cut-off radius and any atom can interact only with another atom within the cut off radius. The simulation box is chosen so that an atom does not interact with more than one image of any given atom.

3.7 Computational procedure

With the configuration described in section 3.3 above, initial energy minimization was done employing periodic boundary condition in all three directions and allowing three degrees of freedom for the relaxation of the computational size using the fortran source code DYNAMO [41]. The relaxed configuration was tested for accuracy by calculating the cohesive energy, the lattice parameters and vacancy formation energy for pure Ni, Al and pure Ni_3Al before the two layers were combined (these details appear in the appendix). The multilayer obtained by bringing the two layers together was then relaxed using the same conditions. The unrelaxed structure does not have any significant meaning, as the atoms are not in their stable equilibrium energy configuration until the relaxation is performed, hence no analysis is done on the unrelaxed structure. After this initial relaxation the bilayered structure had two pure edge misfit dislocation lying vertically above one another (At points A and B) along the interface as shown in Figure 3.7.

This configuration was termed a high energy configuration as a lower energy can be obtained by moving the misfit dislocations around using the elastic displacement field of a dislocation dipole [5] and relaxing the new configuration until the lowest energy configuration is obtained. The final configuration (Figure 3.8) shows the misfit dislocation

Figure 3.7: Position of the misfit dislocations (at points A and B) along the interface after the initial relaxation. Also shown are the slip planes

Figure 3.8: Lowest energy configuration showing the misfit dislocations 48 Å apart along the interface

at their equilibrium position, 48 Å apart along the interface.

3.7.1 Externally introduced dislocations on $(1\bar{1}1)$ plane

Based on the Thompson tetrahedron (Figure 2.9), there are three possible dislocations on the $(1\bar{1}1)$ plane. Two of them are mixed dislocations and the third pure screw for our chosen line direction ($[110]$). For the work done in this thesis, the $\frac{1}{2} \langle 10\bar{1} \rangle$ (mixed) and the $\frac{1}{2} \langle 110 \rangle$ (pure screw) dislocations were considered, and their interaction with the interface in the presence of the misfit dislocations was studied.

Figure 3.9: Diagram showing the positions of the introduced dislocations with reference to the misfit dislocation at A

Each of these two dislocations is introduced into the already relaxed cell discussed in section 3.4 above. Five different positions were considered for each dislocation such that the dislocation cuts through the interface at 0 Å, 10 Å, 25 Å, 50 Å, and 80 Å away from the misfit dislocation. Each of these positions is termed A, B, C, D and E respectively for ease of reference as shown in Figure 3.9.

The external dislocations were specifically introduced in the relaxed structure of section 3.7 with the initial position of the core at about the center of the softer Ni layer. This is to ensure that there is minimal or no interaction with the boundary while the computation is performed. For each of the position considered, the dislocation was introduced using the elastic displacement fields of equations 3.14, 3.15 and 3.16:

$$u_x = \frac{b}{2\pi} \left[\arctan \frac{y}{x} + \frac{xy}{2(1-\nu)(x^2 + y^2)} \right] \quad (3.14)$$

$$u_y = \frac{-b}{2\pi} \left[\frac{1-2\nu}{4(1-\nu)} \ln(x^2 + y^2) + \frac{x^2 - y^2}{4(1-\nu)(x^2 + y^2)} \right] \quad (3.15)$$

$$u_z = \frac{b}{2\pi} \arctan \frac{y}{x} \quad (3.16)$$

3.7.2 Barrier strength of the interface

The dislocation core was relaxed employing periodic boundary condition only in the z direction by increasing the size of the simulation cell in the x and y direction by 12 Å (greater than $2r_{cut}$). As shown in Figure 3.10, the atoms in the inner cell feel the interactions from all their neighboring atoms and therefore behaves as atoms in an infinite crystal. The atoms outside the inner cell (boundary atoms) are held fixed at their original position during relaxation. Farther away from the inner cell, the atoms do not feel the interaction from all their neighbors as the periodic box is much larger in the x and y direction thereby losing periodicity along these directions. Though periodicity is lost in the x and y direction, holding the boundary atoms fixed results in “*a trick*” that make atoms in the inner cell unaware of the free surface such that no complex energy (such as interface energy) term is associated with them. The energy obtained from only the inner cell atoms is used in the analysis done. The simulation is therefore two dimensional in nature but with with periodicity in the z direction and therefore the dislocation line is confined to be in the z direction with an infinite length.

To determine the barrier strength of the interface, a homogeneous shear strain was imposed on the computational cell acting on the slip plane in the slip direction according to equation 3.17:

$$x_i = X_i + \epsilon b_i m_j X_j \quad (3.17)$$

Where X_i is the ith co - ordinate of the position of the atom, ϵ is the applied strain, b_i , is the ith component of the unit Burgers vector of dislocation, m_j is the ith component of

Figure 3.10: Schematic diagram showing the simulation cell, periodicity is lost in the x and y direction as the periodic box is elongated in these directions

the normal to the slip plane. After applying each small increment of strain, the structure is then relaxed, again with periodic boundary only in z direction and keeping the boundary atoms fixed. The resulting shear stress acts in the direction of the Burgers vector such that the dislocation moves towards the interface. The simulation is started with imposing a shear strain corresponding to a small stress. Larger stresses were built up by repeating the process. The results obtained after each increment of strain and relaxation were inspected and the critical stress at which the dislocation crosses through the interface is interpreted as the *barrier strength* of the interface. This critical stress is the resolved shear stress on the slip plane and is obtained from Schmid's expression [5]. It states that the resolved shear stress (τ_{res}) on a dislocation is given by:

$$\tau_{res} = \vec{m}_i \sigma_{ij} \vec{s}_j \quad (3.18)$$

where $\vec{m}_i$ is the slip plane normal, $\vec{s}_j$ is the slip direction and σ_{ij} is the stress tensor. This law can be applied to the present case by evaluating the stresses acting on the

structure for each applied strain and the value at the point when the barrier obstacle is overcome gives a measure of the strength of the interface. For each relaxed configuration, the stress σ_{kl} is obtained from the atomic level stress [42] acting on the entire inner cell, and is given by:

$$\sigma_{kl} = \frac{1}{\Omega} \sum_i \sum_{j \neq i} [\phi'_{ij}(r_{ij}) + F'_i(\rho_{h,i})\rho'_j(r_{ij}) + F'_j(\rho_{h,j})\rho'_i(r_{ij})] \frac{r_{ij}^k r_{ij}^l}{r_{ij}} \quad (3.19)$$

where ϕ'_{ij} , F'_i and F'_j are the partial derivatives of the functions, Ω is the volume of the inner cell, r_{ij}^k is the k th component of the vector extending from atom i to atom j and i is summed over the atoms in the inner cell only.

Chapter 4

Results and Discussion

4.1 Pictorial representation of results

Analysis of the results obtained from the simulations described in chapter 3 is made possible by pictorial views of the positions of the dislocations after each simulation. To clearly illustrate these views, the atoms in their initial configuration have been joined together by triangles resulting in a mesh plot. Figure 4.1 shows a portion of the γ layer without any dislocation, this is the perfect arrangement of atoms without the defect and serves as a reference. Figure 4.2 shows the same portion of the γ layer with the introduced full $\frac{a}{2}[10\bar{1}]$ dislocation labelled X in the figure. The deformed mesh up to the position of the dislocation correspond to the slipped region, while after this position the triangles are undeformed corresponding to the unslipped portion of the structure.

Figure 4.3 shows exactly the same configuration with the externally introduced dislocation X just as in Figure 4.2 but without the mesh. The importance of these meshes in our analysis is therefore seen when Figure 4.2 is compared with Figure 4.3. The position of the dislocation and events leading to it cannot easily be seen in Figure 4.3. Finally the mesh allow us to trace the path of the dislocations as the applied strain on the simulation cell

Figure 4.1: The mesh plot of a portion of the γ layer without any dislocation.

Figure 4.2: A full $\frac{a}{2}[10\bar{1}]$ dislocation (X) inserted into the γ phase.

Figure 4.3: Figure showing the introduced $\frac{a}{2}[10\bar{1}]$ dislocation (X) but without the mesh.

is increased and helps to locate the position of the dislocation core through the stacking fault obtained between partial dislocations.

4.2 Interface interaction with a $[10\bar{1}]$ mixed dislocation

The relaxed structure of the dislocation cores for the structure described in section 3.7.1 were analyzed and the result show that the introduced full dislocation splits into two partial dislocations with a core spreading of the dislocation on the $(1\bar{1}1)$ plane (Figure 4.4) and with a separation distance of 30.25 Å between the partial dislocations.

This is in agreement with similar analysis done by Rao, [16] where a full dislocation on the $(1\bar{1}1)$ plane dissociate into two Shockley partial dislocation with a ribbon of stacking

Figure 4.4: Core spreading of the dislocation on the slip plane in nickel after the initial relaxation at no applied strain (the two partial dislocations are separated by stacking fault).

fault between then according to equation 4.1:

$$\frac{a}{2}[10\bar{1}] = \frac{a}{6}[1\bar{1}\bar{2}] + SF + \frac{a}{6}[21\bar{1}], \quad (4.1)$$

where SF is the stacking fault.

A complete analysis of the results show that for the dislocations which glide down and cut through the interface at points B through E as shown in Figure 3.9, the leading partial extends towards the interface with the band of stacking fault left behind over the region passed through and between it and the trailing partial (Figure 4.5). The motion of the dislocations is such that, before the leading dislocation cuts through the interface, both partial dislocations move together, maintaining the same separation distance between them. In all these cases the leading dislocations continue to move until they get to the interface where they remain until sufficient stress is applied to drive them through. When the resolved shear stress reaches a critical value as the applied shear strain increases, the leading dislocation gets across but the trailing dislocation remain in the Ni layer. This led to the stacking fault extending from the Ni layer into Ni_3Al layer. Further increase in the applied shear strain pushes the trailing dislocation up to the interface where it remained temporarily till the the resulting shear stress is high enough to drive it across into the γ' layer. Once this stage is reached an antiphase boundary is created in Ni_3Al between the trailing dislocation and the interface, as a result of the atoms on the slip plane having slipped by one atomic distance in the slip direction.

Since the results for dislocations cutting through the interface at points B through E are qualitatively very similar, a complete analysis is given for only one of them (D) in this section. Also, since the behaviour of the dislocation introduced in the path of the misfit dislocation at A is considerably different from that of B - E, a detailed analysis of the result obtained from this case is given in section 4.2.1

Figure 4.5: On application of a shear strain the leading partial dislocation extends towards the interface (the interface is identified by the portion where the alternate coloured atoms begins). The position of the trailing dislocation is out of the page of the picture.

Figure 4.6: Plot showing the resolved shear stress on the slip plane vs the applied strain for case A.

4.2.1 Analysis of dislocation interaction

Figure 4.6 is a plot of the resolved shear stress on the slip plane against the applied strain for a dislocation striking the interface at A, directly at the location of the misfit dislocation. At a strain of 0.006, the resolved stress of $0.003037 \text{ eV}/\text{\AA}^3$ acts on the slip plane³. This is shown as point P1 in the figure, this peak corresponds to the critical stress required to break the $[1\bar{1}0]$ misfit dislocation into partials as seen in Figure 4.7 and illustrated in equation 4.2:

$$\frac{a}{2}[1\bar{1}0] = \frac{a}{6}[1\bar{1}\bar{2}] + \frac{a}{6}[1\bar{1}2] + \frac{a}{6}[1\bar{1}0]. \quad (4.2)$$

From Thompson's tetrahedron (Figure 2.9), the $[1\bar{1}\bar{2}]$ and $[1\bar{1}2]$ dislocations lie on the

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³where $1 \text{ eV}/\text{\AA}^3$ equals $16.022 \times 10^4 \text{ MPa}$

Figure 4.7: The misfit dislocation emanates partial dislocations (a and b) on the $(\bar{1}\bar{1}1)$, and $(\bar{1}11)$ planes respectively as the applied strain increased beyond 0.006, for configuration A.

($1\bar{1}1$) and ($\bar{1}11$) slip planes respectively. The result obtained in Figure 4.7 shows the dislocations labelled a and b as the $[1\bar{1}\bar{2}]$ and $[1\bar{1}2]$ dislocations respectively which is in agreement with Thompson's analysis. To conserve the Burgers vector of the dislocation, a $\frac{a}{6}[1\bar{1}0]$ Lomer-Cottrell sessile dislocation is formed at the interface with its core right at the previous position of the misfit dislocation. This dislocation has its Burgers vector on neither of the two slip planes of our structure and therefore it is sessile (cannot glide) [5].

On increment of the applied shear strain to a value of 0.012, the corresponding resolved shear stress is $0.003356 \text{ eV}/\text{\AA}^3$ (point P2, Figure 4.6). This is the stress that has to be overcome in order to move the gliding (external) dislocation up to the interface. What follows after this point is a complex dislocation interaction which is explained as follows; The leading partial dislocation (which is also a $[1\bar{1}\bar{2}]$ dislocation), on getting to the interface (Figure 4.8) restores the interfacial misfit dislocation to its initial configuration (the partial dislocation b, seen on the ($\bar{1}11$) plane in Figure 4.7 is not seen any more). This can be explained as the leading dislocation summing up with the Lomer-Cottrell sessile dislocation to form a $\frac{a}{3}[1\bar{1}\bar{1}]$ dislocation which attracts the partial b extending from the interface on to the ($\bar{1}11$) plane in a reversed reaction of equation 4.2 to restore the misfit dislocation.

After this point, further increment of the applied strain only increased the resulting shear stress without any further noticeable change occurring in the crystal. The trailing dislocation (dislocation labelled c in Figure 4.8 which is still further up in the Ni layer as shown by the arrow) remained in Ni, conserving the stacking fault length as the motion of the leading partial has been stopped by the reaction leading to restoring the interfacial misfit dislocation. The resulting dislocation interaction leading to the restoration of the misfit dislocation demonstrates the disadvantage of an incoherent interface, as the $[1\bar{1}\bar{2}]$ dislocation moved into the γ' phase at a relatively low value of stress.

For the dislocation passing through the interface at position D, Figure 4.9 shows the plot of the resolved shear stress against the applied strain. Using this figure as a reference,

Figure 4.8: The gliding leading dislocation interacts with the dislocation at the interface restoring the misfit dislocation. The position of the trailing partial dislocation c , and the partial dislocation a , are out of the picture as depicted by the arrows.

we define the following important stress values which will be consistently used throughout the remainder of this thesis: σ_o ; the stress required to move the leading dislocation up to the interface, σ_l ; the stress required to move the leading dislocation across the interface into the γ' layer, σ_t ; the stress required to move the trailing dislocation up to the interface, and σ_b ; the stress required to move the trailing dislocation across the interface into the γ' layer. Furthermore, we will use the term “*barrier strength*” to describe the stress required to completely drive both the leading and trailing dislocations into the γ' layer (hence the b subscript for σ_b). Quantitatively, this stress value serves as a measure of the strength of the interface.

The first peak in the figure (point *i*) corresponds to the shear stress (σ_o) required to move the leading dislocation from the starting position up to the interface (as shown in Figure 4.10) and has a value of (0.00177 eV/Å³). The motion of the dislocation is prevented by the interface at this value of stress and further increase in the applied strain was not able to drive the dislocation through until the critical shear stress (σ_l) of 0.00566 eV/Å³ (point *ii*, Figure 4.9) is surpassed.

As the applied strain is increased and the resulting shear stress exceeds σ_l , the leading partial dislocation cuts across the interface into the γ' precipitate (Figure 4.11). At this point, the resulting applied stress was insufficient to drive the trailing dislocation across into the γ' layer. This therefore results in the formation of stacking fault in Ni_3Al (Figure 4.11), shown by the deformed mesh between the two dislocation as seen in the diagram. At point *iii* in Figure 4.9, the resulting shear stress of 0.00675 eV/Å³ was obtained, corresponding to the stress (σ_t) to move the trailing dislocation up to the interface. The stacking fault distance continues to increase until the trailing dislocation was finally able to completely break free from the interfacial resistance at a stress of 0.00723 eV/Å³, which is the barrier strength of the interface (σ_b) for this case (point *iv* Figure 4.9). At this point, an antiphase boundary (shown by the variation in the horizontal arrangement of the atoms

Figure 4.9: Plot showing the resolved shear stress on the slip plane vs the applied strain for case D.

across the slip plane in Figure 4.12) was formed and the interface showed no complex network of dislocations. The dislocation shown in the figure is the trailing dislocation, the leading dislocation is out of the page of the picture as shown by the arrow.

Contrary to expectation from the energy point of view that the partial dislocations should not be too far apart because the farther they are the higher the crystal energy, a long ribbon of stacking fault was obtained in Ni_3Al (indicating the dislocations were far apart) before the trailing dislocation was able to cut across the interface. This could be attributed to the high antiphase boundary energy in Ni_3Al when compared with the stacking fault energy as seen in table 3.3. Therefore, since much higher energy is required to produce an antiphase boundary, the stacking fault separation distance continue to increase until the resulting applied stress was sufficient for the formation of an antiphase boundary.

Figure 4.13 show a summary of the results from the analysis for cases A through E,

Figure 4.10: The leading partial dislocation blocked by the interface when the applied strain was insufficient to overcome the barrier.

Figure 4.11: Leading dislocation extends through the interface into Ni_3Al but the trailing dislocation is still in Ni.

Figure 4.12: Antiphase boundary created in Ni_3Al (from the position of the trailing dislocation to the interface) after the trailing dislocation passed through the interface. Note: No complex dislocation at the interface as a result of this motion.

the plot of the resolved shear stress acting on the slip plane against the applied strain is shown. The plots labelled A through E corresponds to the different dislocation positions considered. The behaviour leading to the shape of these curves is quantitatively similar except for case A, hence only case D was explained as a representative for B - E. The plot of the required stress σ_o to move the leading dislocation up to the interface with respect to the spacing relative to the misfit dislocation is depicted in Figure 4.14. Figure 4.15 shows the plot of the critical stress σ_l required to move the leading dislocations across interface as a function of separation distance from the misfit dislocation.

It can be seen that there is a uniform trend of a decrease in the stress required to move the dislocations up to the interface (Figure 4.14). The rate at which the leading dislocation approaches the interface generally increase from cases A - E, indicating an increased rate of motion when the gliding dislocation is farther from misfit dislocation. For the dislocation considered in case A for example, there was virtually no motion until the applied strain was increased to a value of 0.0045.

Further more, from Figure 4.15, σ_l was very low when the introduced dislocation glides directly on to the misfit dislocation and then increases as the introduced dislocations are further away, reaching a peak at a distance of about 25 Å . After this position it starts to decrease as the distance from the misfit dislocation to the gliding dislocation increases. This shows that the misfit dislocation plays less significant role on the motion of the gliding dislocations when the distance between them is far enough that little or no interaction exist between them. The stress value obtained at point P1 of Figure 4.6 is taken as σ_l for that case since it is the stress required to move the same partial dislocation as in the other cases into the γ' layer.

The plot of the barrier strength σ_b to move the trailing dislocation across the interface into Ni_3Al is shown in Figure 4.16. Comparing corresponding values from this plot to those of σ_o in figure 4.15, it is seen that for each dislocation position, the barrier stress

Figure 4.13: Plot showing the resulting resolved shear stress on application of shear strain.

Figure 4.14: Plot showing the stress required to drive the leading dislocation to the interface.

Figure 4.15: Figure showing the stress required to move the leading dislocation across the interface vs distance from misfit dislocation.

σ_b , is only slightly higher than σ_l . For example, when the dislocation crosses through the interface 25 Å away from the misfit dislocation, the value of the stresses are 0.00763 eV/Å³ and 0.00706 eV/Å³ respectively. This show that once σ_l is reached, the interface does not offer a significant resistance to the motion of trailing dislocation.

4.3 Interface interaction with a [110] screw dislocation

Analysis of the results for the screw dislocation shows quantitatively similar results to that of the mixed dislocation in the sense that after the initial relaxation at no applied strain, the full dislocation dissociated into the correct Shockley partials according to equation 4.3, with core spreading of the dislocation on the slip plane.

Figure 4.16: Figure showing the barrier strength of the interface to the $[10\bar{1}]$ dislocation vs distance from misfit dislocation.

$$\frac{a}{2}[110] = \frac{a}{6}[21\bar{1}] + SF + \frac{a}{6}[121]. \quad (4.3)$$

The leading partial dislocation is the $\frac{a}{6}[21\bar{1}]$ dislocation. Also an increase in the applied strain gave a corresponding increase in the resolved shear stress acting on the slip plane. However, (for cases B through E) the interaction of the partials with the interface is different in this case. On application of increasing shear strain, both partials move together towards the interface, the leading partial on getting to the interface glides through without significant hinderance (when compared to the previous case of section 4.2.1). Here once the leading dislocation gets to the interface it crosses through on the next strain increment. The trailing dislocation however, does not simultaneously cross through, it remains in the γ layer and higher stresses are required to gradually move it through before it finally is able to overcome the interface barrier. While the trailing dislocation is still in the γ layer and the applied strain is gradually increased, the leading dislocation moves further down into the γ' layer increasing the length of the stacking fault ribbon as seen in Figure 4.17.

For this case then, the interface offered a relatively low resistance to the leading dislocation from crossing into the γ' layer, unlike in the previous case. However, despite the interface not offering significant resistance to the leading dislocation, the motion of the trailing dislocation was significantly hindered by this interface. This demonstrates that the resistance offered by the interface depends on the Burgers vector of the dislocation approaching it.

For the introduced dislocation gliding down directly towards the misfit dislocation at A of Figure 3.9, the leading partial dislocation was attracted to the misfit dislocation immediately after the dissociation. At this point the leading dislocation got stuck at the interface and as the applied strain is gradually increased, the trailing partial dislocation moved towards the interface reducing the stacking fault length. Figure 4.18 shows the resulting resolved shear stress on the slip plane as the applied strain is increased. The

Figure 4.17: Large separation distance between leading dislocation (in the γ' layer) and trailing dislocation (in the γ layer) by the interface leading to formation of a long stacking fault.

Figure 4.18: Plot showing the resolved shear stress on the slip plane vs the applied strain for case A

result showed that the increased applied strain only lead to an increase in the resulting shear stress on the crystal, as the dislocation has been locked at the interface and therefore no further motion is possible. Figure 4.19 shows this situation with the dislocations locked at the interface, here, unlike in Figures 4.7 and 4.8 the misfit dislocation did not split into partial dislocations, because the stress being applied is different according to equation 3.18.

Qualitatively in this case also, the results for dislocations crossing through the interface at points B through E gave similar results as in the case of the mixed dislocation. Analysis of case D is given as a sample for these cases. Figure 4.20 shows the plot of the resolved shear stress on the slip plane versus the applied strain. The first peak at i corresponds to the stress required to drive the leading partial dislocation up to the interface σ_0 . Immediately after this point, the leading dislocation crosses to the γ' layer while the trailing get stucked in the γ layer by the interface as shown in Figure 4.21

The next peak at ii in Figure 4.20 corresponds to the stress that must be overcome for

Figure 4.19: Interlock of the misfit and the gliding dislocation at the interface with no dissociation of the misfit dislocation.

Figure 4.20: Plot showing the resolved shear stress on the slip plane against the applied strain for case D

the trailing dislocation to overcome the interface resistance (σ_b). It is noticed from the Figure that after peak i when the leading dislocation has crossed to the γ' layer and the trailing is at the interface, several steps of strain increment were taken before the trailing dislocation was able to cross over into the γ' layer. This confirms that the interface is more resistant to the motion of the trailing dislocation than to the leading dislocation in this case.

A summary of the results is shown in Figure 4.22, where the resulting stress is plotted against the applied strain for all the cases considered. The similarity of cases B through D is shown while that of case A is different.

The plot of the barrier strength of the interface (the stress required move the entire dislocation into the γ' layer) and the stress required to move the leading dislocation across the interface in relation to the position of the misfit dislocation is shown in Figure 4.23. It is shown here that apart from the case when the dislocation crossed through the interface about 10 Å away from the misfit dislocation, the distance from the misfit dislocation does

Figure 4.21: Leading dislocation extends well into the γ' while the trailing dislocation remained tangled with the interface.

Figure 4.22: Plot showing the resulting resolved shear stress on application of shear strain for the cases considered.

Figure 4.23: Figure showing the interfacial barrier strength and stress to move the leading dislocation through the interface away from the misfit dislocation

not affect the strength of the interface. The required stress to overcome the interface when the gliding dislocation is closest to the misfit dislocation is however, much higher than in all other cases. For this case, the plot of the stress required to move the leading dislocation up to the interface σ_o is not shown because this occurs immediately on the first applied load. Thus σ_o is smaller than the accuracy dictated by the size of the load increments.

Also from Figure 4.23, it is clearly shown that the corresponding stress required to move the entire dislocation across the interface σ_b for each dislocation position is much higher than the stress (σ_l) to move the leading dislocation across the interface, unlike in the case of the mixed dislocation. This further confirms the resistance of the interface being dependent on the type of dislocation.

Chapter 5

Conclusion

This thesis has been a detailed investigation into the interaction between the γ / γ' interface and gliding dislocation in the γ matrix.

A full $\frac{a}{2}[10\bar{1}]$ dislocation dissociates into two partial dislocations, $\frac{a}{6}[1\bar{1}\bar{2}]$ and $\frac{a}{6}[21\bar{1}]$ as predicted by Frank's rule based on energy considerations. The $\frac{a}{6}[1\bar{1}\bar{2}]$ is the leading dislocation while the $\frac{a}{6}[21\bar{1}]$ is the trailing dislocation.

Under the application of a shear stress the partials move towards the interface. The fact that in all cases considered, a certain critical stress is reached followed by a drop in the resolved shear stresses (as seen in Figure 4.13) before the dislocations actually gets to the interface shows that the motion of the dislocations is retarded as they approach the interface, the interface therefore constitute an initial barrier.

After the dislocation gets to the interface. The interface does not allow it to cross into the harder layer of Ni_3Al until the barrier strength is overcome. This barrier strength gradually reduces as the crossing point becomes farther from the misfit dislocation. This explains the misfit dislocation itself as a further hindrance to dislocation motion.

The position of the misfit dislocation with reference to the point at which the leading gliding dislocation crosses the interface affects the barrier strength of the interface. The

closer the distance between these two points, the higher the interfacial barrier strength (except for case A). Therefore the dislocations would cross through the interface more easily (at lower applied stress) in the absence of misfit dislocations. The trailing dislocation did not simultaneously cross through the interface when the leading dislocation cut through, but required additional applied stress to do so. However, similar to the case of the leading dislocation the trailing dislocation requires lesser energy to overcome the barrier as the distance between it and the misfit dislocation increases along the interface.

The trailing dislocation requiring higher critical stress to cut through the interface and the long stacking fault distance in Ni_3Al (implying a high lattice energy) is as a result of two factors: First, the interface is a strong barrier to dislocation motion, hence the reason why the trailing dislocation does not simultaneously cross the boundary at the same time the leading dislocation crosses, and secondly a high energy (compared to the stacking fault energy) is required to form an antiphase boundary in Ni_3Al since the motion of the trailing dislocation into the Ni_3Al layer is accompanied by the formation of the antiphase boundary.

On the other hand, when the misfit dislocation is directly in the path of the gliding dislocation, a complex dislocation interaction occurs. The misfit dislocation breaks up into partial dislocations on to the $(1\bar{1}1)$ plane and $(\bar{1}11)$. The partial on the $(\bar{1}11)$ plane extending only slightly from the interface onto this plane while the $\frac{a}{6}[1\bar{1}\bar{2}]$ extends well into the γ' phase on the $(1\bar{1}1)$. The gliding dislocation from the γ phase hits the interface and combines with the $\frac{a}{6}[1\bar{1}0]$ and $\frac{a}{6}[1\bar{1}2]$ partials to restore the interfacial misfit dislocation. The barrier strength of the interface for this condition is $0.003356 \text{ eV}/\text{\AA}^3$ which is much lower than $0.007058 \text{ eV}/\text{\AA}^3$ obtained when the gliding dislocation crosses through the interface $25 \text{ \AA}$ away from the misfit dislocation. This therefore shows a disadvantage of having an incoherent interface with misfit dislocations as the resulting structure will be soft (because the co-operative motion of the dislocations lead to a lower energy) and

allow dislocation to pass through easily as in case A of our analysis. However dislocations find it harder to overcome the interface barrier when passing through close to the misfit dislocation. Farther from it the barrier strength is reduced.

A full $\frac{a}{2}[110]$ screw dislocation dissociates into two partial dislocations, $\frac{a}{6}[121]$ and $\frac{a}{6}[21\bar{1}]$ with the leading partial dislocation being the $\frac{a}{6}[21\bar{1}]$. The interface offered little resistance to the leading dislocation but higher resistance to the trailing dislocation. Therefore, a measure of the strength of the interface depends more on the type of dislocation passing through. The resistance of the γ/γ' interface to dislocation motion in this case is hardly affected by the position of the misfit dislocation since in all cases considered (apart from case A) the barrier strength of the interface to the dislocation is approximately the same (about $0.0058 \text{ eV}/\text{\AA}^3$). The barrier strength of the interface to the $\frac{a}{2}[10\bar{1}]$ dislocation is higher than that for the $\frac{a}{2}[110]$ as seen when the dislocation from same distance to the misfit dislocations are considered for both cases.

For the screw dislocation introduced on the slip plane directly in the path of the misfit dislocation, the motion of the leading dislocation is stopped at the interface by the misfit dislocation. A situation which shows that the dislocations were interlocked and in this case, the misfit dislocation further strengthened the interface.

In this thesis we have used atomistic simulation to study and understand the $\text{Ni}/\text{Ni}_3\text{Al}$ interface interaction with two different types of dislocations. We have obtained the mechanisms of the interactions between the misfit dislocation and the gliding dislocations. And we have been able to quantify the barrier strength as a function of position and type of the Burgers vector of dislocation. We therefore conclude that the dislocation - interface interaction depends on the dislocation considered and the position of the misfit dislocation.

Future extensions to the work done in this thesis can be made as follows . Performing the computations with a much larger cell having the z axis increased to obtain a full 3 dimensional analysis would introduce more realistic dislocation-interface interactions, but

would require parallel computing facilities and more complex visualization tools to analyse the results. This will also help to determine if dislocations with more screw than edge components find it relatively easier to cross through the interface and vice-versa. Another improvement will be to use the correct thickness and dislocation spacing as predicted by continuum mechanics in the work of Shoyket and Hazzledine [38]. Again this requires larger simulations and possibly parallel computing.

Having more of the externally introduced dislocations on planes close to the misfit dislocations and farther from it may help to determine if there is a certain spacing between the dislocations that give the highest barrier strength of the interface. Also comparing this results with the case of a fully coherent interface and one in which the lattice parameter(s) has been altered to change the lattice parameter misfit (δ) may provide insight into the optimal value of δ and the optimal degree of interface coherency for enhanced strength. Finally a simulation with periodicity in all directions which will allow the gliding dislocations after crossing from the γ layer to the γ' layer to continue to the next γ layer may yield important results.

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Appendix A

Sample calculations

A sample of some of the essential calculations made while putting together the thesis is shown in this section. It should be noted that quite a number of other calculations whose values were used in this work are not shown and they could easily be obtained from references cited where their results were mentioned.

A.0.1 Calculation of cohesive energy

For a block of 256 Aluminium atoms, an initial structure was built with a wrong lattice parameter but with the correct fcc configuration and relaxed using the code Dynamo. The energy of the block of atoms was minimized using the conjugate gradient method. The periodic boundary conditions used makes the simulation behave as if we have an infinite crystal and therefore the final energy of the system is just that associated with each atom. Also the periodic box was allowed to relax in all direction to confirm that the returned lattice parameter is the correct value. The final potential energy returned after the minimization is the total relaxed energy ($E_{relaxed}$) of the configuration. The cohesive energy of aluminium E_{coh} is therefore given by

$$E_{coh} = \frac{E_{relaxed}}{N} \quad (A.1)$$

where $N = 256$, the number of atoms and for this particular simulation:

$$E_{coh} = \frac{-860.15954}{256} = -3.36eV \quad (A.2)$$

Applying the same analysis to a block of nickel and Ni_3Al atoms gave the correct cohesive energy for each structure.

A.0.2 Calculation of vacancy formation energy

Repeating the same steps as described in section A.0.1 but now with 500 nickel atoms. The cohesive energy for nickel was obtained as -4.45 eV. Taking this relaxed configuration now and removing one atom such that a vacant site is created, relaxation is then done with this defect in place. The new energy obtained with the vacant site is E_{defect} and the vacancy formation energy E_{vac} calculated as:

$$E_{vac} = E_{defect} - E_{perfect} - E_{coh} \quad (A.3)$$

$E_{perfect}$ is the energy of a perfect structure containing 500 nickel atoms. The values obtained are put in equation A.3 and the vacancy formation energy is obtained as

$$E_{vac} = -2218.948 + 2224.9978 - 4.45 = 1.6eV \quad (A.4)$$

This is in agreement with the published result of the work done by Voter [36]. Similar calculations performed on a block of aluminium and Ni_3Al gave the expected result. In the case of Ni_3Al , however, taking out a nickel atom to create the vacancy is different from when an aluminium atom is taken out due to their different chemical properties.

A.0.3 Calculation of (111) stacking fault energy

To obtain the (111) stacking fault energy in Nickel, a block of atoms stacked in such a way that the (111) planes lie on top of one another in the z direction was built and a stacking fault obtained by removing one layer of atoms such that instead of the ABCABCABC.. fcc closed packed configuration we have ABCBCABC.. pattern. The structure was again relaxed with periodic boundary conditions in all 3 directions. The total energy of the relaxed configuration is sum of the cohesive energy and the stacking fault energy and is given by equation A.5.

$$E_{rel} = E_{coh} \times N + A \times \gamma_{SF} \quad (A.5)$$

The stacking fault energy is therefore,

$$\gamma_{SF} = \frac{E_{rel} - E_{coh} \times N}{A} \quad (A.6)$$

Where A is the area of each (111) plane ($14.9341 \text{ \AA} \times 17.244 \text{ \AA}$). and γ_{SF} is the stacking fault energy. For a block of nickel atoms with 1104 atoms the stacking fault energy per unit area was obtained as

$$\gamma_{SF} = \frac{-4911.876 - (-4.45) \times 1104}{257.524} = 0.003588 \text{ eV/\AA}^2 = 57.49 \text{ mJ/m}^2 \quad (A.7)$$

A.1 Calculation of the thickness of simulation box

The calculations leading to the size of the simulation box described in section 3.3, is shown in this section. Subscript 1 and 2 refers to Ni and Ni_3Al properties respectively.

$$M_1 = 2\mu_1 \frac{1 + \nu_1}{1 - \nu_1} \quad (\text{A.8})$$

$$M_2 = 2\mu_2 \frac{1 + \nu_2}{1 - \nu_2} \quad (\text{A.9})$$

$$H_a = 2C_{44} + C_{12} - C_{11} \quad (\text{A.10})$$

For nickel

$$H_a = [2(1.26) + 1.49 - 2.44] \times 10^{12} \text{erg/cm}^3$$

$$H_a = 1.57 \times 10^{12} \text{erg/cm}^3 = 0.9799 \text{eV/\AA}^3$$

$$\mu = 1.26 - \frac{1}{5}(1.57) \times 10^{12} \text{erg/cm}^3$$

$$\mu = 0.946 \times 10^{12} \text{erg/cm}^3 = 0.59 \text{eV/\AA}^3$$

$$\lambda = C_{12} - \frac{1}{5}H_a \quad (\text{A.11})$$

$$\lambda = [1.49 - \frac{1.57}{5}] \times 10^{12} \text{erg/cm}^3$$

$$\lambda = 1.176 \times 10^{12} \text{erg/cm}^3 = 0.73399 \text{eV/\AA}^3$$

For Ni_3Al ,

$$H_a = [2(1.23) + 1.37 - 2.46] \times 10^{12} \text{erg/cm}^3$$

$$H_a = 1.37 \times 10^{12} \text{erg/cm}^3 = 0.8549 \text{eV/\AA}^3$$

$$\begin{aligned}
\mu &= 1.23 - \frac{1}{5}(1.37) \times 10^{12} \text{erg/cm}^3 \\
\mu &= 0.956 \times 10^{12} \text{erg/cm}^3 = 0.5967 \text{eV}/\text{\AA}^3 \\
\lambda &= [1.37 - \frac{1.37}{5}] \times 10^{12} \text{erg/cm}^3 \\
\lambda &= 1.096 \times 10^{12} \text{erg/cm}^3 = 0.6841 \text{eV}/\text{\AA}^3 \\
\nu &= \frac{\lambda}{2(\mu + \lambda)} \tag{A.12}
\end{aligned}$$

For nickel,

$$\begin{aligned}
\nu &= \frac{0.73399}{2(0.59 + 0.73399)} \\
\nu &= 0.2772 \\
M_1 &= \frac{2 \times 0.59(1 + 0.2772)}{1 - 0.2772} \\
M_1 &= 2.0851 \text{eV}/\text{\AA}^3
\end{aligned}$$

For Ni_3Al ,

$$\begin{aligned}
\nu &= \frac{0.6841}{2(0.5967 + 0.6841)} \\
\nu &= 0.267 \\
M_2 &= \frac{2 \times 0.5967(1 + 0.267)}{1 - 0.267} \\
M_2 &= 2.06281 \text{eV}/\text{\AA}^3
\end{aligned}$$

$$f_1 = \frac{a_1}{a_1 + a_2} \tag{A.13}$$

$$f_2 = \frac{a_1}{a_1 + a_2} \tag{A.14}$$

$$f_1 = \frac{3.52}{3.52 + 3.573}$$

$$f_1 = 0.4963$$

$$f_2 = \frac{3.573}{3.52 + 3.573}$$

$$\begin{aligned}
f_1 &= 0.5037 \\
M^* &= f_1 M_1 + f_2 M_2 \\
M^* &= 0.496264 \times 2.0851 + 0.503736 \times 2.06281 \\
M^* &= 2.07387 eV/\text{\AA}^3 \\
\nu_{avg} &= \frac{\nu_1 + \nu_2}{2} \\
\nu_{avg} &= \frac{0.2772 + 0.267}{2} = 0.2721
\end{aligned} \tag{A.15}$$

The expression for the critical thickness is given by [38] as;

$$\frac{H_c}{b} = \frac{\mu M^* \ln(f_1 \frac{H_c}{b})}{2\pi(1-\nu)\delta M_1 M_2 f_1 f_2} \tag{A.16}$$

$$\tag{A.17}$$

where b is obtained as;

$$b = \frac{a_1}{\sqrt{2}} \tag{A.18}$$

Substituting all the derived values into equation A.16, we get

$$\begin{aligned}
0.401765 H_c &= \frac{1.23053 \ln(0.199383 H_c)}{0.074265433} \\
H_c &= 136.1563 \text{ \AA}
\end{aligned}$$

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with the γ/γ' (Ni/Ni₃Al) interface of a
nickel based single crystal super alloy**

by

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Obafemi Awolowo University.

A thesis submitted to
the Faculty of Graduate Studies and Research
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the requirements for the degree of

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Ottawa-Carleton Institute for
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**An atomistic study of dislocation interactions with the γ/γ'
(Ni/Ni₃Al) interface of a nickel based single crystal super alloy**

submitted by

Adeyemi James Akangbe, B.Sc.
in partial fulfilment of the requirements for
the degree of Master of Applied Science

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Carleton University
April 2003

Abstract

Dislocation interactions are known to be responsible for the ductility and brittleness of materials. A study of how dislocation activities is affected by the interface between two phases of a nickel based single crystal super alloy is presented here.

Atomistic simulations were performed to study the interactions of a $\langle 110 \rangle$ externally introduced dislocations in presence of misfit dislocations on the $\text{Ni}/\text{Ni}_3\text{Al}$ (γ/γ') interface in the super alloy, with the interface between these phases. The Embedded Atom Method (EAM) has been used for the energy simulation and minimization with the Conjugate Gradient Method (CGM).

Dislocations were generated at appropriate spacings in relation to the misfit dislocation in simulation cells relaxed using rigid boundary conditions in two directions and periodicity along the direction of the dislocation line. Shear strains leading to shear stresses were applied in small steps on the computational cell to drive the dislocations across the interface.

Based on the resulting configurations, each $\langle 110 \rangle$ dislocation dissociates into $\langle 121 \rangle$ shockley partials with core spreading of the partial dislocations on the $\{111\}$ slip plane. From the resulting stresses and observation of the relaxed configurations, it was concluded that the interface acts as a barrier to dislocation motion. Also the resistance of the interface is dependent on the dislocation type and the position of the misfit dislocation.

The $\frac{a}{6}[1\bar{1}\bar{2}]$ partial dislocation encounters a significant barrier to its motion across the interface unlike the $\frac{a}{6}[21\bar{1}]$ partial dislocation. Also the interfacial misfit dislocation when directly in the path of a gliding dislocation could either completely stop the motion of the dislocation or allow it to pass through the interface with relative ease depending on the nature of the dislocation.

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List of Symbols

γ	Nickel phase
γ'	Ni_3Al phase
δ	Lattice parameter misfit
τ	Shear stress
G	Shear modulus
$\vec{b}$	Burgers vector of dislocation
τ_{th}	Theoretical shear stress
E_{pp}	Pair potential energy
E_o	Constant reference volumetric energy
r_{ij}	Interatomic distance between atoms
V_2^{eff}	Effective pair potential
E_{tot}	Total energy
F_i	Embedding energy
ρ	Density
ϕ	Interatomic interaction
a	Lattice parameter
E_{coh}	Cohesive energy
C_{11}, C_{12}, C_{44}	Elastic constants
ΔE_v	Vacancy formation energy
H	Thickness
H_a	Anisotropic factor
f_i	Fraction of thickness
s	Dislocation spacing
H_c	Critical thickness

M^*	Average bi axial modulus
ν	Poisson's ratio
μ	Shear modulus
λ	Lame's constant
U_i	Displacement of atom i
X_i	Co-ordinate of the position of atom i
ϵ	Applied strain
N	number of atoms
m_1	Slip plane normal
τ_{res}	Resolved shear stress
σ_{ij}	Atomic level stress tensor
S_j	Slip direction vector
$E_{relaxed}$	Relaxed energy of the atoms
σ_0	Stress to move leading dislocation up to the interface
σ_l	Stress to move leading dislocation across the interface
σ_t	Stress to move trailing dislocation to the interface
σ_b	Barrier strength of the interface
Ω	Volume of inner cell

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Chapter 1

Introduction

1.1 The single crystal nickel based super alloy

Highly-alloyed, precipitate-hardened, nickel-based super alloys have unique properties for use as structural materials at elevated temperatures. Their creep, fatigue, thermal fatigue and corrosion resistance have been significantly improved through chemistry modifications. Many materials which require resistance to high temperatures such as turbine blades are made from these alloys.

Polycrystalline turbine blades with equiaxed grain structures often fail due to creep and environmental induced cracking along the grain boundaries that are aligned perpendicular to the stress axis of the blade [1]. This led to the development of directional solidification processes which eliminate the transverse grain boundaries. Finally a break through was made by completely eliminating the grain boundaries through the use of carefully fabricated single crystal super alloys. These super alloys have superior creep resistance over the polycrystalline and the directional solidified alloys.

Single crystal nickel based super alloys are used in nuclear reactors, submarines, airframes, steam power plants, chemical plants and other applications with the largest portion

being in marine, and aircraft gas turbines due to their high temperature strength, resistance to creep, adequate ductility, and resistance to oxidation and hot corrosion. These alloys consist of two phases, γ and γ' , which in combination produce an alloy of higher strength. A significant factor in this strength increase is the interface between the two phases [2]. The γ phase is nickel rich fcc solid solution matrix, while the γ' phase is an ordered precipitate of Ni_3Al having a $L1_2$ type structure. The volume fraction of the γ' phase in modern nickel based single crystal super alloys (NBSCS) is about 50 - 70 percent [3] which is embedded in the nickel rich solid solution matrix γ .

There exist misfit dislocations at the γ/γ' interface due to the lattice parameter mismatch δ , which is defined from the lattice parameters of the matrix and precipitate γ and γ' respectively as

$$\delta = \frac{a_{\gamma'} - a_{\gamma}}{a_{\gamma'}} \quad (1.1)$$

where a_{γ} and $a_{\gamma'}$ are the lattice parameters of Ni and Ni_3Al respectively. Figure 1.1 shows two blocks of atoms having different lattice constants. Putting the two blocks together leads to subjecting block B to tension (i.e., it is strained) and the block A to compression if a coherent interface with no dislocations is formed. Therefore the lattice misfit introduces a significant internal stress in the crystal. These stresses may be relieved by misfit dislocations at the interface, leading to an incoherent or semicoherent interface [4].

In this research, a computational study using atomic scale modelling is used to study this interface, specifically its resistance to dislocation transmission from γ to γ' and thus its role in the strength of nickel based single crystal super alloys (NBSCS). In the simulations a dislocation is introduced into the softer γ layer, followed by application of shear strain resulting in shear stresses which drives this externally introduced dislocation across this interface in the presence of the interfacial misfit dislocations. This is done along specific

Figure 1.1: Showing two blocks of atoms strained when brought together due to different lattice parameters. A and B shows the configuration before and after being brought together respectively (taken from [4])

planes and at different positions relative to the misfit dislocation. An estimate of the stress required to overcome the interface barrier will serve as a measure of the strength of this interface. Also the interaction between the two dislocations (the misfit and the introduced dislocation) will be studied.

An atomistic approach is used for this study using the embedded atom method (section 3.1.1) to obtained the total energy of the configuration and energy minimization of each structure based on the conjugate gradient method (section 3.2).

1.2 Objective of thesis

This thesis focuses on the Ni/ Ni_3Al super alloy which has found use especially in turbine engines. As the interface between Ni and Ni_3Al has been shown to play an important role in the creep resistance of this alloy, the atomic scale details of this interface and its strength are the focus of this study.

This thesis therefore focuses on this interface with the aim of getting a better understanding of how dislocations interact with it. Since dislocation activities are known to affect whether a material will be ductile or not, a proper understanding of the dislocations interacting with this interface is expected to shed more light on the strength of this alloy.

In getting a detailed understanding of this interface then, the critical stress required to move dislocations across from Ni into the Ni_3Al phase will be determined. Furthermore since the difference in the lattice parameters of the constituents of this alloy has led to misfit dislocations being formed naturally at the interface, the relationship between the introduced dislocation and the misfit dislocations will be studied. That is, we shall find out if the positions of the introduced dislocation relative to the misfit dislocation has any effect on its motion and on the stress to move it across the interface.

1.3 Overview of the thesis

The remainder of chapter 1 include the description of the fcc and the $L1_2$ crystal structures, a brief explanation of plastic deformation and how it is linked with dislocation motion is also explained. Also included in this chapter is the continuum and atomistic approach to computer simulations, the areas where each of these methods has been used and some of the advantages and disadvantages of both methods.

Chapter 2 gives a summary of similar work done in this field and related fields on this alloy and the likes. An in-depth look of how the alloy fails is examined from different perspectives: atomistic simulation, and microscopic analysis using high resolution transmission electron microscopes (microscopy) and diffraction methods. Also, a detailed explanation of dislocations in fcc crystals is explained.

Chapter 3 gives the detailed computational procedure. It showed how the structure was built and the determining parameters. It also gives an explanation of the embedded

atom method and the conjugate gradient method as a means of calculating the energy of the structure and its minimization respectively. Conclusions drawn from the simulations and discussion of results is covered in chapter 4 while the last chapter (chapter 5) gives the final conclusions. Details of calculations not shown in the body of the thesis which are of importance and applicable to future work are given in the appendix.

1.4 The face centered cubic and the $L1_2$ crystal structures

A lot of engineering materials including metals and ceramics are made up of small crystals or grains where atoms are packed in a regular repeating three dimensional pattern. This periodically repeating pattern of arrangement of the atoms is termed crystalline and the actual arrangement of the atoms is called the crystal structure. In visualizing the crystalline structures, atoms are represented as solid spheres having well defined diameters. This is termed the atomic hard sphere model in which spheres representing nearest neighbor atoms touch one another as in Figure 1.2.

Most pure metals have a simple crystal structure usually simple cubic, face centered cubic, body centered cubic or the hexagonal structures, while most alloys and non metallic compounds have a more complex structure. Figures 1.3 and 1.4 show the fcc crystal structure as in Ni and the $L1_2$ structure as in Ni_3Al respectively. Quite a number of engineering materials are however, not pure metals but alloys of two or more metals and solid solutions. The lattice structure of some solid solutions are such that the atoms are arranged randomly on the atomic positions, therefore, for such an arrangement, the two atoms A and B constituting the solid solution can occupy any of the available atomic sites. But in some cases however, each type of the constituting atoms only occupy specific lattice point such that a well defined distribution of the atoms is obtained. Such a situation can

Figure 1.2: Hard sphere model for atomic arrangement

Figure 1.3: The fcc crystal Structure, having atoms at the centre of each face of the cube and at the corners

Figure 1.4: The $L1_2$ crystal structure of Ni_3Al . Similar to the fcc structure in Figure 1.3 but the corner atoms now are the aluminium atoms while the faces of the cube has nickel atoms

be explained as a lattice of crystal A interpenetrating that of crystal B [5] and the result is an ordered solid solution whose lattice structure is now termed a “*super lattice*”. The γ' structure is a typical example of a super lattice. The size of a cube of Ni_3Al is slightly larger than that of Ni and smaller than that of Al due to the difference in the atomic size of the two atoms (Al atoms being bigger than Ni atoms). Therefore since larger Al atoms replace the corner atoms in the fcc structure of Ni there exist an elongation in the length of each side of the cube to accommodate the larger Al atoms and hence the increase in the cube size.

For the face centered cubic (fcc) structure, the atoms are positioned at the corners of a cube referred to as the unit cell and at the centre of each of the six faces of the cube. The atoms touch along the $[011]$ directions and this is termed the closed packed direction.

The (111) planes are the most important in the fcc structure as they are the close packed planes (Figure 1.5) and contain the closed packed directions which are 60° apart.

Figure 1.5: The (111) closed packed planes of atoms in fcc structure

The stacking sequence of the (111) planes is the ABCABCABC arrangement as shown in Figure 1.6. This particular arrangement is one in which the atoms take up the least volume and is called a closed packed structure [6].

It is important to note that there is another alternative for stacking the close packed planes one on another. After the first two layers A and B are obtained there are two possibilities for the third layer, either into the position C as in fcc structure or directly above those atoms in the first layer, thereby generating a ABABAB sequence. This second possibility gives rise to the hexagonal closed packed (hcp) structure. Quite a number of metals belong to either of these structures, for example Ca, Ni, Cu, Ag, Al have the fcc crystal structure while Ti, Mg, Be, Zr, Zn have the hcp structure. The choice of what structure an element takes is a function of that which gives it the lowest energy. Generally then, materials do not necessarily have to be closed packed but take on the structure which

Figure 1.6: The closed pack stacking sequence of fcc crystals

results in the lowest energy configuration [6], as determined by the quantum mechanics of atomic bonding.

1.5 Plastic deformation

Plastic deformation occurs in a perfect crystal when a plane of atoms slides over the atoms on the adjacent plane (Figure 1.7a and b). For this to take place a sufficient amount of stress has to be applied to the structure. The shear stress required for this was first calculated by Frenkel [5]. He assumed that there is a periodic shearing stress to slide one layer over the other given by:

$$\tau = \frac{Gb}{2\pi a} \sin \frac{2\pi x}{b} \quad (1.2)$$

Where G is the shear modulus, b the spacing between atoms in the direction of the shear stress, a , the spacing of the rows of atoms and x , the distance away from the low

Figure 1.7: Illustration of how atoms slide over one another in estimating the stress for slip. (a) atoms at their equilibrium position, (b) the top layer has slipped a distance x relative to the lower layer.

energy equilibrium position. The theoretical critical stress τ_{th} is thus obtained when $\sin\frac{2\pi x}{b}$ is maximum, therefore:

$$\tau_{th} = \frac{Gb}{2\pi a} \quad (1.3)$$

Real crystals however, are not perfect, they have defects which reduces their strength. The calculated resolved shear stresses measured in real crystals, (even in the well annealed ones) are many order of magnitudes smaller than the theoretical critical stress τ_{th} . The wide variation between the predicted value and the experimentally calculated value is attributed to imperfection in the crystal. The dislocation is a defect that has the effect of allowing materials to deform plastically (yield) at stresses much lower than the predicted theoretical stress.

1.6 Continuum models

The branch of mechanics which focuses on the stresses in the three states of matter (solid, liquid and gas) and their deformation is termed mechanics of a continuous medium [7]. The continuum theory is the form of partial differential equations describing the conservation laws and constitutive relations. It is assumed that all mathematical functions based on this theory are continuous and the derivatives also continuous. Further more continuum theories rest on the assumption that the relevant fields that describe the state of the material vary slowly on the atomic scale. Therefore the theory breaks down in the vicinity of lattice defects and cannot model any phenomenon on the atomistic scale such as dislocation nucleation and material fracture [8].

The continuum approach has been successful in quite a number of areas such as solid and fluid mechanics. It is very efficient, simple and often involves very few material parameters, but it becomes inaccurate for problems in which the detailed atomistic processes affect the macroscopic behavior of the material, or when the scale of the medium becomes small enough that the continuum approximations becomes unsuitable [4].

However, despite the lapses, the continuum model has been used in conjunction with continuum field models of dislocations, and finite element methods to solve several dislocation problems [8], such as computing the overall stresses due to dislocations, interactions between dislocations and the stress driven motion of dislocations. Other features such as stress concentration due to dislocation pile up [8], hardening by inclusions impeding dislocation motion and fatigue crack growth have been modelled using the combination of continuum and atomistic models.

1.7 Atomistic simulation

From section 1.6 above, it is clear that to fully understand the behavior and responses of materials, a detailed atomistic modelling may be required. Macroscopic properties of materials are obtained from atomistic observations, especially for small models in the nanometer range. The explanation to why materials are brittle or ductile is linked to bond breaking and the deformation that takes place due to dislocations. Such details cannot be revealed by the continuum approach and hence require atomistic explanations.

The breakthrough by physicists in the 1920's gave the knowledge to describe the behaviour of nature down to the atomistic scale in terms of atoms and electrons [9]. The improved development in the computer world which has led to the production of faster and cheaper computers has also significantly aided this process. This improved knowledge obtained using computers for atomistic simulations has led to it being a major field in physics, chemistry and biology [9].

Several methods exist for performing various calculations using atomistic simulations. In most cases the methods differ from one another in terms of the speed, accuracy and ability to describe specific phenomena. These atomistic simulations give the exact nature of the study being done as the results are obtained from the most fundamental possible approach. However, it must be realized that despite the accuracy and significance of computer simulations, a simulation is not nature [9] and it is therefore essential that which ever simulation method is being used, the result should in as much as possible be compared with experimental values.

1.7.1 Atomistic modelling

The structure to be modelled is built by representing each atom in the structure by their co-ordinates in three dimensions and placing them in a simulation box. Each atom interacts

with its neighboring atoms according to known forces and the energy associated with each atom is computed. By summing up the energies of the individual atoms the overall energy for the structure is determined. The energy of the configuration is described using inter-atomic potentials, which are function of the position of the atomic nuclei. Also included in the potentials is the electron - nucleus interaction, since the positions of the nuclei affects those of the electrons. Various atomic potentials have been developed for these simulations, with each one having its up side and down side as will be discussed in chapter 3.

Quite a number of methods exist for performing atomistic modelling and the choice depends on the goal and the available method. In molecular dynamics approach an assembly consisting of N atoms for example is governed by $3N$ simultaneous equations of motion which are derived as a function of time for simulating the movement of each atom [10]. Several other methods have been used for these simulations, the quasi-dynamic method, the direct variation method and Monte Carlo methods are a few examples.

The quasi-dynamic method of simulation is employed at zero Kelvin, and the equilibrium (lowest energy) configuration obtained by minimizing the kinetic energy of each atom and allowing them to converge to the minimum energy position [4]. The direct variation method involves adjusting the atomic co-ordinates of each atom until the net force on all atoms reaches the minimal.

For the present work, after building the block of atoms (based on the structure of the alloy considered, such as the lattice type and lattice parameter), the energy of the configuration so obtained is taken as the starting point for the minimization process. The atoms are then moved around using the the conjugate gradient method to minimize the energy. The final configuration is thus the one with the entire structure in the lowest possible energy based on the atomic potentials used and is termed the “*relaxed*” configuration. The difference between the energies of the new position and the previous one is taken and the

process is continued until this difference becomes insignificant. This method of atomistic simulation works well in getting accurate results but requires significant computer memory and time for each simulation (a function of the size and starting configuration).

Chapter 2

Background and Literature Review

2.1 Previous studies on Ni/Ni_3Al and related structures

Despite the high temperature properties of these alloys, it has been found that under the application of uniaxial stress at elevated temperatures the morphology of the precipitate changes, ultimately leading to failure [11]. This change is termed "rafting" of the γ' precipitate which is as a result of coarsening of the precipitates. Previous work done by Kolbe, Dlouhy and Eggeler has shown experimental evidence of a relationship between the susceptibility to coarsening and dislocation interactions with the interface [12]. The study of dislocations in these alloys is therefore necessary to get a better knowledge on this change in morphology, with an eye toward explaining the effect of dislocations on future coarsening. Several approaches has been taken to explain this phenomenon, atomistic simulations, experimental creep test and investigation of effect of other alloying elements among others are examples of the different approaches taken to get a better understanding of these alloys.

2.1.1 Computational approach

Atomistic simulations have been used in great detail to study dislocation emission and motion and to predict strength of materials. The formation and characteristics of misfit dislocation in heterostructures has been done extensively by Nandekar [13]. Using the f.c.c. Au/Ni (15.9% mismatch) as a case study, he concluded that nucleation of misfit dislocations in compressed films begin by formation of vacancies near the film surface. The simulation also demonstrated that the site of nucleation of the dislocation is near the free surfaces and also showed the differences in energies for the 60 degrees and 90 degrees dislocations for the (111) and (110) interfaces. The activation energy barrier for misfit dislocations in his work was then interpreted to be the energy required to generate vacancies leading to the misfit dislocations, and that dislocation types depended on interface orientations.

The interaction of $\frac{1}{2}\langle 110 \rangle$ screw dislocations with symmetric $[110]$ tilt boundaries was investigated by a group of researchers using atomistic simulations [14]. They came up with useful information on the attraction of a lattice Shockley partial dislocation towards grain boundary and transmission through the grain boundary under the influence of a shear stress in Cu_3Au .

The Coupled Atomistic and Discrete Dislocation (CADD) method described by [15] has been used for multiscale modelling of plasticity, combining simultaneously atomistic and continuum degrees of freedom. This method combines atomistic and continuum regions that communicate across a coherent interface. CADD is able to track dislocations as they pass through the atom / continuum boundary. It is specifically useful in the study of problems involving a large number of dislocation which would be too cumbersome for fully atomistic modelling, and is able to produce accurate atomistic details when required.

A fully atomistic simulations of dislocation / interface interactions was done by Rao and Hazzledine [16] using Cu-Ni multilayer as an example. They investigated four parameters

that attribute to the fact that a nanolayered structure of two types of metals possesses increased strength as the layer thickness is reduced. The parameters responsible for this were the elastic moduli, lattice parameter, gamma surface and slip plane mismatches between adjacent layers. The barrier strengths of various interfaces was studied and the strength of misfit dislocations as barriers to glide dislocations investigated.

An atomistic structural study of the mechanism responsible for the improved ductility in polycrystalline Ni_3Al was studied by Da Chen, Min Lu and Lin T. [17]. They concluded that Boron enhances the cohesive strength of the grain boundaries and simultaneously eases the slip transfer across the boundary. This conclusion was based on their results which show that Boron segregation facilitates the Ni rich layer to serve as a source and sink of dislocation, thereby easing the slip transfer across grain boundary. Stress concentration across the boundary by pile up of dislocations is therefore relieved and thus the tendency for intergranular fracture is reduced.

2.1.2 Experimental approach

The microstructure of the single crystal super alloy as obtained by the work of Pierre carron and Tasadduq [18] is shown in Figure 2.1. Previous work done on determining the locally acting loads during service life of a turbine blade by investigation of the microstructure revealed that the γ/γ' precipitates of which the blade is made of are oriented on a cuboid to cuboid bases in same orientation [19]. The picture seen in Figure 2.1 shows the microstructure in 2-D, but in 3-D, each of the flat plate seen is actually a cuboid and the orientation of the cuboid in both phases are same, e.g the $\langle 110 \rangle$ direction in the γ' phase is parallel to that of the γ phase and same to all other directions.

At very high operating temperatures of about 900° centigrade, it has been experimentally found that the γ' cuboidal precipitates become unstable and link together to form plates called "rafts". This process, "*coarsening*" of γ' precipitates leads to the instability

Figure 2.1: The γ/γ' microstructure of a first generation single crystal superalloy. The large whitish blocks are the γ' precipitates and the dark patches in between them is the γ matrix (taken from [18])

of this strengthening phase and therefore a reduction in the creep resistance of the alloy [20].

A study of the coarsening of the strengthening γ' phase was studied by T.M Pollock and S. Argon [21]. Two samples of the super alloy containing about 70 % volume of the γ' was used with one sample containing a higher fraction of Ta and Ti to alter the lattice parameter misfit. Creep tests were performed on the samples and the results were analyzed using the transmission electron microscope. They concluded that the orientation of the rafts formed on application of stress depends on the positive / negative sense of the misfit of the alloy, they also found that the coarsening which is directional does not occur at a significant rate until some amount of creep has occurred introducing dislocations into the microstructure, and that rafting occurs by the coalescence of the γ' phase on well defined planes.

A dislocation based criterion for the raft formation in Nickel based single crystal super

alloys was reported by Buffiere and Ingot [3], and supported by experimental observations. They found that the precipitate face which exhibit dislocations will grow during creep by coarsening of the γ' phase. Also, the mechanism responsible for this relationship can be linked to the effect of these dislocations on coherency stresses.

Aoki and Izumi [22] also did a study on the effect of Boron as an alloying element in Ni_3Al , as it accounts for an improved ductility at ambient temperature. The effect of other alloying elements on the super alloy has also been done by Linruo Zhao [1]. A high temperature strengthening was linked to the addition of Re. This was attributed to the the slow diffusion of Re thereby reducing the γ' coarsening rate at high temperatures. The formation of of Re rich clusters in the γ matrix and Re-induced negative $\gamma - \gamma'$ misfits has been linked to a prolonged stress ruptured life [1].

2.2 Dislocations

Dislocations are the phenomenon used to explain the ductility in metals as it accounts for the plastic deformation. A simple illustration of a dislocation begins with the idea of slip. In an ideal case, a crystal deforms by planes of atoms sliding over one another. There is one unit of slip on a slip plane when all the atoms on one side of the plane moved to a position initially occupied by the nearest neighbor in the direction of slip. Therefore a unit slip does not disturb the crystal perfection as the atoms are left in register across the slip plane [23].

For most real crystals, however, a uniform slip across the slip plane does not occur. An illustration is shown in Figure 2.2 where a unit slip has occurred only over a portion of the crystal, with an unslipped region on the other part of the crystal. The slipped region and the unslipped region are separated by the dislocation. From the figure, line AD (dislocation line) is the boundary within the crystal separating the slipped area ABCD

Figure 2.2: Slip leading to edge dislocation. A unit slip has occurred over the area ABCD and the dislocation line AD separates the slipped and unslipped regions (taken from [23])

from the unslipped area.

Putting the atoms in the structure of Figure 2.2 and looking in along line AD, shows the position of the dislocation (Figure 2.3). This type of dislocation is called edge dislocation. If now the dislocation was able to move across the slip plane from one side of the crystal to the other then the crystal will deform as shown in Figure 2.4. This shows how slip, dislocation and dislocation motion leads to plastic deformation.

This same idea could be more clearly seen from atomistic view by considering Figure 2.5 where the edge dislocation has moved from plane A (a), to plane B (b) and finally to produce a unit step of slip as shown in (c) under the application of shear stress. The plane along which the dislocation line moves is the slip plane and the final result gives a permanent deformation.

Dislocations are linear imperfections (line defects) that occurs at places where the crystal stacking has been disrupted such as to produce an extra half plane as in edge dislocation or a spiral as in screw dislocation. Figure 2.3 shows an edge dislocation with

Figure 2.3: Showing a plane of atoms normal to the dislocation line of Figure 2.2 and the dislocation formed as a result of slip (taken from [23])

an extra half plane of atoms. The dislocation line is defined along the edge of the extra plane of atoms. Atoms above the dislocation lines are compressed while those below are pulled apart as seen in the slight curvature for the vertical planes of atoms which bends around the extra half plane of atoms. The distortion decreases as one move away from the dislocation and far away from it the crystal is in its perfect form. When the extra half plane is above the slip plane as in Figure 2.3 is referred to as positive edge dislocation and when it is below, a negative edge dislocation.

A screw dislocation can be though of as formed when a shear stress is applied on a block as to produce the distortion shown in Figure 2.6, the upper front region of the crystal has been shifted by one atomic distance to the right relative to the bottom part.

One very important definition of a dislocation is expressed in terms of the Burgers circuit. Any atom to atom path taken in a crystal containing dislocations which forms a closed loop is termed Burgers circuit. An example of a Burgers circuit is shown in Figure

Figure 2.4: Dislocation motion leading to plastic deformation. (a) application of shear stress to deform the crystal. (b) and (c) dislocation has moved a fraction of the offset b . (d) dislocation has moved to the other end of the crystal (taken from [23])

Figure 2.5: Motion of edge dislocation on the slip plane resulting in a step being formed on the surface of the crystal (taken from [24])

Figure 2.6: Illustration of a screw dislocation (taken from [24])

2.7 a i.e path MNOPQ. When the same path is taken in a material without a dislocation, the circuit does not close Figure 2.7 b. This shows that the first case encloses at least one dislocation. The vector required to close the circuit as shown in 2.7 b is termed the Burgers vector $\vec{b}$, also defined as the magnitude and direction of the lattice distortion associated with a dislocation.

When this atom to atom movement is made in two crystals, one having an edge dislocation and the other a screw dislocation, the Burgers vectors are found to have different directions with respect to the dislocation line. The Burgers vector is perpendicular to the dislocation line for edge dislocations and parallel to the dislocation line for screw dislocations.

Most dislocations found in materials are, however, neither pure edge nor pure screw but a combination of both. This condition is termed a mixed dislocation. The Burgers vector and dislocation line in this case are neither parallel nor perpendicular. All the three

Figure 2.7: Burgers circuit of dislocation, (a) Burgers circuit enclosing a dislocation, (b) the same Burgers circuit drawn in a perfect crystal shows the closure failure (taken from [5])

Figure 2.8: Showing the 3 dislocation types. At point A it is pure screw, while at point B it is pure edge, for regions between A and B the character is mixed (taken from [24])

different types of dislocations (edge, screw and mixed) are shown in Figure 2.8, the lattice distortion produced away from the two faces is mixed, with the dislocation having both edge and screw character. It is worthy to note that even though a dislocation changes direction and type (e.g edge to screw or mixed), the Burgers vector will be the same at all points along the dislocation line.

2.2.1 Dislocations in fcc crystals

Many of the important metals used in engineering have the fcc crystal structure. The energetically favoured dislocation in fcc has the $\frac{a}{2}[110]$ Burgers vector of dislocation and the slip plane is the $\{111\}$ plane [5]. The slip plane and the direction of motion of dislocation

Figure 2.9: Thompsons Tetrahedron showing the various slip systems in a fcc structure (taken from [5])

is termed the *slip system*. This depends on the the crystal structure of the given metal and it is that which gives the minimum atomic distortion on the motion of the dislocation [24]. As stated in section 1.4, the slip plane has the most dense atomic packing (see Figure 1.5), i.e the greatest planar density. The direction of slip has the highest linear density. For the FCC crystal structure, the $\{111\}$ planes and $[110]$ directions are the slip planes and directions respectively. There are four (111) type planes and each consists of three possible $[110]$ directions. Each combination of a plane and a direction constitute a slip system thus there are twelve slip systems in the fcc structure as shown in Figure 2.9 (*Thompson's Tetrahedron*). Folding the big triangle DDD (Figure 2.9) along lines AB, BC and AC brings all the points D together to form the tetrahedron. This resulting tetrahedron contains four triangles representing the four (111) type slip planes of the fcc structure. The orientation of each of the planes in the crystal is as seen in Figure 1.5

Heidenreich and Shockley suggested that a unit dislocation would dissociate into two half (*partial*) dislocations [25]. This has been shown to be true and could be explained

using the Thompson tetrahedron. Considering the triangle at about the centre of the Figure for example, it shows the (111) plane and the three possible full dislocations on this plane with their corresponding partial dislocations. The following dissociation takes place:

$$\frac{a}{2}[0\bar{1}1] = \frac{a}{6}[1\bar{2}1] + \frac{a}{6}[\bar{1}\bar{1}2] \quad (2.1)$$

$$\frac{a}{2}[1\bar{1}0] = \frac{a}{6}[1\bar{2}1] + \frac{a}{6}[2\bar{1}\bar{1}] \quad (2.2)$$

$$\frac{a}{2}[\bar{1}01] = \frac{a}{6}[\bar{1}\bar{1}2] + \frac{a}{6}[\bar{2}11] \quad (2.3)$$

The terms on the left hand side are the full Burgers vector of dislocation, while those on the right are the Schockley partials.

As the two partials separate they leave a a band of stacking fault between them on the slip plane. Elastic interactions between the partials suggest that the two half dislocations should move further apart but as they do, the area of the fault increases and so does the energy of the crystal. Therefore, an equilibrium configuration is reached with a finite spacing between the dislocations and having a fixed stacking fault width. Crystals with a high stacking fault energy therefore, have closely spaced partials e.g Al and those with a low stacking fault energy (such as Au) have widely spaced partials.

2.2.2 Dislocations in Ni_3Al super lattice

Figure 1.4 is the Ni_3Al super lattice structure, if the aluminium atoms do not occupy well defined positions then the dislocation in the crystal will be similar to that of an fcc structure as described in section 2.2.1. But since the atoms are in an ordered position,

Figure 2.10: Positions of atoms on two adjacent (111) planes of Ni_3Al superlattice (taken from [5])

this introduces a difference in the dislocation of this structure. This $L1_2$ structure is quite similar to that of the fcc but for the different atoms, and so it has the same slip planes and slip directions. Figure 2.10 is the arrangement of atoms on a (111) plane of Ni_3Al superlattice, the shaded circles are the aluminium atoms and the open circles are the nickel atoms.

In a pure metal having an fcc structure, the slip $\frac{a}{2}[\bar{1}10]$ produces a unit dislocation, but in Figure 2.10 above, such motion leads to moving the atom at position X to Y and thus there is a change in the arrangement of atoms across the slip plane mainly due to a Ni atom now occupying the position of an Al atom. Such a distortion in the arrangement of atoms creates an antiphase boundary. However, this distortion is removed when the atoms are further moved by another displacement of $\frac{a}{2}[\bar{1}10]$ which brings the atom initially at X

to Z. Therefore in the Ni_3Al lattice, a full dislocation termed “*superlattice dislocation*” is a combination of two $\frac{a}{2}[\bar{1}10]$ joined by an antiphase boundary. From the energetic point of view, the $\frac{a}{2}[\bar{1}10]$ dislocations will then dissociate into Schockley partial dislocations of type $\frac{a}{6}[1\bar{2}1]$. The dislocation in the $L1_2$ crystal structure is thus termed “*super dislocation*” because of the longer repeat distance in the lattice. Dislocations from Ni cannot easily cross the interface into Ni_3Al because of the super lattice nature of Ni_3Al .

2.2.3 Precipitation hardening

Precipitation hardening is one of the heat treatment method used to increase the strength of metals and alloys. Such metals and alloys have a solid solubility which decreases as the temperature falls, they therefore have the potentials for precipitation hardening [26]. These precipitates are second phases which is not dissolved but dispersed in the matrix and are the source of strength in most Aluminium and Titanium alloys [27]. These precipitates obstructs dislocation motion during deformation by making the dislocation bow between them leaving a dislocation loop around the particle. Alternatively the dislocation could be forced to cut through the precipitate [28] but this is usually though to do as the precipitates are stronger than the matrix. By this restricted motion of the dislocation during deformation, the alloy is thus strengthened.

Precipitation strengthening involves heating the alloy to a temperature where the second phase is completely dissolved such that there exist only one phase as shown in Figure 2.11.

An alloy of composition Co is heated and held at temperature T_o till all the β phase is dissolved. The alloy is then cooled rapidly to room temperature (T_1), usually by quenching in cold water such that the β phase is prevented from being formed, thus in this condition the alloy consist of supper saturated solid solution of α phase. The final step is the formation of the tiny uniformly dispersed precipitates (β phase) which is obtained after leaving the alloy for a sufficiently long time at T_1 (natural aging). Alternately the super saturated solution could the heated to temperature T_2 at which there is increased diffusion and held till the precipitates are formed (artificial aging). Figure 2.12 shows the products obtained during the process of aging the supersaturated solution. In order to achieve a lower energy state, the precipitates are spontaneously formed until the equilibrium phase is obtained and this is accompanied by a reduction in energy of the alloy.

It should be noted that the strength of the final product is a function of the properties

Figure 2.11: A hypothetical Binary Phase diagram for two metals A and B. Note the solid solution α has a decreasing solid solubility in A as the temperature decreases

Figure 2.12: Stages in precipitate formation from the high energy supersaturated phase to the equilibrium position through the spontaneous release of energy [taken from [28]]

Figure 2.13: A schematic curve showing the strength of a precipitation hardened alloy with aging time at a given temperature[taken from [28]]

of the β phase, the precipitation temperature and aging time. Different precipitates will therefore have a different combination of these conditions for optimum strength. Figure 2.13 shows the relationship between the aging time at a given temperature and strength of the alloy.

Chapter 3

Simulation tools and computational procedure

3.1 Atomic potentials

The pair potential method, a two - body inter - atomic potential derived from fundamental considerations or by empirical means [29, 30] has been used by many physicists for atomistic simulation. The Lennard-Jones potentials, Born-Mayer potential, etc. are based on this method [4]. This method gives the total energy of a block of atoms directly but requires the use of an accompanying volume dependent energy to describe the elastic properties of a metal [31]. Any uncertainty therefore in the volume may automatically affect the reliability of the results of a pair potential calculation since the elastic properties of the solid may not be accurately represented. This problem arises in calculations involving surfaces, due to the fact that the exact termination of the volume on an atomic scale at the surface is not well defined.

Finally, the pair potential, though has been very successful in applications to inert elements such as Helium, fails when it comes to application on chemically active metals.

It was shown that the energy of hydrogen atom in a transition metal cluster cannot be represented by pair interactions [32] but that of helium can be represented.

For a given block of atoms the total energy of all atoms using the pair potential method is obtained by summing up the energy of each pair of atom. Each pair of atom has an atomic interaction which contributes to the total energy of the structure. The configuration energy of the structure based on the pair potential is given by equation 3.1 [33, 34].

$$E_{pp} = E_o + \frac{1}{2} \sum \sum V_2^{eff}(r_{ij}) \quad (3.1)$$

E_o is a constant reference energy or volumetric energy, r_{ij} is the interatomic distance between atoms i and j and $V_2^{eff}(r_{ij})$ is the effective pair potential.

A better potential for treating metallic systems is the embedded atom method [35] which can be applied to inert and chemically active metals and also to crystal structures which includes defects. This is made possible since the problem of volume-dependent energy is replaced by the embedding energy which is electron density dependent and the density is always clearly defined. A detailed explanation of the embedded atom method is given next.

3.1.1 Embedded atom method

As stated in chapter 1, the embedded atom method is used for the atomistic computation in this thesis. This method is adequate for treating most metallic systems where dislocations, fractures, surfaces, impurities, etc are important [35]. The embedded atom method was developed on the assumption that each atom in a given configuration can be viewed as an impurity in the host of other atoms, and from the quasiautom concept the total energy of the atoms is given by

$$E_{tot} = \sum F_i(\rho_{h,i}) \quad (3.2)$$

Where F_i is the embedding energy, $\rho_{h,i}$ is the density of the host at the position $\vec{r}_i$ but without atom i, and therefore, the total energy is the sum of the individual contribution from each atom. Equation 3.2 however, neglects the core-core repulsion which is corrected by including an additional term which takes the form of a short range pairwise repulsion between the cores. The total energy now including this term is

$$E_{tot} = \sum F_i(\rho_{h,i}) + \frac{1}{2} \sum \phi_{ij}(r_{ij}), \quad (3.3)$$

where ϕ_{ij} is the pair potential, r_{ij} is the distance between atoms i and j. Comparing equation 3.3 with equation 3.1 for the pair potential method, the volumetric energy E_o has been replaced with the density dependent F_i which helps to overcome the ambiguity associated with defining the volume in the pair potential method. Taking Nickel as an example, a plot showing the relationship between the density and the embedding energy is shown in figure 3.1.

On the assumption that the host density is approximately equal to the sum of the contribution from each neighbor's electron density (ρ) of the constituting atoms, then

$$\rho_{h,i} = \sum \rho_j(r_{ij}) \quad (3.4)$$

The energy is thus a function of only the position of the atoms. ρ_j is the contribution to the total density from atom j, $\rho_{h,i}$ is the total host electron density at atom i. Figure 3.2 shows the relationship between the density and inter - atomic distance in Ni.

Figure 3.3 shows the relationship between the interatomic interaction ϕ_{ij} and the interatomic distance in Ni. It is clear from the figure that the interatomic repulsive force between the atoms are greatest when atoms are closer together.

Figure 3.1: Plot showing the embedding energy $F(\rho)$ against density (ρ) in Nickel

Figure 3.2: Plot showing a reduction in the density as the inter - atomic distance increases

Figure 3.3: Graph showing the interatomic interaction vs atomic distance in Nickel

$F(\rho)$ and $\phi(r)$ are determined from the properties of the pure metal for each element, such as the lattice constants, cohesive energy, vacancy formation energy, heat of sublimation etc. In the case of an alloy the unlike atom pair potential is taken as the geometric mean of the interaction between like atoms $\phi_{(ii)}$ and $\phi_{(jj)}$. The inter atomic pair potential for dissimilar atoms is therefore given by

$$\phi_{ij}(r) = \sqrt{\phi_{(ii)}\phi_{(jj)}} \quad (3.5)$$

where $\phi_{(ii)}(r)$ and $\phi_{(jj)}(r)$ are the interatomic interactions between like atoms.

Some constraints are imposed on these functions to give satisfactory results. F is linear at higher densities and constrained to zero at zero density. The cut off radius was chosen to be the shortest distance to give an acceptable fit such that beyond this distance atoms are assumed not to interact and $\phi(r)$, $\rho(i)$ and ϕ are all zero at distances greater than the cut off radius.

3.1.2 Interatomic potentials for Ni, Al, and Ni_3Al

Accurate potentials for the NiAl system of alloys using the EAM approach have been produced by [36] and is used for the simulation in this work. These potentials have been fitted to treat Ni, Al and Ni_3Al alloys. Only the essential results from the fit is presented below, a detailed result and procedure is found in article [36].

For the properties shown in tables 3.2, 3.1 and 3.3, a is the lattice parameter, E_{coh} ¹ is the cohesive energy, B is the bulk modulus², C_{11} , C_{12} and C_{44} are the elastic constants. ΔE_{vac} is the vacancy formation energy, SISF and APB are the super intrinsic stacking fault and the antiphase boundary energy respectively. The calculated values are obtained using the potentials and from the tables it can be seen that these values are in reasonable

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¹where 1 eV equals 1.6022×10^{-19} Joules

²where 1 erg/cm³ equals 0.1 Pa

Table 3.1: Metal properties used in fit for *Ni* with the calculated and experimental values.

<i>Ni</i> properties	Experimental values	calculated values
a (Å)	3.52	3.52
$E_{coh}(eV)$	4.45	4.45
$B(10^{12} \text{ erg/cm}^3)$	1.81	1.81
$C_{11}(10^{12} \text{ erg/cm}^3)$	2.47	2.44
$C_{12}(10^{12} \text{ erg/cm}^3)$	1.47	1.49
$C_{44}(10^{12} \text{ erg/cm}^3)$	1.25	1.26
$\Delta E_v(eV)$	1.6	1.6

Table 3.2: Metal properties used in fit for *Al* with the calculated and experimental values

<i>Al</i> properties	Experimental values	calculated values
$a(\text{Å})$	4.05	4.05
$E_{coh}(eV)$	3.36	3.36
$B(10^{12} \text{ erg/cm}^3)$	0.79	0.79
$C_{11}(10^{12} \text{ erg/cm}^3)$	1.14	1.07
$C_{12}(10^{12} \text{ erg/cm}^3)$	0.619	0.652
$C_{44}(10^{12} \text{ erg/cm}^3)$	0.316	0.322
$\Delta E_v(eV)$	0.75	0.73

Table 3.3: Metal properties used in fit for *Ni₃Al* with the calculated and experimental values

<i>Ni₃Al</i> properties	Experimental values	calculated values
$a(\text{Å})$	3.567	3.53
$E_{coh}(eV)$	4.57	4.59
$C_{11}(10^{12} \text{ erg/cm}^3)$	2.30	2.46
$C_{12}(10^{12} \text{ erg/cm}^3)$	1.50	1.37
$C_{44}(10^{12} \text{ erg/cm}^3)$	1.31	1.23
$\Delta E_v(eV)$	1.6 ± 0.2	1.64(Ni),1.87(Al)
SISF (111) (mJ/m^2)	140 ± 14	83
APB (111) (mJ/m^2)	180 ± 30	142

agreement with the experimental values.

3.2 Conjugate gradient method

The conjugate gradient method is one of the techniques used for energy minimization of a set of atoms under a given interaction model. It is used here to obtain the equilibrium state configuration of a group of atoms. This method proceeds by generating vector sequences of iterates (i.e., successive approximations to the solution), residuals corresponding to the iterates, and search directions used in updating the iterates and residuals. It uses the gradient of the function in locating the minimum as the gradient predicts the path and how the function changes. After obtaining the initial gradient, the process continues by searching for a lower value of the function in a direction which is conjugate to the old gradient. A comprehensive explanation of this method is given in [37].

3.3 The computational cell

The computational cell consists of Ni and Ni_3Al constructed on a cuboid to cuboid basis with the same orientation and the boundary plane being the (001) as is known from diffraction pattern results from experimental analysis done on samples by Richard and Fonda [2].

The dimensions of the box (as justified in a section 3.5) is 167 Å by 155 Å by 5 Å in the x, y and z directions respectively and having a total of 11,704 atoms. The axes of the two crystals were oriented such that $x = [1\bar{1}0]$, $y = [001]$ and $z = [110]$. This is obtained by rotating the crystal from the standard xyz [100] orientation to this preferred orientation to aid visualization. The use of periodic boundary conditions means that the cell contains two interfaces, one at the middle and one on the top / bottom as shown schematically in figure 3.4. The rectangle (2-d view of the box containing the atoms) shown in the picture

Figure 3.4: Two interfaces formed in the simulation cell as a result of applying periodic boundary conditions.

represent the simulation cell, periodic copies are made by placing a duplicate copy of one rectangle on the other such that the two lines labelled as interface 1 match each other. With this configuration, two interfaces are thus obtained in our simulation cell. The use of the minimum periodic length ($5 \text{ \AA}$) in the z direction means that our simulation will only contain straight dislocations with infinite line length along the z direction.

3.4 Determining the right computational cell

From the preliminary understanding of the structures of the γ / γ' interface, the first step in the simulation is to build the appropriate starting structure. With knowledge of the crystal structures, we could simply build a block of Ni atoms and that of Ni_3Al and bring them together to obtain the desired interface. However, due to the difference in lattice parameters of the two materials there arises the difficulty of the size to build such that when brought together they match exactly in length along the interface. This is required so that periodic boundary conditions can be applied to the simulations and the result of this is depicted in Figure 3.4. To obtain the correct structure, and ensure that misfit dislocations are correctly introduced, the number of columns of Ni has to be at least one more than that of Ni_3Al in the x direction. Also, to maintain the correct ratio of 3:1; Ni:Al, in γ' , a minimum of two different layers of atoms is required in the z direction such that the smallest size of simulation box will have a thickness of two atomic distance along this direction.

After obtaining the correct size of the crystals and bringing them together there exist the interface dislocations as expected, but upon relaxation, spacing between the dislocations on the adjacent interfaces in the y direction will vary depending on the initial configuration used for the simulation. Thus we systematically varied the initial configuration until the lowest energy arrangement of the misfits was obtained. This final structure is shown in Figure 3.8, and more detail is given in section 3.7.

Analysis of multilayers [38] show that there exist for every given thickness a correct dislocation spacing along the interface, we were therefore faced with the difficulty of building a structure with the right size and dislocation spacing for our case. For example, by building the same structure as shown in Figure 3.8, but with 10 more Ni and Ni_3Al layers along the x direction, the spacing between dislocations along the interface will increase

by approximately 25Å. This led to reviewing the work done by Shoykhet, Grinfeld and Hazzledine [38] where a detailed study of the correct thickness and dislocation spacing for similar analysis has been done, as shown in the next section.

3.5 The critical thickness and correct dislocation spacing

A detailed study of the internal stresses and strains in coherent multilayers has been performed by [38]. Of interest to us in this study is that of equi-biaxial case in a regular bilayered material as in this study. Considering a bilayered material with thickness H , with one layer f_1H thick and the other f_2H thick, where f_1 and f_2 are the fraction of the total thickness for layers 1 and 2 respectively. The multilayer loses coherency when a grid of edge dislocations with Burgers vector $\vec{b}$ appears on each interface, and the dislocations are spaced at a distance s apart.

By minimizing the sum of the dislocation energy and the uniform elastic energy per unit area with respect to the dislocation spacing s , the dislocation mismatch was found to be :

$$\frac{b}{s} = \delta - \frac{\mu M^* b \ln(f_1 \frac{H}{b})}{2\pi(1-\nu)H M_1 M_2 f_1 f_2} \quad (3.6)$$

$$M_1 = 2\mu_1 \frac{1+\nu_1}{1-\nu_1} \quad (3.7)$$

$$M^* = f_1 M_1 + f_2 M_2 \quad (3.8)$$

Where M^* is the average biaxial modulus for the two layers and subscripts 1 and 2 for

layers 1 and 2 respectively. Equation 3.6 becomes zero and therefore s becomes infinite at a critical value (H_c) of H obtained from:

$$\frac{H_c}{b} = \frac{\mu M^* \ln(f_1 \frac{H_c}{b})}{2\pi(1-\nu)\delta M_1 M_2 f_1 f_2} \quad (3.9)$$

H_c is the largest thickness of the bi layer before the coherent interface becomes unstable and misfit dislocations will occur.

Solving equation 3.9 for H_c as applied to our case we obtained the critical height at which misfit dislocation exists to be 136.16 Å . The corresponding dislocation separation distance s for values of H greater than H_c is obtained by solving equation 3.6. In order to solve equations 3.6 and 3.9, we have used Voigt averages [39] to convert the anisotropic material properties into two isotropic elastic constants λ and μ . Where λ is Lamé constant and μ is the shear modulus. The average value of the elastic constants for the two materials is then used in equations 3.6 and 3.9. The anisotropic factor H_a according to [39] is given by:

$$H_a = 2C_{44} + C_{12} - C_{11} \quad (3.10)$$

The Voigt averages are calculated as shown below

$$\lambda + 2\mu = C_{11} + \frac{2}{5}H_a \quad (3.11)$$

$$\mu = C_{44} - \frac{1}{5}H_a \quad (3.12)$$

$$\lambda = C_{12} - \frac{1}{5}H_a \quad (3.13)$$

In order to verify the accuracy of the results obtained from equations 3.6 and 3.9 (which

are based on continuum elasticity) with atomistic results, we built different structures with a thickness $H = 489.47 \text{ \AA}$, a convenient value that is greater than the critical thickness H_c , and we then varied the dislocation spacing. Figure 3.5 shows the plot of the surface energy per unit area against dislocation spacing s for this simulation. The lowest energy value was obtained at $s = 272.23 \text{ \AA}$. This was in good agreement with equations 3.6 and 3.9 which predict $s = 269.35 \text{ \AA}$ at this value of H . This suggests that the continuum analysis of [38] accurately predicts the equilibrium dislocation spacing as a function of H , but suggest that very large s or very large H are required in atomistic simulations to study an elastically ideal interface.

Therefore using the ideal s will give us a very large computational cell with too many atoms, which will take much longer to simulate than is practical. A compromise was thus reached and a smaller cell was used with a thickness of $1.15H_c$, and spacing $s = 157.92 \text{ \AA}$. This is smaller than the correct spacing, and therefore one limitation of our simulations is the existence of excess elastic strain in the crystal. This gives us the largest reasonable dislocation spacing and ensures that our thickness is above the critical thickness for the material.

3.6 Periodic boundary conditions

A periodic boundary is an important technique used in atomistic simulations. It involves making a simulation that consist of a few hundreds or thousands of atoms behave as if it was infinite. This is done to eliminate the effect of free surfaces which finite samples have. This will ensure that the internal structure of the sample is dominated by internal (bulk) forces rather than surface forces.

Figure 3.6 illustrates this condition. The atoms in the shaded box represents the system being simulated while the surrounding boxes gives the exact copies (in all details) of each

Figure 3.5: Showing the plot of energy per unit area vs dislocation separation

Figure 3.6: Figure showing periodic boundary position of atoms. The shaded square (unit cell) has periodic copies all around it (taken from [40])

atom in the reference cell. The arrows, for example, represent the motion of each atom and it must be same in atoms of all adjacent cells. Therefore, if an atom leaves the simulation cell it is replaced by another with exactly identical properties on the opposite side, and the number of atoms in the cell is always constant. As explained in section 3.1.1 and shown in Figure 3.6, r_{cut} is the cut-off radius and any atom can interact only with another atom within the cut off radius. The simulation box is chosen so that an atom does not interact with more than one image of any given atom.

3.7 Computational procedure

With the configuration described in section 3.3 above, initial energy minimization was done employing periodic boundary condition in all three directions and allowing three degrees of freedom for the relaxation of the computational size using the fortran source code DYNAMO [41]. The relaxed configuration was tested for accuracy by calculating the cohesive energy, the lattice parameters and vacancy formation energy for pure Ni, Al and pure Ni_3Al before the two layers were combined (these details appear in the appendix). The multilayer obtained by bringing the two layers together was then relaxed using the same conditions. The unrelaxed structure does not have any significant meaning, as the atoms are not in their stable equilibrium energy configuration until the relaxation is performed, hence no analysis is done on the unrelaxed structure. After this initial relaxation the bilayered structure had two pure edge misfit dislocation lying vertically above one another (At points A and B) along the interface as shown in Figure 3.7.

This configuration was termed a high energy configuration as a lower energy can be obtained by moving the misfit dislocations around using the elastic displacement field of a dislocation dipole [5] and relaxing the new configuration until the lowest energy configuration is obtained. The final configuration (Figure 3.8) shows the misfit dislocation

Figure 3.7: Position of the misfit dislocations (at points A and B) along the interface after the initial relaxation. Also shown are the slip planes

Figure 3.8: Lowest energy configuration showing the misfit dislocations 48 Å apart along the interface

at their equilibrium position, 48 Å apart along the interface.

3.7.1 Externally introduced dislocations on $(1\bar{1}1)$ plane

Based on the Thompson tetrahedron (Figure 2.9), there are three possible dislocations on the $(1\bar{1}1)$ plane. Two of them are mixed dislocations and the third pure screw for our chosen line direction ($[110]$). For the work done in this thesis, the $\frac{1}{2} \langle 10\bar{1} \rangle$ (mixed) and the $\frac{1}{2} \langle 110 \rangle$ (pure screw) dislocations were considered, and their interaction with the interface in the presence of the misfit dislocations was studied.

Figure 3.9: Diagram showing the positions of the introduced dislocations with reference to the misfit dislocation at A

Each of these two dislocations is introduced into the already relaxed cell discussed in section 3.4 above. Five different positions were considered for each dislocation such that the dislocation cuts through the interface at 0 Å, 10 Å, 25 Å, 50 Å, and 80 Å away from the misfit dislocation. Each of these positions is termed A, B, C, D and E respectively for ease of reference as shown in Figure 3.9.

The external dislocations were specifically introduced in the relaxed structure of section 3.7 with the initial position of the core at about the center of the softer Ni layer. This is to ensure that there is minimal or no interaction with the boundary while the computation is performed. For each of the position considered, the dislocation was introduced using the elastic displacement fields of equations 3.14, 3.15 and 3.16:

$$u_x = \frac{b}{2\pi} \left[\arctan \frac{y}{x} + \frac{xy}{2(1-\nu)(x^2 + y^2)} \right] \quad (3.14)$$

$$u_y = \frac{-b}{2\pi} \left[\frac{1-2\nu}{4(1-\nu)} \ln(x^2 + y^2) + \frac{x^2 - y^2}{4(1-\nu)(x^2 + y^2)} \right] \quad (3.15)$$

$$u_z = \frac{b}{2\pi} \arctan \frac{y}{x} \quad (3.16)$$

3.7.2 Barrier strength of the interface

The dislocation core was relaxed employing periodic boundary condition only in the z direction by increasing the size of the simulation cell in the x and y direction by 12 Å (greater than $2r_{cut}$). As shown in Figure 3.10, the atoms in the inner cell feel the interactions from all their neighboring atoms and therefore behaves as atoms in an infinite crystal. The atoms outside the inner cell (boundary atoms) are held fixed at their original position during relaxation. Farther away from the inner cell, the atoms do not feel the interaction from all their neighbors as the periodic box is much larger in the x and y direction thereby losing periodicity along these directions. Though periodicity is lost in the x and y direction, holding the boundary atoms fixed results in “*a trick*” that make atoms in the inner cell unaware of the free surface such that no complex energy (such as interface energy) term is associated with them. The energy obtained from only the inner cell atoms is used in the analysis done. The simulation is therefore two dimensional in nature but with with periodicity in the z direction and therefore the dislocation line is confined to be in the z direction with an infinite length.

To determine the barrier strength of the interface, a homogeneous shear strain was imposed on the computational cell acting on the slip plane in the slip direction according to equation 3.17:

$$x_i = X_i + \epsilon b_i m_j X_j \quad (3.17)$$

Where X_i is the ith co - ordinate of the position of the atom, ϵ is the applied strain, b_i , is the ith component of the unit Burgers vector of dislocation, m_j is the ith component of

Figure 3.10: Schematic diagram showing the simulation cell, periodicity is lost in the x and y direction as the periodic box is elongated in these directions

the normal to the slip plane. After applying each small increment of strain, the structure is then relaxed, again with periodic boundary only in z direction and keeping the boundary atoms fixed. The resulting shear stress acts in the direction of the Burgers vector such that the dislocation moves towards the interface. The simulation is started with imposing a shear strain corresponding to a small stress. Larger stresses were built up by repeating the process. The results obtained after each increment of strain and relaxation were inspected and the critical stress at which the dislocation crosses through the interface is interpreted as the *barrier strength* of the interface. This critical stress is the resolved shear stress on the slip plane and is obtained from Schmid's expression [5]. It states that the resolved shear stress (τ_{res}) on a dislocation is given by:

$$\tau_{res} = \vec{m}_i \sigma_{ij} \vec{s}_j \quad (3.18)$$

where $\vec{m}_i$ is the slip plane normal, $\vec{s}_j$ is the slip direction and σ_{ij} is the stress tensor. This law can be applied to the present case by evaluating the stresses acting on the

structure for each applied strain and the value at the point when the barrier obstacle is overcome gives a measure of the strength of the interface. For each relaxed configuration, the stress σ_{kl} is obtained from the atomic level stress [42] acting on the entire inner cell, and is given by:

$$\sigma_{kl} = \frac{1}{\Omega} \sum_i \sum_{j \neq i} [\phi'_{ij}(r_{ij}) + F'_i(\rho_{h,i})\rho'_j(r_{ij}) + F'_j(\rho_{h,j})\rho'_i(r_{ij})] \frac{r_{ij}^k r_{ij}^l}{r_{ij}} \quad (3.19)$$

where ϕ'_{ij} , F'_i and F'_j are the partial derivatives of the functions, Ω is the volume of the inner cell, r_{ij}^k is the k th component of the vector extending from atom i to atom j and i is summed over the atoms in the inner cell only.

Chapter 4

Results and Discussion

4.1 Pictorial representation of results

Analysis of the results obtained from the simulations described in chapter 3 is made possible by pictorial views of the positions of the dislocations after each simulation. To clearly illustrate these views, the atoms in their initial configuration have been joined together by triangles resulting in a mesh plot. Figure 4.1 shows a portion of the γ layer without any dislocation, this is the perfect arrangement of atoms without the defect and serves as a reference. Figure 4.2 shows the same portion of the γ layer with the introduced full $\frac{a}{2}[10\bar{1}]$ dislocation labelled X in the figure. The deformed mesh up to the position of the dislocation correspond to the slipped region, while after this position the triangles are undeformed corresponding to the unslipped portion of the structure.

Figure 4.3 shows exactly the same configuration with the externally introduced dislocation X just as in Figure 4.2 but without the mesh. The importance of these meshes in our analysis is therefore seen when Figure 4.2 is compared with Figure 4.3. The position of the dislocation and events leading to it cannot easily be seen in Figure 4.3. Finally the mesh allow us to trace the path of the dislocations as the applied strain on the simulation cell

Figure 4.1: The mesh plot of a portion of the γ layer without any dislocation.

Figure 4.2: A full $\frac{a}{2}[10\bar{1}]$ dislocation (X) inserted into the γ phase.

Figure 4.3: Figure showing the introduced $\frac{a}{2}[10\bar{1}]$ dislocation (X) but without the mesh.

is increased and helps to locate the position of the dislocation core through the stacking fault obtained between partial dislocations.

4.2 Interface interaction with a $[10\bar{1}]$ mixed dislocation

The relaxed structure of the dislocation cores for the structure described in section 3.7.1 were analyzed and the result show that the introduced full dislocation splits into two partial dislocations with a core spreading of the dislocation on the $(1\bar{1}1)$ plane (Figure 4.4) and with a separation distance of 30.25 Å between the partial dislocations.

This is in agreement with similar analysis done by Rao, [16] where a full dislocation on the $(1\bar{1}1)$ plane dissociate into two Shockley partial dislocation with a ribbon of stacking

Figure 4.4: Core spreading of the dislocation on the slip plane in nickel after the initial relaxation at no applied strain (the two partial dislocations are separated by stacking fault).

fault between then according to equation 4.1:

$$\frac{a}{2}[10\bar{1}] = \frac{a}{6}[1\bar{1}\bar{2}] + SF + \frac{a}{6}[21\bar{1}], \quad (4.1)$$

where SF is the stacking fault.

A complete analysis of the results show that for the dislocations which glide down and cut through the interface at points B through E as shown in Figure 3.9, the leading partial extends towards the interface with the band of stacking fault left behind over the region passed through and between it and the trailing partial (Figure 4.5). The motion of the dislocations is such that, before the leading dislocation cuts through the interface, both partial dislocations move together, maintaining the same separation distance between them. In all these cases the leading dislocations continue to move until they get to the interface where they remain until sufficient stress is applied to drive them through. When the resolved shear stress reaches a critical value as the applied shear strain increases, the leading dislocation gets across but the trailing dislocation remain in the Ni layer. This led to the stacking fault extending from the Ni layer into Ni_3Al layer. Further increase in the applied shear strain pushes the trailing dislocation up to the interface where it remained temporarily till the the resulting shear stress is high enough to drive it across into the γ' layer. Once this stage is reached an antiphase boundary is created in Ni_3Al between the trailing dislocation and the interface, as a result of the atoms on the slip plane having slipped by one atomic distance in the slip direction.

Since the results for dislocations cutting through the interface at points B through E are qualitatively very similar, a complete analysis is given for only one of them (D) in this section. Also, since the behaviour of the dislocation introduced in the path of the misfit dislocation at A is considerably different from that of B - E, a detailed analysis of the result obtained from this case is given in section 4.2.1

Figure 4.5: On application of a shear strain the leading partial dislocation extends towards the interface (the interface is identified by the portion where the alternate coloured atoms begins). The position of the trailing dislocation is out of the page of the picture.

Figure 4.6: Plot showing the resolved shear stress on the slip plane vs the applied strain for case A.

4.2.1 Analysis of dislocation interaction

Figure 4.6 is a plot of the resolved shear stress on the slip plane against the applied strain for a dislocation striking the interface at A, directly at the location of the misfit dislocation. At a strain of 0.006, the resolved stress of $0.003037 \text{ eV}/\text{\AA}^3$ acts on the slip plane³. This is shown as point P1 in the figure, this peak corresponds to the critical stress required to break the $[1\bar{1}0]$ misfit dislocation into partials as seen in Figure 4.7 and illustrated in equation 4.2:

$$\frac{a}{2}[1\bar{1}0] = \frac{a}{6}[1\bar{1}\bar{2}] + \frac{a}{6}[1\bar{1}2] + \frac{a}{6}[1\bar{1}0]. \quad (4.2)$$

From Thompson's tetrahedron (Figure 2.9), the $[1\bar{1}\bar{2}]$ and $[1\bar{1}2]$ dislocations lie on the

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³where $1 \text{ eV}/\text{\AA}^3$ equals $16.022 \times 10^4 \text{ MPa}$

Figure 4.7: The misfit dislocation emanates partial dislocations (a and b) on the $(1\bar{1}1)$, and $(\bar{1}11)$ planes respectively as the applied strain increased beyond 0.006, for configuration A.

$(\bar{1}\bar{1}1)$ and $(\bar{1}11)$ slip planes respectively. The result obtained in Figure 4.7 shows the dislocations labelled a and b as the $[1\bar{1}\bar{2}]$ and $[1\bar{1}2]$ dislocations respectively which is in agreement with Thompson's analysis. To conserve the Burgers vector of the dislocation, a $\frac{a}{6}[1\bar{1}0]$ Lomer-Cottrell sessile dislocation is formed at the interface with its core right at the previous position of the misfit dislocation. This dislocation has its Burgers vector on neither of the two slip planes of our structure and therefore it is sessile (cannot glide) [5].

On increment of the applied shear strain to a value of 0.012, the corresponding resolved shear stress is $0.003356 \text{ eV}/\text{\AA}^3$ (point P2, Figure 4.6). This is the stress that has to be overcome in order to move the gliding (external) dislocation up to the interface. What follows after this point is a complex dislocation interaction which is explained as follows; The leading partial dislocation (which is also a $[1\bar{1}\bar{2}]$ dislocation), on getting to the interface (Figure 4.8) restores the interfacial misfit dislocation to its initial configuration (the partial dislocation b, seen on the $(\bar{1}11)$ plane in Figure 4.7 is not seen any more). This can be explained as the leading dislocation summing up with the Lomer-Cottrell sessile dislocation to form a $\frac{a}{3}[1\bar{1}\bar{1}]$ dislocation which attracts the partial b extending from the interface on to the $(\bar{1}11)$ plane in a reversed reaction of equation 4.2 to restore the misfit dislocation.

After this point, further increment of the applied strain only increased the resulting shear stress without any further noticeable change occurring in the crystal. The trailing dislocation (dislocation labelled c in Figure 4.8 which is still further up in the Ni layer as shown by the arrow) remained in Ni, conserving the stacking fault length as the motion of the leading partial has been stopped by the reaction leading to restoring the interfacial misfit dislocation. The resulting dislocation interaction leading to the restoration of the misfit dislocation demonstrates the disadvantage of an incoherent interface, as the $[1\bar{1}\bar{2}]$ dislocation moved into the γ' phase at a relatively low value of stress.

For the dislocation passing through the interface at position D, Figure 4.9 shows the plot of the resolved shear stress against the applied strain. Using this figure as a reference,

Figure 4.8: The gliding leading dislocation interacts with the dislocation at the interface restoring the misfit dislocation. The position of the trailing partial dislocation c , and the partial dislocation a , are out of the picture as depicted by the arrows.

we define the following important stress values which will be consistently used throughout the remainder of this thesis: σ_o ; the stress required to move the leading dislocation up to the interface, σ_l ; the stress required to move the leading dislocation across the interface into the γ' layer, σ_t ; the stress required to move the trailing dislocation up to the interface, and σ_b ; the stress required to move the trailing dislocation across the interface into the γ' layer. Furthermore, we will use the term “*barrier strength*” to describe the stress required to completely drive both the leading and trailing dislocations into the γ' layer (hence the b subscript for σ_b). Quantitatively, this stress value serves as a measure of the strength of the interface.

The first peak in the figure (point *i*) corresponds to the shear stress (σ_o) required to move the leading dislocation from the starting position up to the interface (as shown in Figure 4.10) and has a value of (0.00177 eV/Å³). The motion of the dislocation is prevented by the interface at this value of stress and further increase in the applied strain was not able to drive the dislocation through until the critical shear stress (σ_l) of 0.00566 eV/Å³ (point *ii*, Figure 4.9) is surpassed.

As the applied strain is increased and the resulting shear stress exceeds σ_l , the leading partial dislocation cuts across the interface into the γ' precipitate (Figure 4.11). At this point, the resulting applied stress was insufficient to drive the trailing dislocation across into the γ' layer. This therefore results in the formation of stacking fault in Ni_3Al (Figure 4.11), shown by the deformed mesh between the two dislocation as seen in the diagram. At point *iii* in Figure 4.9, the resulting shear stress of 0.00675 eV/Å³ was obtained, corresponding to the stress (σ_t) to move the trailing dislocation up to the interface. The stacking fault distance continues to increase until the trailing dislocation was finally able to completely break free from the interfacial resistance at a stress of 0.00723 eV/Å³, which is the barrier strength of the interface (σ_b) for this case (point *iv* Figure 4.9). At this point, an antiphase boundary (shown by the variation in the horizontal arrangement of the atoms

Figure 4.9: Plot showing the resolved shear stress on the slip plane vs the applied strain for case D.

across the slip plane in Figure 4.12) was formed and the interface showed no complex network of dislocations. The dislocation shown in the figure is the trailing dislocation, the leading dislocation is out of the page of the picture as shown by the arrow.

Contrary to expectation from the energy point of view that the partial dislocations should not be too far apart because the farther they are the higher the crystal energy, a long ribbon of stacking fault was obtained in Ni_3Al (indicating the dislocations were far apart) before the trailing dislocation was able to cut across the interface. This could be attributed to the high antiphase boundary energy in Ni_3Al when compared with the stacking fault energy as seen in table 3.3. Therefore, since much higher energy is required to produce an antiphase boundary, the stacking fault separation distance continue to increase until the resulting applied stress was sufficient for the formation of an antiphase boundary.

Figure 4.13 show a summary of the results from the analysis for cases A through E,

Figure 4.10: The leading partial dislocation blocked by the interface when the applied strain was insufficient to overcome the barrier.

Figure 4.11: Leading dislocation extends through the interface into Ni_3Al but the trailing dislocation is still in Ni.

Figure 4.12: Antiphase boundary created in Ni_3Al (from the position of the trailing dislocation to the interface) after the trailing dislocation passed through the interface. Note: No complex dislocation at the interface as a result of this motion.

the plot of the resolved shear stress acting on the slip plane against the applied strain is shown. The plots labelled A through E corresponds to the different dislocation positions considered. The behaviour leading to the shape of these curves is quantitatively similar except for case A, hence only case D was explained as a representative for B - E. The plot of the required stress σ_o to move the leading dislocation up to the interface with respect to the spacing relative to the misfit dislocation is depicted in Figure 4.14. Figure 4.15 shows the plot of the critical stress σ_l required to move the leading dislocations across interface as a function of separation distance from the misfit dislocation.

It can be seen that there is a uniform trend of a decrease in the stress required to move the dislocations up to the interface (Figure 4.14). The rate at which the leading dislocation approaches the interface generally increase from cases A - E, indicating an increased rate of motion when the gliding dislocation is farther from misfit dislocation. For the dislocation considered in case A for example, there was virtually no motion until the applied strain was increased to a value of 0.0045.

Further more, from Figure 4.15, σ_l was very low when the introduced dislocation glides directly on to the misfit dislocation and then increases as the introduced dislocations are further away, reaching a peak at a distance of about 25 Å . After this position it starts to decrease as the distance from the misfit dislocation to the gliding dislocation increases. This shows that the misfit dislocation plays less significant role on the motion of the gliding dislocations when the distance between them is far enough that little or no interaction exist between them. The stress value obtained at point P1 of Figure 4.6 is taken as σ_l for that case since it is the stress required to move the same partial dislocation as in the other cases into the γ' layer.

The plot of the barrier strength σ_b to move the trailing dislocation across the interface into Ni_3Al is shown in Figure 4.16. Comparing corresponding values from this plot to those of σ_o in figure 4.15, it is seen that for each dislocation position, the barrier stress

Figure 4.13: Plot showing the resulting resolved shear stress on application of shear strain.

Figure 4.14: Plot showing the stress required to drive the leading dislocation to the interface.

Figure 4.15: Figure showing the stress required to move the leading dislocation across the interface vs distance from misfit dislocation.

σ_b , is only slightly higher than σ_l . For example, when the dislocation crosses through the interface 25 Å away from the misfit dislocation, the value of the stresses are 0.00763 eV/Å³ and 0.00706 eV/Å³ respectively. This show that once σ_l is reached, the interface does not offer a significant resistance to the motion of trailing dislocation.

4.3 Interface interaction with a [110] screw dislocation

Analysis of the results for the screw dislocation shows quantitatively similar results to that of the mixed dislocation in the sense that after the initial relaxation at no applied strain, the full dislocation dissociated into the correct Shockley partials according to equation 4.3, with core spreading of the dislocation on the slip plane.

Figure 4.16: Figure showing the barrier strength of the interface to the $[10\bar{1}]$ dislocation vs distance from misfit dislocation.

$$\frac{a}{2}[110] = \frac{a}{6}[21\bar{1}] + SF + \frac{a}{6}[121]. \quad (4.3)$$

The leading partial dislocation is the $\frac{a}{6}[21\bar{1}]$ dislocation. Also an increase in the applied strain gave a corresponding increase in the resolved shear stress acting on the slip plane. However, (for cases B through E) the interaction of the partials with the interface is different in this case. On application of increasing shear strain, both partials move together towards the interface, the leading partial on getting to the interface glides through without significant hinderance (when compared to the previous case of section 4.2.1). Here once the leading dislocation gets to the interface it crosses through on the next strain increment. The trailing dislocation however, does not simultaneously cross through, it remains in the γ layer and higher stresses are required to gradually move it through before it finally is able to overcome the interface barrier. While the trailing dislocation is still in the γ layer and the applied strain is gradually increased, the leading dislocation moves further down into the γ' layer increasing the length of the stacking fault ribbon as seen in Figure 4.17.

For this case then, the interface offered a relatively low resistance to the leading dislocation from crossing into the γ' layer, unlike in the previous case. However, despite the interface not offering significant resistance to the leading dislocation, the motion of the trailing dislocation was significantly hindered by this interface. This demonstrates that the resistance offered by the interface depends on the Burgers vector of the dislocation approaching it.

For the introduced dislocation gliding down directly towards the misfit dislocation at A of Figure 3.9, the leading partial dislocation was attracted to the misfit dislocation immediately after the dissociation. At this point the leading dislocation got stuck at the interface and as the applied strain is gradually increased, the trailing partial dislocation moved towards the interface reducing the staking fault length. Figure 4.18 shows the resulting resolved shear stress on the slip plane as the applied strain is increased. The

Figure 4.17: Large separation distance between leading dislocation (in the γ' layer) and trailing dislocation (in the γ layer) by the interface leading to formation of a long stacking fault.

Figure 4.18: Plot showing the resolved shear stress on the slip plane vs the applied strain for case A

result showed that the increased applied strain only lead to an increase in the resulting shear stress on the crystal, as the dislocation has been locked at the interface and therefore no further motion is possible. Figure 4.19 shows this situation with the dislocations locked at the interface, here, unlike in Figures 4.7 and 4.8 the misfit dislocation did not split into partial dislocations, because the stress being applied is different according to equation 3.18.

Qualitatively in this case also, the results for dislocations crossing through the interface at points B through E gave similar results as in the case of the mixed dislocation. Analysis of case D is given as a sample for these cases. Figure 4.20 shows the plot of the resolved shear stress on the slip plane versus the applied strain. The first peak at i corresponds to the stress required to drive the leading partial dislocation up to the interface σ_0 . Immediately after this point, the leading dislocation crosses to the γ' layer while the trailing get stucked in the γ layer by the interface as shown in Figure 4.21

The next peak at ii in Figure 4.20 corresponds to the stress that must be overcome for

Figure 4.19: Interlock of the misfit and the gliding dislocation at the interface with no dissociation of the misfit dislocation.

Figure 4.20: Plot showing the resolved shear stress on the slip plane against the applied strain for case D

the trailing dislocation to overcome the interface resistance (σ_b). It is noticed from the Figure that after peak i when the leading dislocation has crossed to the γ' layer and the trailing is at the interface, several steps of strain increment were taken before the trailing dislocation was able to cross over into the γ' layer. This confirms that the interface is more resistant to the motion of the trailing dislocation than to the leading dislocation in this case.

A summary of the results is shown in Figure 4.22, where the resulting stress is plotted against the applied strain for all the cases considered. The similarity of cases B through D is shown while that of case A is different.

The plot of the barrier strength of the interface (the stress required move the entire dislocation into the γ' layer) and the stress required to move the leading dislocation across the interface in relation to the position of the misfit dislocation is shown in Figure 4.23. It is shown here that apart from the case when the dislocation crossed through the interface about 10 Å away from the misfit dislocation, the distance from the misfit dislocation does

Figure 4.21: Leading dislocation extends well into the γ' while the trailing dislocation remained tangled with the interface.

Figure 4.22: Plot showing the resulting resolved shear stress on application of shear strain for the cases considered.

Figure 4.23: Figure showing the interfacial barrier strength and stress to move the leading dislocation through the interface away from the misfit dislocation

not affect the strength of the interface. The required stress to overcome the interface when the gliding dislocation is closest to the misfit dislocation is however, much higher than in all other cases. For this case, the plot of the stress required to move the leading dislocation up to the interface σ_o is not shown because this occurs immediately on the first applied load. Thus σ_o is smaller than the accuracy dictated by the size of the load increments.

Also from Figure 4.23, it is clearly shown that the corresponding stress required to move the entire dislocation across the interface σ_b for each dislocation position is much higher than the stress (σ_l) to move the leading dislocation across the interface, unlike in the case of the mixed dislocation. This further confirms the resistance of the interface being dependent on the type of dislocation.

Chapter 5

Conclusion

This thesis has been a detailed investigation into the interaction between the γ / γ' interface and gliding dislocation in the γ matrix.

A full $\frac{a}{2}[10\bar{1}]$ dislocation dissociates into two partial dislocations, $\frac{a}{6}[1\bar{1}\bar{2}]$ and $\frac{a}{6}[21\bar{1}]$ as predicted by Frank's rule based on energy considerations. The $\frac{a}{6}[1\bar{1}\bar{2}]$ is the leading dislocation while the $\frac{a}{6}[21\bar{1}]$ is the trailing dislocation.

Under the application of a shear stress the partials move towards the interface. The fact that in all cases considered, a certain critical stress is reached followed by a drop in the resolved shear stresses (as seen in Figure 4.13) before the dislocations actually gets to the interface shows that the motion of the dislocations is retarded as they approach the interface, the interface therefore constitute an initial barrier.

After the dislocation gets to the interface. The interface does not allow it to cross into the harder layer of Ni_3Al until the barrier strength is overcome. This barrier strength gradually reduces as the crossing point becomes farther from the misfit dislocation. This explains the misfit dislocation itself as a further hindrance to dislocation motion.

The position of the misfit dislocation with reference to the point at which the leading gliding dislocation crosses the interface affects the barrier strength of the interface. The

closer the distance between these two points, the higher the interfacial barrier strength (except for case A). Therefore the dislocations would cross through the interface more easily (at lower applied stress) in the absence of misfit dislocations. The trailing dislocation did not simultaneously cross through the interface when the leading dislocation cut through, but required additional applied stress to do so. However, similar to the case of the leading dislocation the trailing dislocation requires lesser energy to overcome the barrier as the distance between it and the misfit dislocation increases along the interface.

The trailing dislocation requiring higher critical stress to cut through the interface and the long stacking fault distance in Ni_3Al (implying a high lattice energy) is as a result of two factors: First, the interface is a strong barrier to dislocation motion, hence the reason why the trailing dislocation does not simultaneously cross the boundary at the same time the leading dislocation crosses, and secondly a high energy (compared to the stacking fault energy) is required to form an antiphase boundary in Ni_3Al since the motion of the trailing dislocation into the Ni_3Al layer is accompanied by the formation of the antiphase boundary.

On the other hand, when the misfit dislocation is directly in the path of the gliding dislocation, a complex dislocation interaction occurs. The misfit dislocation breaks up into partial dislocations on to the $(1\bar{1}1)$ plane and $(\bar{1}11)$. The partial on the $(\bar{1}11)$ plane extending only slightly from the interface onto this plane while the $\frac{a}{6}[1\bar{1}\bar{2}]$ extends well into the γ' phase on the $(1\bar{1}1)$. The gliding dislocation from the γ phase hits the interface and combines with the $\frac{a}{6}[1\bar{1}0]$ and $\frac{a}{6}[1\bar{1}2]$ partials to restore the interfacial misfit dislocation. The barrier strength of the interface for this condition is $0.003356 \text{ eV}/\text{\AA}^3$ which is much lower than $0.007058 \text{ eV}/\text{\AA}^3$ obtained when the gliding dislocation crosses through the interface $25 \text{ \AA}$ away from the misfit dislocation. This therefore shows a disadvantage of having an incoherent interface with misfit dislocations as the resulting structure will be soft (because the co-operative motion of the dislocations lead to a lower energy) and

allow dislocation to pass through easily as in case A of our analysis. However dislocations find it harder to overcome the interface barrier when passing through close to the misfit dislocation. Farther from it the barrier strength is reduced.

A full $\frac{a}{2}[110]$ screw dislocation dissociates into two partial dislocations, $\frac{a}{6}[121]$ and $\frac{a}{6}[21\bar{1}]$ with the leading partial dislocation being the $\frac{a}{6}[21\bar{1}]$. The interface offered little resistance to the leading dislocation but higher resistance to the trailing dislocation. Therefore, a measure of the strength of the interface depends more on the type of dislocation passing through. The resistance of the γ/γ' interface to dislocation motion in this case is hardly affected by the position of the misfit dislocation since in all cases considered (apart from case A) the barrier strength of the interface to the dislocation is approximately the same (about $0.0058 \text{ eV}/\text{\AA}^3$). The barrier strength of the interface to the $\frac{a}{2}[10\bar{1}]$ dislocation is higher than that for the $\frac{a}{2}[110]$ as seen when the dislocation from same distance to the misfit dislocations are considered for both cases.

For the screw dislocation introduced on the slip plane directly in the path of the misfit dislocation, the motion of the leading dislocation is stopped at the interface by the misfit dislocation. A situation which shows that the dislocations were interlocked and in this case, the misfit dislocation further strengthened the interface.

In this thesis we have used atomistic simulation to study and understand the $\text{Ni}/\text{Ni}_3\text{Al}$ interface interaction with two different types of dislocations. We have obtained the mechanisms of the interactions between the misfit dislocation and the gliding dislocations. And we have been able to quantify the barrier strength as a function of position and type of the Burgers vector of dislocation. We therefore conclude that the dislocation - interface interaction depends on the dislocation considered and the position of the misfit dislocation.

Future extensions to the work done in this thesis can be made as follows . Performing the computations with a much larger cell having the z axis increased to obtain a full 3 dimensional analysis would introduce more realistic dislocation-interface interactions, but

would require parallel computing facilities and more complex visualization tools to analyse the results. This will also help to determine if dislocations with more screw than edge components find it relatively easier to cross through the interface and vice-versa. Another improvement will be to use the correct thickness and dislocation spacing as predicted by continuum mechanics in the work of Shoyket and Hazzledine [38]. Again this requires larger simulations and possibly parallel computing.

Having more of the externally introduced dislocations on planes close to the misfit dislocations and farther from it may help to determine if there is a certain spacing between the dislocations that give the highest barrier strength of the interface. Also comparing this results with the case of a fully coherent interface and one in which the lattice parameter(s) has been altered to change the lattice parameter misfit (δ) may provide insight into the optimal value of δ and the optimal degree of interface coherency for enhanced strength. Finally a simulation with periodicity in all directions which will allow the gliding dislocations after crossing from the γ layer to the γ' layer to continue to the next γ layer may yield important results.

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Appendix A

Sample calculations

A sample of some of the essential calculations made while putting together the thesis is shown in this section. It should be noted that quite a number of other calculations whose values were used in this work are not shown and they could easily be obtained from references cited where their results were mentioned.

A.0.1 Calculation of cohesive energy

For a block of 256 Aluminium atoms, an initial structure was built with a wrong lattice parameter but with the correct fcc configuration and relaxed using the code Dynamo. The energy of the block of atoms was minimized using the conjugate gradient method. The periodic boundary conditions used makes the simulation behave as if we have an infinite crystal and therefore the final energy of the system is just that associated with each atom. Also the periodic box was allowed to relax in all direction to confirm that the returned lattice parameter is the correct value. The final potential energy returned after the minimization is the total relaxed energy ($E_{relaxed}$) of the configuration. The cohesive energy of aluminium E_{coh} is therefore given by

$$E_{coh} = \frac{E_{relaxed}}{N} \quad (A.1)$$

where $N = 256$, the number of atoms and for this particular simulation:

$$E_{coh} = \frac{-860.15954}{256} = -3.36eV \quad (A.2)$$

Applying the same analysis to a block of nickel and Ni_3Al atoms gave the correct cohesive energy for each structure.

A.0.2 Calculation of vacancy formation energy

Repeating the same steps as described in section A.0.1 but now with 500 nickel atoms. The cohesive energy for nickel was obtained as -4.45 eV. Taking this relaxed configuration now and removing one atom such that a vacant site is created, relaxation is then done with this defect in place. The new energy obtained with the vacant site is E_{defect} and the vacancy formation energy E_{vac} calculated as:

$$E_{vac} = E_{defect} - E_{perfect} - E_{coh} \quad (A.3)$$

$E_{perfect}$ is the energy of a perfect structure containing 500 nickel atoms. The values obtained are put in equation A.3 and the vacancy formation energy is obtained as

$$E_{vac} = -2218.948 + 2224.9978 - 4.45 = 1.6eV \quad (A.4)$$

This is in agreement with the published result of the work done by Voter [36]. Similar calculations performed on a block of aluminium and Ni_3Al gave the expected result. In the case of Ni_3Al , however, taking out a nickel atom to create the vacancy is different from when an aluminium atom is taken out due to their different chemical properties.

A.0.3 Calculation of (111) stacking fault energy

To obtain the (111) stacking fault energy in Nickel, a block of atoms stacked in such a way that the (111) planes lie on top of one another in the z direction was built and a stacking fault obtained by removing one layer of atoms such that instead of the ABCABCABC.. fcc closed packed configuration we have ABCBCABC.. pattern. The structure was again relaxed with periodic boundary conditions in all 3 directions. The total energy of the relaxed configuration is sum of the cohesive energy and the stacking fault energy and is given by equation A.5.

$$E_{rel} = E_{coh} \times N + A \times \gamma_{SF} \quad (A.5)$$

The stacking fault energy is therefore,

$$\gamma_{SF} = \frac{E_{rel} - E_{coh} \times N}{A} \quad (A.6)$$

Where A is the area of each (111) plane ($14.9341 \text{ \AA} \times 17.244 \text{ \AA}$). and γ_{SF} is the stacking fault energy. For a block of nickel atoms with 1104 atoms the stacking fault energy per unit area was obtained as

$$\gamma_{SF} = \frac{-4911.876 - (-4.45) \times 1104}{257.524} = 0.003588 \text{ eV/\AA}^2 = 57.49 \text{ mJ/m}^2 \quad (A.7)$$

A.1 Calculation of the thickness of simulation box

The calculations leading to the size of the simulation box described in section 3.3, is shown in this section. Subscript 1 and 2 refers to Ni and Ni_3Al properties respectively.

$$M_1 = 2\mu_1 \frac{1 + \nu_1}{1 - \nu_1} \quad (\text{A.8})$$

$$M_2 = 2\mu_2 \frac{1 + \nu_2}{1 - \nu_2} \quad (\text{A.9})$$

$$H_a = 2C_{44} + C_{12} - C_{11} \quad (\text{A.10})$$

For nickel

$$H_a = [2(1.26) + 1.49 - 2.44] \times 10^{12} \text{erg/cm}^3$$

$$H_a = 1.57 \times 10^{12} \text{erg/cm}^3 = 0.9799 \text{eV/\AA}^3$$

$$\mu = 1.26 - \frac{1}{5}(1.57) \times 10^{12} \text{erg/cm}^3$$

$$\mu = 0.946 \times 10^{12} \text{erg/cm}^3 = 0.59 \text{eV/\AA}^3$$

$$\lambda = C_{12} - \frac{1}{5}H_a \quad (\text{A.11})$$

$$\lambda = [1.49 - \frac{1.57}{5}] \times 10^{12} \text{erg/cm}^3$$

$$\lambda = 1.176 \times 10^{12} \text{erg/cm}^3 = 0.73399 \text{eV/\AA}^3$$

For Ni_3Al ,

$$H_a = [2(1.23) + 1.37 - 2.46] \times 10^{12} \text{erg/cm}^3$$

$$H_a = 1.37 \times 10^{12} \text{erg/cm}^3 = 0.8549 \text{eV/\AA}^3$$

$$\begin{aligned}
\mu &= 1.23 - \frac{1}{5}(1.37) \times 10^{12} \text{erg/cm}^3 \\
\mu &= 0.956 \times 10^{12} \text{erg/cm}^3 = 0.5967 \text{eV}/\text{\AA}^3 \\
\lambda &= \left[1.37 - \frac{1.37}{5}\right] \times 10^{12} \text{erg/cm}^3 \\
\lambda &= 1.096 \times 10^{12} \text{erg/cm}^3 = 0.6841 \text{eV}/\text{\AA}^3 \\
\nu &= \frac{\lambda}{2(\mu + \lambda)}
\end{aligned} \tag{A.12}$$

For nickel,

$$\begin{aligned}
\nu &= \frac{0.73399}{2(0.59 + 0.73399)} \\
\nu &= 0.2772 \\
M_1 &= \frac{2 \times 0.59(1 + 0.2772)}{1 - 0.2772} \\
M_1 &= 2.0851 \text{eV}/\text{\AA}^3
\end{aligned}$$

For Ni_3Al ,

$$\begin{aligned}
\nu &= \frac{0.6841}{2(0.5967 + 0.6841)} \\
\nu &= 0.267 \\
M_2 &= \frac{2 \times 0.5967(1 + 0.267)}{1 - 0.267} \\
M_2 &= 2.06281 \text{eV}/\text{\AA}^3 \\
f_1 &= \frac{a_1}{a_1 + a_2}
\end{aligned} \tag{A.13}$$

$$\begin{aligned}
f_2 &= \frac{a_1}{a_1 + a_2} \\
f_1 &= \frac{3.52}{3.52 + 3.573} \\
f_1 &= 0.4963 \\
f_2 &= \frac{3.573}{3.52 + 3.573}
\end{aligned} \tag{A.14}$$

$$\begin{aligned}
f_1 &= 0.5037 \\
M^* &= f_1 M_1 + f_2 M_2 \\
M^* &= 0.496264 \times 2.0851 + 0.503736 \times 2.06281 \\
M^* &= 2.07387 eV/\text{\AA}^3 \\
\nu_{avg} &= \frac{\nu_1 + \nu_2}{2} \\
\nu_{avg} &= \frac{0.2772 + 0.267}{2} = 0.2721
\end{aligned} \tag{A.15}$$

The expression for the critical thickness is given by [38] as;

$$\frac{H_c}{b} = \frac{\mu M^* \ln(f_1 \frac{H_c}{b})}{2\pi(1-\nu)\delta M_1 M_2 f_1 f_2} \tag{A.16}$$

$$\tag{A.17}$$

where b is obtained as;

$$b = \frac{a_1}{\sqrt{2}} \tag{A.18}$$

Substituting all the derived values into equation A.16,we get

$$\begin{aligned}
0.401765 H_c &= \frac{1.23053 \ln(0.199383 H_c)}{0.074265433} \\
H_c &= 136.1563 \text{ \AA}
\end{aligned}$$