THEORY AND MODELING OF THE MECHANICAL BEHAVIOR OF NANOSCALE AND FINESCALE MULTILAYER THIN FILMS

DISSERTATION

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By

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* * * * *

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ABSTRACT

In this work, a 3D Dislocation Cellular Automaton (CA) model is developed and calibrated first; then the model is applied to study the mechanical properties of nanoscale and finescale multilayer thin films. In the 3D dislocation model, the study object has a FCC structure. The structure is divided into cubic cells with edges along crystallographic <100> directions. Crystallographic {111} slip planes with three-fold symmetry are discretized into equilateral triangular patches with sides along <110> directions. Dislocation lines are represented by a set of triangular sides within {111} planes. These triangular patches slip provided there is a sufficient driving force associated with reduction in system energy. Perfect <110>/<{111}> dislocations are considered. The resulting variables are the triangular patch size and dislocation core cut-off, measured relative to Burgers vector magnitude $b$. To calibrate this model, three examples involving operation of a Frank-Read source are chosen. These examples also highlight the benefits and drawbacks of the method. A benefit to discretization is that dislocation evolution may be analyzed via spatial averaging over collections of patches, so that the discrete versus continuum nature of the results may be studied. Further, dislocation reactions and cross slip are accommodated easily and, in principle, Monte-Carlo schemes can be integrated into the evolution formalism. Overall, the discrete nature of the method is
attractive for incorporating the kinetics of thermally activated states and for simplifying
the range of geometries and threshold criteria associated with dislocation reactions.

This 3D Dislocation Cellular Automaton model is employed to simulate yield and
hardening in nanostructured metallic multilayer thin films. Threading and interfacial
dislocation sources are studied. The films are composed of 2 types of alternating single
crystalline FCC layers with a (001) epitaxy, a mismatch in stress-free lattice parameter,
but no elastic modulus mismatch. Interfaces are assigned no additional strength except
that from lattice parameter mismatch and interfacial dislocation arrays. Three regimes of
tensile plastic response are identified based on the evolution of interfaces during tensile
defformation. For smaller individual layer thickness, interfaces are coherent initially and
remain so up to bulk yield (Regime I). For intermediate layer thickness, interfaces are
coherent initially but become semi-coherent prior to bulk yield (Regime IIa). For larger
layer thickness, interfaces are semi-coherent initially and acquire additional dislocation
content prior to bulk yield (Regime IIb). The evolution of interfacial structure during
dereformation in Regimes IIa and IIb occurs due to deposition of dislocation content along
interfaces by confined layer slip (CLS). The overall outcome is that the plastic strength
of multilayer thin films increases with decreasing layer thickness until Regime I is
encountered. Strength in Regime I may increase, reach a plateau, or even decrease. The
results are consistent with experimental measurements of hardness, including the Ag/Al
system in particular.
To my family
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CHAPTER 1

INTRODUCTION

Since Blum [1] first reported enhanced tensile properties in electrochemically-produced alloys consisting of alternating layers of copper and nickel in 1921, multilayered materials attract great interest from researchers [2-12]. Using physical vapor deposition, we have almost unlimited freedom to choose among elements, alloys, and compounds as layering constituents and to design and produce materials with compositional and structural periodicities approaching the atomic scale [13]. With these special properties, multilayered materials become of great interest for applications such as hard coatings, x-ray optical elements, microelectromechanical systems (MEMS), and magnetic recording media and heads [13,14].

Clemens, Barnett, and Kung [13] reviewed hardness vs. bilayer period relationship for many multilayer systems as shown in Figure 1.1. It is clear that hardness increases with bilayer period decrease, and reaches a maximum value when bilayer period is about 10nm. Since plastic deformation and strength of crystalline materials are mainly controlled by dislocation behavior, this research tries to understand the strengthening trend for multilayers based on dislocation model.
Figure 1.1: Plot of hardness vs. bilayer period for several multilayer systems. Also shown are the predicted Hall-Petch behaviors for Cu and Nb using bulk parameters. The designations e- and p- refer to epitaxial and polycrystalline, respectively.
As one of the most important defects in materials, dislocations are extensively studied experimentally [15-21] and computationally [22-34], which contribute greatly to understand properties of materials, especially mechanical properties. **Chapter 2** focuses on reviewing the representation of structure and the evolution process of different computational methods employed in studying dislocation behaviors. Three major existing methods are discussed first. They are molecular dynamics, dislocation dynamics modeling, and phase field method. Then, cellular automaton method is reviewed since it is applied in setting up our dislocation modeling.

To study dislocation motion and plastic deformation of materials, a cellular automaton dislocation motion model is developed first. **Chapter 3** provides the development of this model. FCC (Face Centered Cubic) structure is chosen to be the structure of the study object employed. Other structures can also be studied after some adaptation of this model. How to represent the study system, the rules for system behavior under some external excitation, and how to process simulation results should be specified in the model. In this chapter, the scheme used to discretize and represent the structure is given first. FCC structure is divided into cubes with edges along $<100>$ crystallographic directions, {$111$} slip planes are partitioned into regular triangular patches, and dislocations are expressed as a set of triangular sides. Then, theoretical background for this model is developed. This section includes verification of divisibility of dislocation line into segments, and calculation of system energy change during system evolution. System evolves with slipping of triangular patches adjoining the studying dislocation line in slip plane. Dislocation line front changes with system evolution. System energy change is composed of elastic energy change due to the change in dislocation line configuration, and work
done by internal and external stresses excluding the stress from the studying dislocation. After that, system evolution process is described. In our model, one triangular patch is slipped at each step, and system evolves along the path of steepest decent in energy. However, Monte-Carlo scheme can be incorporated in selecting the evolution path. Last, two stress averaging methods are illustrated. These methods are utilized to process the local instantaneous raw stress data from simulations.

**Chapter 4** focuses on calibration of the 3D dislocation CA model developed in chapter 3. First, triangular patch nucleation on a finite segment is studied. The applied stress needed for this nucleation is derived analytically. Results from simulations agree very well with the analytic results. Next, Frank-Read source operation in an infinite, elastically isotropic medium is analyzed. Three examples are used here. The first example assumes dislocation line energy is isotropic with $\nu = 0$. The second example models dislocation with anisotropic line energy with $\nu = 0.1$. Dislocation propagates in a non-equiaxed mode. The third example includes an infinite long parallel same-signed fixed screw dislocation in the parent slip plane of the Frank-Read source. Gliding dislocation can propagate in parent or cross-slip plane. Simulation results are consistent with analytic understanding.

Since Blum [1] first reported enhanced tensile properties in electrochemically-produced alloys consisting of alternating layers of copper and nickel in 1921, multilayered materials attract great interest of researchers [2-12]. One of the special properties is their extremely high strength, when layer thickness is in nanometer scale. **Chapter 5** focuses on reviewing dislocation-based strengthening mechanisms for multilayers, and the interfacial structure evolution due to misfit dislocation behavior in
multilayers with lattice parameter mismatch between neighboring layers. Dislocation-based strengthening mechanisms can be grouped into two categories: deformation mode and strengthening source. Interfacial structure will become from coherent to semicoherent to incoherent with increase of layer thickness of multilayers, by deposition of interfacial misfit dislocations on the interfaces. Two main theories for evaluating critical layer thickness corresponding to coherent-semicoherent transition are discussed. They are proposed by Merwe and collaborators (based on energy minimization), and Matthews and Blakeslee (based on force balance) respectively.

In Chapter 6, 3D Cellular Automaton Dislocation Model is employed to study mechanical behavior and structure development during deformation in fine-scale metallic multilayers. Multilayers studied in this chapter are composed of alternating (1) and (2) phases with no elastic modulus mismatch. First, geometry and discretization of multilayer structure in the simulations is described. After that, theory on deformation and structure evolution is developed. Dislocation can propagate in confined layer slip mode or transmit through interfaces to multiple layer slip mode. The analytic formulas for the stresses to drive confined layer slip and interfacial transmission are derived. Then, an ideal multilayer structure is studied. This ideal multilayer has no lattice parameter mismatch, same volume fraction of phases (1) and (2), and intransmissible interfaces. Both interfacial and threading dislocation configurations are simulated. The stress needed for confined layer slip is obtained for different layer thickness. The results for threading dislocation agree with theory developed in the former section. The results for interfacial dislocation show the competition between layer thickness and dislocation source length, and the stress is controlled by the smaller one. Next, multilayers with lattice parameter
mismatch are studied. Multilayers with threading dislocation through several layers are modeled. For small lattice parameter mismatch and small layer thickness condition, strength of material is controlled by dislocation source length. For large lattice parameter mismatch and large layer thickness condition, initial confined layer slip will deposit interfacial misfit dislocations on the interfaces, and strength of material is controlled by the propagation of interfacial dislocation and threading dislocation through one layer. So, the motion of interfacial dislocation and threading dislocation through one layer is studied. The simulation and analytic results predict that two regimes exist for multilayers with fine layer thickness. At larger layer thickness, strength depends primarily on layer thickness. This occurs since slip is confined to individual layers, prior to macroscopic yield. At sufficiently small layer thickness, strength depends primarily on lattice parameter mismatch and the dislocation source length scale, rather than layer thickness. This occurs since slip is not confined to individual layers, even during the initial stage of plastic deformation. Last, simulation results are compared with experimental data. The model results capture experimental trends of multilayer yield strength versus layer thickness.

In Chapter 7, conclusions of this research are reported first; then, future work is described. This work is composed of three major parts: 3D dislocation cellular automaton model development, model calibration, and model application in study of multilayer system.
CHAPTER 2

DISLOCATION MODELING METHODS AND
CELLULAR AUTOMATON METHOD
– A REVIEW

As one of the most important defects in materials, dislocations are extensively studied experimentally [15-21] and computationally [22-34], which contribute greatly to understand properties of materials, especially mechanical properties. This chapter focuses on reviewing the representation of structure and the evolution process of different computational methods employed in studying dislocation behaviors. Three major existing methods are discussed first. They are molecular dynamics, dislocation dynamics modeling, and phase field method. Then, cellular automaton method is reviewed since it is applied in setting up our dislocation modeling.

2.1 Molecular Dynamics (MD) in Dislocation Simulation

Molecular Dynamics is an atomic level method. Simulated structure is represented by a number of atoms arranged in some special way. For example, in Rao and Hazzledine [22], dislocation is represented by a group of atoms with differential displacement as shown in Figure 2.1.
Figure 2.1: Differential displacement plots of the relaxed configurations of \((a/2)<110>\) screw dislocation in (a) Cu and (b) Ni
Figure 2.2: (a), (b) HRTEM images showing core structures of two different $a[\overline{1}01]$ dislocations imaged along the [$\overline{1}11$] direction. In both cases, the overall $a[\overline{1}01]$ dislocation (indicated by the closure failure $b_1 = (a/3) [\overline{1}21]$) has decomposed into two $a<100>$ dislocations. The closure failure for $b_2$ is $(a/3) [2 \overline{1}1]$, indicating an $a[\overline{1}00]$ dislocation, while the closure failure of $b_3$ is $(a/3) [1 \overline{1}2]$, consistent with an $a[001]$ dislocation. The individual $a<010>$ cores are separated by about 1.5nm in (a) and about 2 nm in (b)
There is experimental evidence for this kind of representation. Mills et al [16] provided the atomic structure of dislocation in Figure 2.2. This dislocation structure was obtained through High-Resolution TEM.

System evolves by following a minimum energy path. Therefore, it is essential to get the energy for different possible evolution path. Here, system energy for different state is obtained by calculating the interaction energy between atoms. There are different empirical potentials to describe the interaction energy between atoms, such as Morse potential [35], Lennard-Jones potential [36], and EAM (embedded atomic method) potential [22]. The first two potentials are pair potentials without considering many body interactions, while EAM includes many body potential. EAM is a good potential for metals and alloys. In formulating EAM potential, the energy of an ensemble of atoms is calculated as a sum of a pair interaction and a local volume-dependent embedding term [22, 37, 38]

\[
e = \sum_i e_i = \sum_{i,j,i \neq j} V_{ij}(R_{ij}) + \sum_i F_i(\rho_i) \tag{2.1}
\]

where \( V_{ij} \) is the pair interaction between two different atoms \( i \) and \( j \); \( F_i \) is the embedding term for atom \( i \). In the pair interaction term, \( R_{ij} \) is the distance between the two atoms in a pair. In the embedding term, the argument \( \rho_i \) is taken to be a sum of pairwise terms as

\[
\rho_i = \sum_j \phi_j(R_{ij}) \tag{2.2}
\]
For each atom $i$, its embedding term is the sum of its pair interaction with all other atoms $j$. Morse potential [39, 40] is utilized here. The function $\phi$ is taken to be an exponentially decreasing function with distance. The embedding function is obtained from an exact fit to ‘Rose’s equation of state’ [41]. To get an EAM potential for a specific type of metal or alloy, the method is by varying the various Morse potential parameters, as well as the parameter, which describes the rate of decay of the function $\phi$ with distance to fit the properties of studied materials. In Rao and Hazzledine [22], the Cu, Ni, and Cu-Ni Morse pair interaction potentials are developed by fitting to the properties of FCC Cu, FCC Ni, and disordered FCC 0.5Cu-0.5Ni systems respectively.

Atomistic approaches such as static and dynamic versions of the embedded atom method have been employed for several years to compute the core structure of single dislocations or the interaction of a dislocation with point, line, or area defects [22-24]. This scale of study is essential to supply activation energies for glide processes such as kink-pair formation, cross-slip processes dependent on jog-pair formation, and dislocation reactions with products. Currently, molecular dynamics approaches may involve on the order of millions of atoms for hundreds of picoseconds, so that only regions on the scale of nm can be considered.

### 2.2 Dislocation Dynamics Modeling

To study a larger system than that in atomistic simulations, mesoscale dislocation dynamics modeling is employed. Examples of more macroscopic, continuum approaches include those by Kubin et al [25, 26], Zbib et al [27], Chrzan et al [28], and Schwarz et al [29] where macroscopically-curved dislocations are approximated by piecewise-linear
configurations of arbitrary orientation and an approach by Ghoniem [30] employing curved, parametric segments with smoothly varying slope and curvature. Taking Zbib et al [27] as an example, dislocations are partitioned into many segments as shown in Figure 2.3.

These larger-scale continuum formulations attempt to replace atomistic contributions to system energy with phenomenological relations that specify dislocation mobility, cross slip, and annihilation events in terms of macroscopic configurational variables and forces. These methods can compute system energy based on the theory of elasticity for Volterra dislocations in infinite, elastically homogeneous media so that dislocation cores are represented as planar, discontinuous jumps in slip distribution. In some cases, the finite element method or collocation techniques are employed to incorporate the effect of free surfaces or elastically inhomogeneous media [31].

Specifically, system evolution is through some Force-velocity (F-V) relationship. Mostly, power-law F-V relation is used. A linear relation between dislocation glide velocity $v_g$ and effective shear stress $\tau_e$ for a segment can be

$$v_g = \frac{\tau_e b}{B_g}$$

(2.3)

where $B_g$ is the temperature-dependent dislocation glide mobility, and $b$ is the Burgers vector. Effective shear stress is obtained by Peach–Koehler equation [42]. Next, the displacement of each segment is gained by multiply its velocity by time step.
Figure 2.3: Discretization of dislocation curves into a set of straight dislocation segments
At each time increment, these approaches need to track each segment of all dislocation line segments and compute force acting on each segment from all other segments, and each segment is updated. To follow the true evolution process of a system, appropriate time step must be set. Also, some dislocation behavior such as cross-slip is very complex because line sense and Burger’s vector should be compared for each segment to get the segments of screw characteristics.

2.3 Phase Field Method

Recently, phase field method is extended to study dislocation behavior [32-34]. Dislocations are represented by thin coherent inclusions with stress-free strain in Equation (2.4) as shown in Figure 2.4 [33]. The stress-free strain [43] is

\[ \varepsilon_{ij}^o = \frac{b_i n_j}{d} \]

where \( b \) is Burgers vector, \( n \) is the normal to the slip plane, and \( d \) is the thickness of the inclusion plate.
Figure 2.4: Schematic drawing illustrates the presentation of (a) the dislocation line ABC ending on the crystal surface at points A and C, and (b) a dislocation loop, by the thin coherent inclusions with the stress-free strain in Equation (2.4); $b$ is the Burgers vector, $d$ is the thickness of the inclusion, and $n$ is the unit vector normal to the inclusion habit plane coinciding with the slip plane. For a dislocation the thickness $d$ is equal to the interplanar distance of the slip plane.
Here, dislocation is interpreted as one phase. Density function for dislocations with Burgers vector \( b(\alpha, m_\alpha) \) is \( \eta(\alpha, m_\alpha, r) \), where \( \alpha \) is the index of slip plane number, \( m_\alpha \) is the index of elementary Burgers vector, and \( r \) is the position. From \( b(\alpha, m_\alpha) \) and \( \eta(\alpha, m_\alpha, r) \), the total Burgers vector field from all slip planes is the sum over slip planes \([32, 33]\),

\[
b(r) = \sum_{\alpha=1}^{p} b(\alpha, r) = \sum_{\alpha=1}^{p} \sum_{m_\alpha=1}^{q} b(\alpha, m_\alpha) \eta(\alpha, m_\alpha, r) \tag{2.5}
\]

where \( p \) is the total number of slip planes, \( q \) is the total number of elementary Burgers vectors. The stress-free strain \( \varepsilon_{ij}^0(r) \) produced by dislocation with Burgers vector of Equation (2.5) is \([32, 33]\)

\[
\varepsilon_{ij}^0(r) = \frac{1}{d} \sum_{\alpha=1}^{p} \sum_{m_\alpha=1}^{q} b(\alpha, m_\alpha)n(\alpha) \eta(\alpha, m_\alpha, r) \tag{2.6}
\]

The Dislocation evolution is a kind of phase transformation, which is driven by strain energy minimization. Strain energy \([32, 33]\) is the sum of elastic energy \( E^{\text{elast}} \), crystalline energy \( E^{\text{cryst}} \), and gradient energy \( E^{\text{grad}} \)

\[
E = E^{\text{elast}} + E^{\text{cryst}} + E^{\text{grad}} \tag{2.7}
\]
The simplest form of the kinetic equations is obtained by assuming that the evolution rate of a field is a linear function of the thermodynamic driving forces [32, 33]

\[
\frac{\partial \eta(\alpha, m_\alpha, r, t)}{\partial t} = -L \frac{\delta E}{\delta \eta(\alpha, m_\alpha, r, t)} + \xi(\alpha, m_\alpha, r, t) \tag{2.8}
\]

where \( \eta(\alpha, m_\alpha, r, t) \) is the field function (Iro parameter) describing dislocations with the Burgers vector \( b(\alpha, m_\alpha) \), \( L \) is the kinetic coefficient characterizing dislocation mobility, \( E \) is the total energy functional, \( \delta E / \delta \eta(\alpha, m_\alpha, r, t) \) is the thermodynamic driving force, and \( \xi(\alpha, m_\alpha, r, t) \) is the Langevin Gaussian noise term reproducing thermal fluctuations [44].

As a new method in studying dislocation behavior, phase field method has its special advantage in modeling dislocations in terms of smoothly varying distributions of shear transformation within thin planar regions. This more detailed formalism relies on atomistic results to supply the generalized stacking fault energy for candidate slip systems. Consequently, highly non-linear interactions between dislocation cores and the detailed, core-dependent structure of defects such as extended nodes can be computed. A consequence of current implementations with a regular 3-dimensional discretization is that the system size cannot exceed 100 to 200 core dimensions. Thus, only small portions of arrays can be modeled.
2.4 Cellular Automaton Method

For cellular automaton method, system is divided into regular cells, and the status of each cell is determined by its neighbor cells [45]. Cells can be rectangular, hexagonal, and so on. Examples of application of this method include transportation and traffic flow [46], alloy solidification [47, 48], static recrystallization in Aluminum [49], phase transformation [50]. Taken austenite decomposition into ferrite [51] as an example, the system is divided into hexagonal cells as shown in Figure 2.5(a), which are characterized by certain attributes that represent the state of each cell. Transformation rules for each cell are obtained from ferrite nucleation and growth models. The neighbors of a cell are defined as the nearest six cells in Figure 2.5(b) in this CA model. There are six variables for every cell in the lattice in simulating austenite decomposition into ferrite. The six variables are: one crystal orientation variable representing the crystallization orientation of ferrite nucleus; one phase state variable implying that the lattice site whether belongs to ferrite ($\alpha$) phase, austenite ($\gamma$) phase, or interface ($\gamma$-$\alpha$); three concentration variables representing carbon concentration in ferrite, carbon concentration in austenite and average carbon concentration; one phase fraction variable that indicates the ferrite fraction.
Figure 2.5: Schematic illustration of the hexagonal grid in the CA model (a) and the neighborhood of a cell (b)
The initial system state is a unique austenite phase with an average carbon concentration $c_0$, carbon concentration $c_0$ in austenite, zero carbon concentration in ferrite, and zero ferrite fraction. With cooling under transformation temperature, ferrite is nucleated randomly from the austenite cells. Once a cell gets nucleated, its phase state changes into ferrite and its carbon concentration is that in ferrite. The system continues its transformation according to nucleation and growth rules.

In this study, cellular automaton method is employed to study dislocation behaviors. The system is three-dimensional and is divided into cube cells with edges along crystallographic directions $\langle 100 \rangle$. The $\{111\}$ planes are partitioned into regular triangle patches automatically. Dislocation is represented as the frontal edges of the slipped region in the slip planes. Dislocation propagation is realized by changing the status of triangles in front of existing dislocation line from unslipped to slipped. The following chapter focuses on the cellular automaton model development for dislocation study.
CHAPTER 3

CELLULAR AUTOMATON DISLOCATION MODEL

– MODEL DEVELOPMENT

To study dislocation motion and plastic deformation of materials, a cellular automaton dislocation motion model is developed first. This chapter provides the development of this model. FCC (Face Centered Cubic) structure is chosen to be the structure of the study object employed. Other structures can also be studied after some adaptation of this model. How to represent the study system, the rules for system behavior under some external excitation, and how to process simulation results should be specified in the model.

In this chapter, the scheme used to discretize and represent the structure is given first. FCC structure is divided into cubes with edges along <100> crystallographic directions, {111} slip planes are partitioned into regular triangular patches, and dislocations are expressed as a set of triangular sides. Then, theoretical background for this model is developed. This section includes verification of divisibility of dislocation line into segments, and calculation of system energy change during system evolution. System evolves with slipping of triangular patches adjoining the studying dislocation line in slip plane. Dislocation line front changes with system evolution. System energy change is composed of elastic energy change due to the change in dislocation line configuration,
and work done by internal and external stresses excluding the stress from the studying dislocation. After that, system evolution process is described. In our model, one triangular patch is slipped at each step, and system evolves along the path of steepest decent in energy. However, Monte-Carlo scheme can be incorporated in selecting the evolution path. Last, two stress averaging methods are illustrated. These methods are utilized to process the local instantaneous raw stress data from simulations.

3.1 Discretization and Representation of Study Object

A three dimensional FCC crystal as shown in Figure 3.1 is discretized into cubes of edge length $u$ that are aligned to the <100> crystallographic basis. {111} family of crystallographic slip planes in FCC crystals [52] are automatically partitioned into equilateral triangular patches with edge length $L = \sqrt{2}u$, whose three vertices coincide with the cube corners. The perpendicular spacing between parallel slip planes is $2/\sqrt{3}u$. In Figure 3.1, triangular patches PBA and CBA show the (111) and (1 1 1) variants of the four possible slip plane orientations, and the larger triangle DEF shows the seamless extension of individual patches to produce a macroscopic (111) slip plane. Figure 3.2 illustrated a two dimensional representation of partitioned (111) plane. Dislocation loop ABCDEF in Figure 3.2 shows that dislocations are divided into straight segments, which correspond to triangular sides of discretized slip plane. Each dislocation segment has the length of $\sqrt{2}u$. Specifically, dislocation loop ABCDEF is composed of straight segments AB, BC, CD, DE, EF, and FA.
Figure 3.1: Discretization of a FCC crystal into cubes of edge length $u$ aligned to a <100> crystallographic basis
Figure 3.2: Illustration of discretization of (111) plane into regular triangles in 2-dimensional view. ABCDEF represents a dislocation loop with shaded region inside as slipped
The four \{111\} planes are projected onto the (001) plane in Figure 3.3. These slip planes are labeled $a$, $b$, $c$, or $d$ and each has three possible Burgers vectors (1, 2, 3) for a total of 12 perfect \{111\}/<110> slip systems. Table 3.1 lists these 12 systems using the notation $a1$, $a2$, etc. to denote the combination of slip plane and Burgers vector. Also included are 6 \{100\}/<110> pure edge misfit dislocations that may occur as reaction products between \{111\}/<110> dislocations. For example, misfit dislocations $e1$ and $e2$ in Figure 3.3 can be formed by the reactions $e1 = c3 + a1 = -(a3 + c1)$ and $e2 = b1 + d3 = -(b3 + d1)$. 
Figure 3.3: Projection of the $\{110\} / \{111\}$ and $\{110\} / \{001\}$ FCC slip systems listed in Table 3.1
<table>
<thead>
<tr>
<th>slip plane</th>
<th>Burgers vectors</th>
</tr>
</thead>
<tbody>
<tr>
<td>n</td>
<td>b(1)</td>
</tr>
<tr>
<td>(a) [111]</td>
<td>[10 T]</td>
</tr>
<tr>
<td>(b) [T 11]</td>
<td>[01 T]</td>
</tr>
<tr>
<td>(c) [T T 1]</td>
<td>[T 0 T]</td>
</tr>
<tr>
<td>(d) [1 T 1]</td>
<td>[0 T T]</td>
</tr>
<tr>
<td>(e) [001]</td>
<td>[110]</td>
</tr>
<tr>
<td>(f) [010]</td>
<td>[101]</td>
</tr>
<tr>
<td>(g) [100]</td>
<td>[0 T 1]</td>
</tr>
</tbody>
</table>

Table 3.1: FCC slip systems in the CA model.
3.2 Theoretical Background

In the model, dislocation is expressed as a set of straight, equal-length segments, which correspond to triangular cell sides of partitioned slip planes. Dislocation propagates by slipping one triangle neighboring to the slipped region each step. In this section, divisibility of dislocation line into segments is verified analytically first. Then, system energy change due to dislocation propagation is provided. The total energy change $\Delta \phi$ includes elastic energy change of dislocation line $\Delta e$, and work $\Delta w$ done by applied stress and microstructural stress on the newly slipped triangle. $\Delta e$ comes from dislocation configuration change and is composed of variation in dislocation self energy and interaction energy. For multilayered structures, the source of microstructural stress can be lattice parameter mismatch and elastic modulus mismatch between layers of different materials, and misfit dislocation arrays in interfaces.

3.2.1 Divisibility of Dislocation Line

Since a dislocation line is represented by a set of straight segments, the divisibility of dislocation line is very important. This section verifies divisibility of dislocation line. First, a general curved dislocation is studied to show this property of dislocation. Next, a straight screw dislocation is analyzed as an example. As for any dislocation line, the segments representing it can be assumed to be straight if the segments are short.

From Hirth and Lothe [52], self energy $e_{s(C)}$ of a dislocation loop $C$ and interaction energy $e_{\text{int}(C_1-C_2)}$ between two dislocation loops $C_1$ and $C_2$ are
\[ e_{s(C)} = \frac{\mu}{8\pi C_C} \iint \frac{(b \cdot d\ell_1)(b \cdot d\ell_2)}{R} + \frac{\mu}{8\pi(1-v) C_C} \iint (b \times d\ell_1) \cdot T \cdot (b \times d\ell_2) \quad (3.1) \]

\[ e_{\text{int}(C_1-C_2)} = -\frac{\mu}{2\pi C_1 C_2} \iint \frac{(b_1 \times b_2) \cdot (d\ell_1 \times d\ell_2)}{R} + \frac{\mu}{4\pi C_1 C_2} \iint \frac{(b_1 \cdot d\ell_1)(b_2 \cdot d\ell_2)}{R} + \frac{\mu}{4\pi(1-v) C_1 C_2} \iint (b_1 \times d\ell_1) \cdot T \cdot (b_2 \times d\ell_2) \quad (3.2) \]

where \( b, b_1, \) and \( b_2 \) are Burgers vector of dislocation loop \( C, C_1, \) and \( C_2 \) respectively. \( d\ell_1 \) and \( d\ell_2 \) in \( e_{s(C)} \) are two infinitesimal segments on dislocation loop \( C. \) \( d\ell_1 \) and \( d\ell_2 \) in \( e_{\text{int}(C_1-C_2)} \) are two infinitesimal segments on dislocation loop \( C_1 \) and \( C_2 \) respectively. \( R \) is the distance between \( d\ell_1 \) and \( d\ell_2. \) And \( T_{ij} = \frac{\partial^2 R}{\partial x_i \partial x_j}. \)

**Figure 3.4** gives a dislocation loop \( C. \) When \( C \) is divided into \( C_1 \) and \( C_2, \) we have \( C = C_1 + C_2. \) When represented as one loop \( C, \) the energy expression is

\[ e(C) = e_{s(C)} = \frac{\mu}{8\pi C_C} \iint \frac{(b \cdot d\ell_1)(b \cdot d\ell_2)}{R} + \frac{\mu}{8\pi(1-v) C_C} \iint (b \times d\ell_1) \cdot T \cdot (b \times d\ell_2) \quad (3.3) \]

When represented as \( C_1 + C_2, \) the energy is

\[ e(C_1+C_2) = e_{s(C_1)} + e_{s(C_2)} + e_{\text{int}(C_1-C_2)} \quad (3.4) \]

where
\[ e_{s(c_1)} = \frac{\mu}{8\pi c_1 c_1} \int \frac{(b \cdot d\ell_1)(b \cdot d\ell_2)}{R} + \frac{\mu}{8\pi (1-v) c_1 c_1} \int \frac{(b \times d\ell_1) \cdot T \cdot (b \times d\ell_2)}{} \\ (3.5) \]

\[ e_{s(c_2)} = \frac{\mu}{8\pi c_2 c_2} \int \frac{(b \cdot d\ell_1)(b \cdot d\ell_2)}{R} + \frac{\mu}{8\pi (1-v) c_2 c_2} \int \frac{(b \times d\ell_1) \cdot T \cdot (b \times d\ell_2)}{} \\ (3.6) \]

\[ e_{\text{int}(c_1-c_2)} = -\frac{\mu}{2\pi c_1 c_2} \int \frac{(b_1 \times b_2) \cdot (d\ell_1 \times d\ell_2)}{R} + \frac{\mu}{4\pi c_1 c_2} \int \frac{(b_1 \cdot d\ell_1)(b_2 \cdot d\ell_2)}{R} \\
+ \frac{\mu}{4\pi (1-v) c_1 c_2} \int \frac{(b_1 \times d\ell_1) \cdot T \cdot (b_2 \times d\ell_2)}{} \\ (3.7) \]

Since \( b_1 \) and \( b_2 \) are the same as \( b \) in \( e_{\text{int}(c_1-c_2)} \), interaction energy between \( C_1 \) and \( C_2 \) here is

\[ e_{\text{int}(c_1-c_2)} = \frac{\mu}{4\pi c_1 c_2} \int \frac{(b \cdot d\ell_1)(b \cdot d\ell_2)}{R} + \frac{\mu}{4\pi (1-v) c_1 c_2} \int \frac{(b \times d\ell_1) \cdot T \cdot (b \times d\ell_2)}{} \\ (3.8) \]
Figure 3.4: A general curved dislocation for illustration of dislocation divisibility. $b$ is Burgers vector, $A_1A_2$ is dislocation $C$, and $A_1A_3$ and $A_3A_2$ are dislocations $C_1$ and $C_2$. 
Equation (3.3) of $e_{(C)}$ can be expressed as follows:

$$e_{(C)} = \frac{\mu}{8\pi} \oint_{(C_1+C_2)(C_1+C_2)} \oint (b \cdot d\ell_1)(b \cdot d\ell_2) \frac{R}{R}$$

$$+ \frac{\mu}{8\pi(1-v)} \oint_{(C_1+C_2)(C_1+C_2)} \oint (b \times d\ell_1) \cdot T \cdot (b \times d\ell_2)$$

$$= \frac{\mu}{8\pi} \oint_{C_1 C_1} \oint (b \cdot d\ell_1)(b \cdot d\ell_2) + \frac{\mu}{8\pi(1-v)} \oint_{C_1 C_1} \oint (b \times d\ell_1) \cdot T \cdot (b \times d\ell_2)$$

$$+ \frac{\mu}{8\pi} \oint_{C_2 C_2} \oint (b \cdot d\ell_1)(b \cdot d\ell_2) + \frac{\mu}{8\pi(1-v)} \oint_{C_2 C_2} \oint (b \times d\ell_1) \cdot T \cdot (b \times d\ell_2)$$

$$+ \frac{\mu}{8\pi} \oint_{C_1 C_1} \oint (b \cdot d\ell_1)(b \cdot d\ell_2) + \frac{\mu}{8\pi(1-v)} \oint_{C_1 C_1} \oint (b \times d\ell_1) \cdot T \cdot (b \times d\ell_2)$$

$$= \frac{\mu}{8\pi} \oint_{C_1 C_1} \oint (b \cdot d\ell_1)(b \cdot d\ell_2) + \frac{\mu}{8\pi(1-v)} \oint_{C_1 C_1} \oint (b \times d\ell_1) \cdot T \cdot (b \times d\ell_2)$$

$$+ \frac{\mu}{8\pi} \oint_{C_2 C_2} \oint (b \cdot d\ell_1)(b \cdot d\ell_2) + \frac{\mu}{8\pi(1-v)} \oint_{C_2 C_2} \oint (b \times d\ell_1) \cdot T \cdot (b \times d\ell_2)$$

$$+ \frac{2\mu}{8\pi} \oint_{C_1 C_2} \oint (b \cdot d\ell_1)(b \cdot d\ell_2) + \frac{2\mu}{8\pi(1-v)} \oint_{C_1 C_2} \oint (b \times d\ell_1) \cdot T \cdot (b \times d\ell_2)$$

$$= e_{s(C_1)} + e_{s(C_2)} + e_{\text{int}(C_1-C_2)}$$

Therefore, dislocation loop $C$ can be represented as $C_1+C_2$.

Taken a straight screw dislocation in Figure 3.5 as an example, AB is a dislocation line of length $L$, C is a division point on line AB. The following part shows that dislocation AB can be represented as 2 segments AC and CB.
Figure 3.5: Division of dislocation line AB of length $L$ into segments AC and CB of length $L_1$ and $L_2$ respectively. $\mathbf{b}$ is Burgers vector; and $\xi$ is line sense.
Self energy of a screw dislocation of length $L$ and interaction energy between screw dislocations of length $L_1$ and $L_2$ are

\[
e_s = \frac{\mu b^2}{8\pi} \int_0^L dl_1 \left( \int_0^{l_1-p} \frac{dl_2}{l_1-l_2} + \int_0^{l_1+p} \frac{dl_2}{l_2-l_1} \right)
\]

and

\[
e_{\text{int}} = \frac{\mu b^2}{4\pi} \int_0^{L_1} \int_0^{L_2} \frac{dl_2}{l_1+l_2}
\]

where $\rho$ is the cut off spacing below which two differential segments do not interact.

For dislocation line $AB$ in Figure 3.5, when it is expressed as one line, the total system energy is the self energy of $AB$. By elementary integration formula $\int \frac{dx}{x} = \ln \frac{x_2}{x_1}$, and

\[
\int_{x_1}^{x_2} \ln(x)dx = x_2 \ln \frac{x_2}{e} - x_1 \ln \frac{x_1}{e}, \text{ the self energy expression is}
\]

\[
e_{\text{total}} = e_{s(AB)} = \frac{\mu b^2 L}{4\pi} \ln \frac{L}{\rho}
\]

When $AB$ is represented as the combination of line segments $AC$ and $CB$, the total system energy is the summation of the self energy of $AC$ and $CB$, and the interaction energy between $AC$ and $CB$. Similarly with the integration, the energy expressions are
By adding the three parts of energy together, the total system energy is

\[ e_{total} = e_s(AC) + e_s(CB) + e_{int(AC-CB)} = \frac{\mu b^2}{4\pi} L \ln \frac{L}{ep} = e_s(AB) \] (3.16)

From the above results, it is clear that the total energy is the same for the two different representations of the dislocation configuration. Therefore, any true dislocation configuration can be approximated by a set of piecewise dislocation segments. The self energy for each segment and the interaction energy between different segments are much easier to be obtained than the whole line when dislocation configuration is complex. Then, the energy for the approximate configuration can be obtained accurately and much more easily.

### 3.2.2 Energetics of Slipping Patches

The slip of individual patches changes the energy of a stressed crystal by an amount
\[ \Delta \phi = \Delta e - \Delta w \] (3.17)

where \( \Delta e \) is the change in elastic energy of the isolated dislocation configuration. \( \Delta w \) is the work done by applied and internal sources of stress other than the dislocation segments.

### 3.2.2.1 Change in elastic energy of dislocation

\( \Delta e \) is the difference between the energy of dislocation before an individual patch slip and that of dislocation after an individual patch slip. Dislocation is represented as \( N_b \) and \( N_a \) straight segments for the configurations before and after a patch slip respectively. The energy of dislocation contains self energy of segments and interaction energy between segments.

\[
\Delta e = \left\{ \sum_{i=1}^{N_b} e_{s(i)} + \frac{1}{2} \sum_{i=1}^{N_b} \sum_{j=i+1}^{N_b} e_{\text{int}(i-j)} \right\}_{\text{afterslip}} \\
- \left\{ \sum_{i=1}^{N_a} e_{s(i)} + \frac{1}{2} \sum_{i=1}^{N_a} \sum_{j=i+1}^{N_a} E_{\text{int}(i-j)} \right\}_{\text{beforeslip}}
\] (3.18)

where \( i \) and \( j \) refer to dislocation segments. In **Figure 3.6**, the original straight dislocation line EF propagates to EGHIF, and the corresponding elastic dislocation energy change is:

\[
\Delta e = e_{s(GH)} + e_{s(HI)} - e_{s(GL)} + e_{\text{int}(GH\rightarrow EG)} + e_{\text{int}(GH\rightarrow IF)} + e_{\text{int}(GH\rightarrow HI)} + e_{\text{int}(HI\rightarrow EG)} - e_{\text{int}(GI\rightarrow EG)} - e_{\text{int}(GI\rightarrow IF)}
\] (3.19)
where \( e_{s(GH)} \), \( e_{s(HI)} \) and \( e_{s(GI)} \) are the self energies of line segments \( GH \), \( HI \) and \( GI \), respectively, and \( e_{\text{int}(GH-EG)} \), \( e_{\text{int}(GH-IF)} \), \( e_{\text{int}(HI-GE)} \), \( e_{\text{int}(HI-IF)} \), \( e_{\text{int}(GI-EG)} \) and \( e_{\text{int}(GI-IF)} \) are the corresponding interaction energies between two line segments.

The self and interaction energies are obtained using the development provided by Hirth and Lothe [52], and they are described briefly here.

Self energy \( e_{s(i)} \) of a segment with length \( L \) is

\[
e_{s(i)} = \frac{\mu}{4\pi} \left[ (b \cdot \xi)^2 + \frac{|(b \times \xi)|^2}{1 - \nu} \right] L \ln \frac{L}{\varepsilon \rho}
\]  

(3.20)

where \( i = (1, 2, 3, \ldots, N) \), \( N \) is the number of segments, \( b \) is the Burgers vector, and \( \xi \) is the line sense.

The interaction energy between two dislocation segments as shown in Figure 3.7 is

\[
e_{\text{int}}(x_1,y_1,x_2,y_2) = \left[-\frac{\mu}{2\pi}(b_1 \times b_2) \cdot (\xi_1 \times \xi_2) + \frac{\mu}{4\pi}(b_1 \cdot \xi_1)(b_2 \cdot \xi_2)\right] I(x_\alpha,y_\beta) \\
+ \frac{\mu}{4\pi(1 - \nu)}(b_1 \times \xi_1) \cdot T \cdot (b_2 \times \xi_2)
\]  

(3.21)

where \( \xi_3 = \frac{(\xi_1 \times \xi_2)}{|\xi_1 \times \xi_2|} \), \( I(x_\alpha,y_\beta) = I(x_2,y_2) + I(x_1,y_1) - I(x_2,y_1) - I(x_1,y_2) \), and \( x_\alpha \) and \( y_\beta \) are the end coordinates of two dislocation segments, \( \alpha, \beta = 1, 2 \). For two non-coplanar dislocations, \( I \) and \( T \) are defined as
\[
I(x, y) = \frac{x}{2} \ln \frac{z^2 + v^2 \cot \theta (\theta / 2)}{st} + \frac{y}{2} \ln \frac{z^2 + u^2 \cot \theta (\theta / 2)}{st} - z^2 J(x, y) \quad (3.22)
\]

\[
T = -\xi_2 \otimes \xi_1 \frac{\cos \theta}{\sin^4 \theta} \left[ L(x_\alpha, y_\beta) + L(y_\alpha, x_\beta) \right]
- \xi_2 \otimes \xi_1 \frac{1 + \cos^2 \theta}{\sin^4 \theta} R(x_\alpha, y_\beta) + (e_3 \otimes \xi_1 - \xi_2 \otimes e_3 \cos \theta) \frac{z}{\sin^2 \theta} K(y_\alpha, x_\beta)
+ (e_3 \otimes \xi_1 \cos \theta - \xi_2 \otimes e_3) \frac{z}{\sin^2 \theta} K(x_\alpha, y_\beta) + e_3 \otimes e_3 [I(x_\alpha, y_\beta) - z^2 J(x_\alpha, y_\beta)] \quad (3.23)
\]

where

\[
s = y \cos \theta - x + R \quad (3.24)
\]
\[
t = x \cos \theta - y + R \quad (3.25)
\]
\[
u = x - y + R \quad (3.26)
\]
\[
w = x + y + R \quad (3.27)
\]
\[
K(x, y) = -\ln s \quad (3.29)
\]
\[
K(y, x) = -\ln t \quad (3.30)
\]
\[
L(x, y) = -R(x, y) \cos \theta - y \sin^2 \theta \ln s \quad (3.31)
\]
\[
L(y, x) = -R(x, y) \cos \theta - x \sin^2 \theta \ln t \quad (3.32)
\]
\[
J(x, y) = \frac{\tan(\theta / 2)}{2z} \left[ \tan^{-1} \left( \frac{u}{z} \cot \theta \right) \right]
+ \tan^{-1} \left( \frac{v}{z} \cot \theta \right) - \frac{\cot \theta (\theta / 2)}{z} \tan^{-1} \left( \frac{w}{z} \tan \theta \right) \quad (3.33)
\]
\[
R(x, y) = \sqrt{x^2 + y^2 - 2xy \cos \theta + z^2} \quad (3.34)
\]

For two coplanar dislocations, \( z = 0 \) is applied in the above equations.
Figure 3.6: Evolution of initial straight dislocation EF to EGHIF. The shaded area is slipped.
Figure 3.7: Coordinates for interaction energy calculations for two dislocations, used in equation (3.21); $x$ and $y$ are defined along the two dislocations, and $x_1, y_1, x_2, y_2$ are the end points of the two dislocation segments (from Hirth and Lothe [52])
3.2.2.2 Work done by applied and internal stresses

The work done by applied and internal sources of stress other than the dislocation segments is expressed as

\[ \Delta w = \int_{A_s} n_i \left( \sigma_{ij}^a(x) + \sigma_{ij}^m(x) \right) b_j \, d_\Sigma = \lambda \sigma_{nb}^o A_s + \sigma_{nb}^m A_s \]  \tag{3.35} \]

where \( n_i \) and \( b_j \) are the components of the slip plane normal and Burgers vector for the area \( A_s \) to be slipped, and \( \sigma_{ij}^a \) and \( \sigma_{ij}^m \) are the components of applied and microstructural stress that vary spatially in general. Specifically in multilayers, \( \sigma_{ij}^m \) includes stress from particles, misfit dislocations and coherency stress from lattice parameter mismatch [52-54]. The right-hand portion of Equation (3.35) expresses the result in terms of a homogeneous applied stress that is proportional to a reference value,

\[ \sigma_{ij}^a = \lambda \sigma_{ij}^o \]  \tag{3.36} \]

and a microstructural stress \( \sigma_{ij}^m \) averaged over \( A_s \). The subscripts nb simply denote the component of stress that is resolved on the slip plane with normal \( n_i \) in the direction of slip \( b_j \). Combining Equations (3.17) and (3.35),

\[ \Delta \phi = \Delta e - \lambda \sigma_{nb}^o b A_s - \sigma_{nb}^m b A_s \]  \tag{3.37} \]
In this model, the sources contributing to microstructure stress \( \sigma_{ij}^m \) are the coherency stress due to the lattice mismatch of different layers, and the stress field of misfit dislocation arrays on or near the interfaces of the multilayered composites.

\[
\sigma_{ij}^m = \sigma_{ij}^{coh} + \sigma_{ij}^{misfit}
\]

(3.38)

\( \sigma_{ij}^{coh} \) is the alternating compressive and tensile coherency stress due to a mismatch in stress-free lattice parameters \( a_2^0 \) and \( a_1^0 \) of the two kinds of layers in multilayered materials. An equi-biaxial stress state will arise, and the stress in layer type (1) is as in equation (3.39)[54].

\[
\frac{\sigma_{ij}^{coh-1}}{M_1} = \frac{\sigma_{22}^{coh-1}}{M_1} = \frac{(a_2^0 / a_1^0)(1 + \Sigma / v_2M_2) - (1 + b_1 / s)}{1 + (a_2^0 v_1 M_1 / a_1^0 v_2 M_2)}
\]

(3.39)

where \( M_i = E_i / (1 - \nu_i) \) is a function of the elastic modulus \( E_i \) and Poissons ratio of layer type (i), and \( v_i \) is the volume fraction of type (i). To get the stress in layer type (2), the indices 1 and 2 need to be exchanged in equation (3.39). For an FCC structure, the resolved shear stress on a (111) slip plane with [10\( \bar{1} \)] slip direction is \( \tau \equiv \sigma_{ij} n_i s_j = \sigma_{11}^{(i)} / \sqrt{6} \).
Figure 3.8: Schematic interfacial dislocation array with spacing $S$ for equation (3.40)-(3.43) (From Hirth and Lothe[52])
The interfacial misfit dislocation arrays in the model are assumed to be uniformly distributed. The stress field is obtained by summing up that of each array of dislocations as shown in Figure 3.8. The stress field of misfit dislocation array in Figure 3.8 [52] is

\[
\sigma_{xy}^{\text{misfit}} = \sigma_0 \sin 2\pi Y (\cosh 2\pi X - \cos 2\pi Y - 2\pi \chi \sinh 2\pi \chi) \tag{3.40}
\]

\[
\sigma_{xx}^{\text{misfit}} = -\sigma_0 2\pi \chi (\cosh 2\pi \chi \cos 2\pi Y - 1) \tag{3.41}
\]

\[
\sigma_{yy}^{\text{misfit}} = -\sigma_0 [2 \sinh 2\pi \chi (\cosh 2\pi \chi - \cos 2\pi Y) - 2\pi \chi (\cosh 2\pi \chi \cos 2\pi Y - 1)] \tag{3.42}
\]

\[
\sigma_{zz}^{\text{misfit}} = v (\sigma_{xx}^{\text{misfit}} + \sigma_{yy}^{\text{misfit}}) \tag{3.43}
\]

where the array geometry is shown in Figure 3.8, with \(X = x/S, Y = y/S\), and

\[
\sigma_0 = \frac{\mu b}{2S(1-v)(\cosh 2\pi X - \cos 2\pi Y)^2}.
\]

3.3 System Evolution

Several methods exist to update dislocation configurations as a function of time. In the limit of atomic-scale patches, \(\Delta \phi\) may be on the order of \(kT\) so that a Monte-Carlo scheme may be appropriate. In this case, the probability that patch \(k\) is slipped during some time interval \(\Delta t\) is \(P_k(\Delta t) = \eta \Delta t \exp(-\Delta \phi k/kT)\), where \(\eta\) is attempt frequency. The simulation proceeds by determining the time interval \(\Delta t^*\) over which the collective probability \(\Sigma P_k(\Delta t^*)\) over all patches is 1. A random number in the interval [0, 1] is then selected to determine the triangle that slips during \(\Delta t^*\). Thus, the simulation captures the thermal fluctuations of dislocation loops. For example, such methods have been used by
Daehn [55] to study creep behavior and Cai et al [56] to modeled dislocation motion in BCC metals. One significant difference is that the current work uses a 3D space-filling array of patches reflecting the symmetry of the crystal, compared to 2D rectangular grids.

An approach applicable for larger patch sizes is to follow the path of steepest decent in energy, with the constraint that only one patch is slipped at a time. This can be implemented in two forms. The first requires a prescribed stress history. The patch with the most negative $\Delta\phi$ is selected, so that a path of steepest decent in energy is followed, subject to the constraint that only one patch is selected in each step. A relaxation test is an example of a prescribed stress history, in which the dislocation loop relaxes to a stable configuration under a constraint of zero applied stress. A second macroscopic approach is to determine the stress history necessary to reversibly change the shape of a loop. Here, an applied reference stress state $\sigma^0_{ij}$ is prescribed and the applied stress $\sigma_{ij(k)} = \lambda_k \sigma^0_{ij}$ to activate each triangle $k$ adjoining the existing loop is determined subject to the condition $\Delta\phi_k = 0$. The applied stress magnitude necessary to activate a loop is given by

$$\lambda_k = \frac{(\Delta e - \Delta w)_k}{(n_i\sigma_{ij}^0 s_j b A_s)_k}$$

(3.44)

where $n_i, s_j, b, and A_s$ are the unit slip plane normal, unit slip direction, Burgers vector magnitude, and slipped area associated with triangle $k$.

The minimum positive value, $\lambda_{\text{min}}$, among all possible slip events is identified so that $\sigma^\text{rev}_{ij} = \lambda_{\text{min}} \sigma^0_{ij}$ is the stress needed to reversibly expand the loop during that increment.
The method is a physically viable one if $\lambda_{\text{min}}$ monotonically increases from one step to the next, implying that the configuration expands in a stable fashion. However, a decrease in the magnitude of $\lambda_{\text{min}}$ signifies an instability through which there is no stable configuration of the loop. Here, the first form requiring a stress history must be used to study evolution in unstable regimes.

### 3.4 Stress Average

Averaging values of $\lambda_{\text{min}}$ is an important processing step that corresponds to the smoothening out of the discrete patch nature of the simulation. At the atomic scale, it may be reasonable to view dislocation line motion in terms of nucleation and growth of kink pairs via the addition of discrete triangles $1, 2, 3, 4, 5$ to the line $\mathbf{HJ}$ in Figure 3.3. For larger triangles that correspond to several atomic slip distances, the triangular patches lose their physical connection to an atomic lattice and result in the artificial creation and removal of dislocation line length. For example, the addition of triangle 1 on line $\mathbf{AB}$ in Figure 3.9 requires a large positive nucleation stress given by equation (3.44), since the dislocation line length increases by $L$ while slipped area increases only by $A_s$. Typically, the preferred site for the next step is triangle 2 or triangle 4, which is the symmetric counterpart of triangle 2. This also requires a large positive stress since dislocation line length again increases by $L$ while slipped area increases only by $A_s$. The preferred site for the next step is triangle 3 or the symmetric counterpart, which decreases line length by $L$ and increases slipped area by $A_s$. The reversible stress required is negative. The values of resolved shear stress to nucleate individual triangles at each step are reported in Figure
This pattern of two positive values of $\tau$ followed by a negative value typically signifies formation of a new kink-pair-like structure on a straight dislocation line. Subsequent expansion of the structure involves the slip of triangle 4, followed by 5 or the symmetric counterpart. The expansion pattern thus has alternating positive-negative 
values of $\tau$ as shown in Figure 3.10.

This discussion suggests two-levels at which to average successive $\tau$. A smaller-scale, or microstructural process is to average over triplets consisting of positive/positive/negative values so that in the example here, $\tau_1 = \text{Avg}(\tau_1, \tau_2, \tau_3)$, and also to average over pairs of positive/negative values so that $\tau_p = \text{Avg}(\tau_4, \tau_5)$. These two average values ($\tau_t$, $\tau_p$) define the nucleation of a triplet and the expansion of it in a row via nucleation of pairs, respectively. Figure 3.11 presents the result of this triplets/doublets averaging. A larger, macroscopic average is over all $\tau$ from one triplet nucleation to the next. This average ($\tau_r$) typically defines the forward motion of a linear portion of a macroscopic loop via the slip of an entire row ($r$) of triangles. Additional smoothening is achieved by computing

$$T_r = 0.25\tau_{r-1} + 0.50\tau_r + 0.25\tau_{r+1} \quad (3.45)$$

where subscript $r$ denotes the row over which the average has occurred. This averaging result is shown in Figure 3.12. Thus, unlike methods employing continuous motion of front-tracking nodes, the CA approach described here permits a rich hierarchy of
energetics and length scales, within which averages over small clusters or entire dislocation fronts are possible, depending on the physical scale of the triangular patches.
Figure 3.9: Schematic illustration of dislocation propagation from initial configuration of line AB to ACDEFB
Figure 3.10: Instantaneous local applied shear stress $\frac{\tau^{(k)}}{\mu}$ needed for dislocation propagation in Figure 3.9; evolution steps refer to the sequence of triangles activated.
Figure 3.11: Kink-pair averaging stress $\frac{\tau}{\mu}$ for operating a Frank-Read source; (t1) and (t2) are the average stresses for nucleating a kink pair, (p1), (p2), and so on are the average stresses for growing a kink pair.
Figure 3.12: Window averaging stress $\frac{\tau}{\mu}$ for operating a Frank-Read source; $\tau_{row(a)}$ and $\tau_{row(b)}$ are the average stress for a whole row.
3.5 Summary

A 3D dislocation cellular automaton (CA) model is developed in which FCC crystalline material is discretized into a 3D array of cube cells. \{111\} slip planes are partitioned into regular triangles, each of which can slip. Discretization matches the crystallographic structure and symmetry of materials. Dislocations are represented by a set of triangular sides in slip planes. This makes dislocation line senses along \textless 110\textgreater only. This discrete line sense is very beneficial in modeling cross-slip. Meanwhile, line sense of a dislocation does not change continuously. The energy of a dislocated system is computed exactly within the limits of elasticity theory for the self and interaction energies of Volterra dislocation segments in elastically homogeneous material. Additional contributions to the system energy stem from the work done by the applied stress and internal sources of stress due to inclusions or other inhomogeneities. The dislocation configuration is updated by successively slipping triangular patches according to a path of steepest decent in energy, with the constraint that only one triangle slips at a time. At each step, only one new triangle is added to the record. There is no need to update for each dislocation segment. From the recorded resolved shear stress for each triangular patch slip, micro- and macro-level averaging can be employed to get continuum result.

The primary benefit to a CA approach is that complicated evolution of dislocation loops, including cross slip, can be modeled in a geometrically simple manner. Computational complexities associated with the singular interaction between Volterra dislocation segments are avoided using a discrete system. The approach has a microstructural appeal since, in the limit of decreasing patch size, the discretization
mimics the nucleation and growth of kink or jog pairs. Thus, the model lends itself to a Monte-Carlo approach for system evolution. The 3D space filling discretization permits kink and jog formation at arbitrary locations along a dislocation line, and even loop formation at arbitrary volume sites. The operation of a Frank-Read source near a barrier highlights the 3D cross slip configurations that evolve using this approach.
CHAPTER 4

CELLULAR AUTOMATON DISLOCATION MODEL

—MODEL CALIBRATION

This chapter focuses on calibration of the 3D dislocation CA model developed in chapter 3. First, triangular patch nucleation on a finite segment is studied. The applied stress needed for this nucleation is derived analytically. Results from simulations agree very well with the analytic results. Next, Frank-Read source operation in an infinite, elastically isotropic medium is analyzed. Three examples are used here. The first example assumes dislocation line energy is isotropic with $\nu = 0$. The second example models dislocation with anisotropic line energy with $\nu = 0.1$. Dislocation propagates in a non-equiaxed mode. The third example includes an infinite long parallel same-signed fixed screw dislocation in the parent slip plane of the Frank-Read source. Gliding dislocation can propagate in parent or cross-slip plane. Simulation results are consistent with analytic understanding.

4.1. Triangular Patch Nucleation on a Finite Segment

An initial test of the 3D dislocation cellular atomaton (CA) model is to compare the CA and analytic results for the critical applied stress to nucleate a triangular patch
Figure 4.1: Nucleation and growth of triangular slip on a straight dislocation line
with side length \( L \) onto a straight screw segment of length \( L_{\text{seg}} = L_1 + L + L_2 \) in isotropic, homogeneous media. The relevant geometry is shown in Figure 4.1 in terms of the nucleation of triangle \( l \) onto line \( OZ \). Since microstructural stress \( \sigma_{ij}^m \) is zero, Equation (3.37) becomes

\[
\Delta \phi = \Delta e - \lambda \sigma_{n_b}^a b A_s = \Delta e - \sigma_{n_b}^a b A_s \quad (4.1)
\]

The critical applied stress \( \sigma_{n_b}^a \) is the stress, which makes \( \Delta \phi \) equal zero. Therefore, \( (\sigma_{n_b}^a)_c \) is

\[
(\sigma_{n_b}^a)_c = \frac{\Delta e}{b A_s} \quad (4.2)
\]

where \( A_s \) is the area of triangle PAB in Figure 4.1, and \( A_s = \frac{1}{2} L^2 \sin(60^\circ) \). \( \Delta e \) is derived analytically for the configuration in Figure 4.1.

\[
\Delta e = \frac{\mu b^2}{8\pi} \left(2L \ln \left(\frac{8L}{8\text{lep}}\right) + \sum_{i=1}^{2} -L_i \ln \left(\frac{3}{4}\right)\right) \\
+ L_i \ln \left(\sqrt{L_i^2 + L_i^2 + L_i L + L + 0.5L_i} \right)
\]
\begin{equation}
+(L_i + L) \ln \left( \frac{\sqrt{L_i^2 + L^2 + L_i L + 0.5L} - 0.5L_i}{L_i + L} \right) \tag{4.3}
\end{equation}

\begin{equation}
+2L \ln \left( \frac{\sqrt{L_i^2 + L^2 + L_i L + L + 0.5L}}{L} \right)
- 2[-L_i \ln (2L_i) + (L_i + L) \ln (2L_i + 2L) - L \ln (2L)]] \end{equation}

In the limit $L_1, L_2 \to \infty$ so that the screw dislocation is infinitely long, the above expression may be reduced to

\begin{equation}
\Delta e = \frac{\mu b^2}{8\pi} 2L \ln \left( \frac{16L}{81\pi \rho} \right) \tag{4.4}
\end{equation}

By putting the formula for $\Delta e$ into Equation (4.2), the analytic resolved shear stress needed to nucleate a regular triangle can be calculated.

An important feature to note is that the analytic solution models OA and BZ in Figure 4.1 as segments of arbitrary length $L_1$ and $L_2$ while the CA approach models these segments as several smaller segments of triangular side length $L$. As discussed in Section 6-2 of Hirth and Lothe [52] and proved in Chapter 3, the energy of a straight dislocation segment such as $L$ is independent of whether $L$ is expressed as a single segment or $i = 1$ to $N$ multiple segments, so that
\[
e_s(b, \xi, L) = \frac{\mu}{4\pi} \left[ \left( b \cdot \xi \right)^2 + \left( \frac{b \times \xi}{1 - \nu} \right)^2 \right] \ln \frac{L}{\varepsilon \rho} = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} e_{ij}(b, \xi, L_i, L_j)
\]

(4.5)

The CA results reproduce the analytic results over a large range of \((L_1 + L_2)/L\) and \(L/\rho\), confirming that the program accurately computes the self and interaction energies of dislocation segments. In Table 4.1, a comparison of the analytic and CA results confirms that the energy of a configuration can be computed by discretization of longer segments into several shorter ones.

For the condition of an infinitely long screw segment with \(L_1, L_2 \to \infty\), the resolved shear stress to nucleate a triangular patch along its midpoint is denoted as \(\tau_n^\infty\). Combining Equations (4.2) and (4.4), \(\tau_n^\infty\) is

\[
\tau_n^\infty = \frac{\Delta e}{A_s b} = \frac{\mu b}{2\pi L \sin(60^\circ)} \ln \left( \frac{16L}{81\varepsilon \rho} \right)
\]

(4.6)

By plotting \(\tau_n^\infty/\mu\) verses \(L/b\) for different values of \(\rho/b\) in Figure 4.2, it is clear that there is a maximum value of \(\tau_n^\infty\). The criterion \(\frac{\partial \tau_n^\infty}{\partial L} = 0\) is used to obtain the corresponding \(L\) at the maximum \(\tau_n^\infty\). Specifically,

\[
\frac{\partial \tau_n^\infty}{\partial L} = \frac{\mu b}{2\pi \sin(60^\circ)L^2} \left[1 - \ln \left( \frac{16L}{81\varepsilon \rho} \right) \right] = 0
\]

(4.7)
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<th>$L/b$</th>
<th>$\rho/b$</th>
<th>$\tau^{\text{analytic}}/\mu$</th>
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<tr>
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<tr>
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<td>$10\sqrt{2}$</td>
<td>0.3</td>
<td>0.016</td>
<td>0.016</td>
</tr>
</tbody>
</table>

Table 4.1: Resolved shear stress to nucleate a regular triangle on an initial straight dislocation line.

* $N$ is the number of initial dislocation segments, and $N = \frac{L_{\text{seg}}}{L}$. 
Equation (4.7) can be reduced to

\[ 1 - \ln\left(\frac{16L}{81\rho}\right) = \ln\left(\frac{81e^2\rho}{16L}\right) = 0 \] (4.8)

Solving Equation (4.8) gives us the value of \( \frac{L}{\rho} \) at the maximum \( \tau_n^\infty \),

\[ \frac{L}{\rho} = \frac{81e^2}{16} \approx 37 \] (4.9)

By setting \( \tau_n^\infty = 0 \), another \( \frac{L}{\rho} \) value is gained.

\[ \frac{L}{\rho} = \frac{81e}{16} \approx 14 \] (4.10)

Therefore, \( \tau_n^\infty \) increases monotonically with decreasing patch size \( L \) until \( \frac{L}{\rho} \approx 37 \), and then monotonically decreases to 0 at \( \frac{L}{\rho} \approx 14 \). For \( \rho = b \) and 0.3\( b \), \( \tau_n^\infty \) is less than 0.5\%\( \mu \) and 2\%\( \mu \), respectively, for all values of \( L \).

**Figure 4.3** shows that the resolved shear stress to nucleate a triangular patch is larger for a finite compared to infinite segment. The difference between \( \tau_n^\infty \) and \( \tau_n \) increases with decrease of \( L/L_1 \). Further, \( \tau_n \) is a minimum for nucleation at the midpoint of a segment \((L_1 = L_2)\) compared to nucleation off of the midpoint \((L_1 = 3L_2)\).
Figure 4.2: Resolved shear stress $\tau_n^\infty$ to nucleate a triangular patch along the midpoint of an infinitely long screw segment where $L_1, L_2 \to \infty$ in Figure 4.1
Figure 4.3: Difference, $\tau_n - \tau_n^\infty$, in resolved shear stress to nucleate a triangular patch on a finite length versus infinite length screw dislocation geometry shown in Figure 4.1
4.2 Frank-Read Simulation in an Infinite, Elastically Isotropic Medium

This section compares predictions of the CA code and the corresponding analytic continuum solution for the critical stress to operate a Frank-Read source [57],

$$\tau_{\text{FR}} = \frac{A \mu b}{2\pi S} \frac{S}{r_0}, \quad A = 1 + \frac{\nu}{1 - \nu} \sin^2 \theta$$

(4.11)

where $S$ is the initial length of the source as shown in Figure 4.4, $\nu$ is Poisson's ratio, $r_0$ is dislocation core cut-off, and $\theta$ is the angle subtended by the dislocation line sense $\xi$ and Burgers vector $b$. The relation between dislocation core cut-off $r_0$ and $\rho$ is

$$\rho = \frac{r_0}{2A}, \quad A = \begin{cases} 1 & \text{screw} \\ e^{(1-2\nu)/4(1\nu)} & \text{edge} \end{cases}$$

(4.12)

These equalities ensure that the energy of a pair of infinitely long, opposite-sign dislocation lines is the same, regardless of whether a formulation based on $\rho$ or $r_0$ is used.

An initial screw segment is considered so that $\theta = 0$, and $\rho = 0.3b$ is used so that, according to Equation (4.12), $r_0 = 0.6 \ b$. First, an isotropic analysis is considered for which $\nu = 0$, so that dislocation line energy is independent of screw versus edge character. The convergence of the solution with decreasing triangular patch size is studied, using the reversible evolution procedure described in chapter 3 and macroscopic smoothening defined in Equation (3.45). Frank-Read sources with different initial length
are modeled, and the critical stress for their propagation from simulations is consistent with the analytic values. Second, an anisotropic line energy analysis is considered for which \( \nu = 0.1 \), so that line energy is a minimum for pure screw character. A non-equiaxed mode of expansion is highlighted in this case. Third, an infinitely long fixed screw dislocation is introduced into the media. This dislocation in the parent plane is parallel to and has the same sign as the Frank-Read source. Frank-Read propagation in front of this dislocation obstacle is studied.

4.2.1 Isotropic Dislocation Line Energy (\( \nu = 0 \))

This analysis reveals several features about the sequential slip of triangular patches during operation of a Frank-Read source and the effect of averaging over triangles as discussed in chapter 3, in order to get a continuum measure of critical operating stress for the source. These features are present in all analyses but are identified most easily by considering a limiting case of isotropic dislocation line energy. Figure 4.4 shows the expansion sequence of an initially straight screw dislocation of length \( S = 300 \sqrt{2} b \). The number of initial segments used in the simulation is 20. The dislocation propagates by adding triangles 1, 2, 3, 4, 5, 6, 7, … sequentially. One triangle is slipped at each step. At 39th step, the first entire row \( r_1 \) is slipped. This process of row nucleation and completion continues in the order indicated by the labeled row numbers in Figure 4.4.
Figure 4.4: Operation of a Frank-Read source of length $S = 300 \sqrt{2} b$ using triangular patches of side length $L = 15 \sqrt{2} b$, $\rho = 0.3 b$, and $v = 0$, showing the sequence of expansion
Figure 4.5: Average stress to evolve rows of patches ($T_r$) according to Equation (3.45). The critical resolved shear stress to operate the source is denoted by $\tau_{FR}$.
Macro averaging described in Chapter 3 and Equation (3.45) is used to compute the resolved shear stress $T_r$. Figure 4.5 shows that $T_r$ increases monotonically to a maximum value at row $r9$, oscillates between rows $r10$ to $r14$, and then monotonically decreases. The maximum stress at $r9$ is defined to be $T_{FR}$, which is the critical stress to operate a Frank-Read source from the simulation. The corresponding stress from analytic equation (4.11) is also reported as $\tau_{FR}$ in Figure 4.5. The simulation result agrees pretty well with the analytic value. The stress decrease after reaching $T_{FR}$ value indicates that this model captures the unstable expansion of Frank-Read operation.

For the Frank-Read source shown in Figure 4.1, different initial number $N_i$ of segments is used for its representation. For the maximum $N_i = 40$ here, $L/\rho \sim 35$, so that the simulations are stable. As shown in Figure 4.6, the error of the $\tau_{FR}$ prediction from simulations decreases exponentially with increasing $N_i$. Therefore, within the limit, increasing $N_i$ improves the accuracy of simulation prediction.

Figure 4.7 shows good agreement between $T_{FR}$ computed from the CA model and $\tau_{FR}$ from the analytic expression (Equation (4.11)), over the range $S = (106$ to $636) \ b$. A fixed triangular size $L = 15 \sqrt{2} b$ is used so that the initial number, $N_i$ of segments varies from 5 for the smallest $S$ to 30 for the largest $S$ considered.
Figure 4.6: error in CA model predictions as a function of $N_i$ for $S = 300 \sqrt{2} b$
Figure 4.7: The critical resolved shear stress $\tau_{FR}$ to operate a Frank-Read source as a function of source length $S$, as given by Equation (4.11) with $v = 0$ and $r_0 = 0.6 \ b$. Corresponding predictions, $T_{FR}$, from the CA simulation are shown as points, with numbers in parentheses denoting the initial number of segments, $N_i$. 
4.2.2 Anisotropic Dislocation Line Energy ($\nu \neq 0$)

This analysis shows that the CA model and continuum results can vary substantially due to system evolution rules. In particular, the case for $\nu = 0.1$ and $S = 300\sqrt{2} b$ involves an initial expansion as outlined in Figure 4.4, where rows $r1$ to $r5$ slip successively by the formation of a triplet of triangles in the middle of the row, followed by row expansion due to triangular pairs. Rather than nucleate a new triangle $c$ in row $r6$, triangles $a$ and $b$ form and expand as to extend the loop in the $\pm 2$ direction. This mode of expansion continues, so that a pair of oppositely signed screw dislocation lines is generated with perpendicular spacing $s_\perp \approx 92 b$. The mode of expansion is artificially trapped by the system evolution rule to select the triangle with the smallest value of $\tau$. In particular, nucleation of triangle $c$ in row $r6$ generates two mixed segments and removes one screw segment while nucleation of triangle $a$ or $b$ generates one mixed and one screw segment but removes one mixed segment. Thus, for $\nu = 0.1$, the smaller self energy of a screw segment favors continued nucleation at $a$ and $b$ and therefore continued expansion along the $\pm 2$ direction. The CA model predicts a macroscopic resolved shear stress $T_r$ that monotonically increases to $8.7 \times 10^{-3} \mu$, which compares well with $8.4 \times 10^{-3} \mu$, obtained if Equation (4.11) is used with $S = s_\perp \approx 92 b$, $\theta = 0$, and $\nu = 0.1$. However, the CA result is substantially different from $2.7 \times 10^{-3} \mu$, obtained if Equation (4.11) is used with $S = 300\sqrt{2} b$ instead.
4.2.3 Simulation of Cross-Slip During Operation of a Frank-Read Source

This section shows that the CA model is capable of capturing basic features of cross slip. The particular geometry is shown in Figure 4.8, in which a Frank-Read source involving an ends-pinned screw dislocation $OZ$ with line direction and Burgers vector along $[10\bar{1}]$ is positioned a distance $s_\perp$ from a fixed, infinitely long screw dislocation of the same sign. The two screw dislocations lie in the same (111) parent slip plane so that a local coordinate system $(1', 2', 3')$ can be defined with $s_\perp$ measured along the 1'-direction. Therefore, the crystallographic directions for 1', 2', and 3' are $[\bar{1}2\bar{1}]$, [111], and $[10\bar{1}]$. Normal operation of the Frank-Read source involves the bow out of line $OZ$ along the 1'-direction in the (111) parent plane. However, the same-signed fixed dislocation will repel the bow-out. Line $OZ$ is also contained within a (111) cross-slip plane so that screw portions of the bow out can circumvent the repulsion from the fixed dislocation by cross-slipping. Thus, Figure 4.8 shows that the source may expand by slip on the parent plane $(p)$, slip onto the positive portion of the cross slip plane $(+c)$, or slip onto the negative portion of the cross slip plane $(-c)$.

The elastic stress, applied stress, and microstructural stress terms will compete to determine whether mode $p$, $+c$, or $-c$ prevails in the initial bow-out process. A map can be constructed to highlight the trade-off in these terms and provide groundwork for evaluation of the CA results to follow. The stress field produced by the fixed, infinitely long dislocation is viewed as a microstructural stress and takes the form [52]

$$\sigma_{1'3'}^m = \sigma_{3'1'}^m = -\frac{\mu b}{2\pi} \frac{x_{2'}}{x_1'^2 + x_2'^2}, \quad \sigma_{2'3'}^m = \sigma_{3'2'}^m = \frac{\mu b}{2\pi} \frac{x_1'}{x_1'^2 + x_2'^2}, \quad \text{all other } \sigma_{ij}^m = 0 \quad (4.13)$$
Combination of Equations (3.37) and Equation (4.13) can be used to solve for the critical values \( \lambda_{(p)} \), \( \lambda_{(c)} \), \( \lambda_{(-c)} \) needed to nucleate a triangular patch along the paths \( p \), \(+c\), \(-c\), respectively. In particular, the condition \( \Delta \phi = 0 \) is applied with \( \Delta e \) approximated by the energy change to nucleate a triangular patch on an infinitely long screw dislocation, given in Equation (4.4). The microstructural work term for the triangle is evaluated at a point along the line \( OZ \),

\[
\mathbf{\bar{\sigma}}_{mb}^m b = n_i \mathbf{\sigma}_{ij}^m (x_i' = -s_\perp, x_2' = 0) b_j' = f^m \frac{\mu b^2}{2\pi s_\perp} \quad (4.14)
\]

where \( f^m = 1 \), \( 1/3 \), and \(-1/3\) for paths \( p \), \(+c\), \(-c\), respectively. Equation (3.37) then yields the critical values of \( \lambda_{(k)} \) for nucleation of a triangle along paths \( k = p \), \(+c\), and \(-c\)

\[
\lambda_{(k)} = \frac{\mu}{2\pi \sigma_{mb(k)}^o} \left[ \frac{b}{L \sin(60^\circ)} \ln \left( \frac{16L}{81c\rho} \right) + \frac{b f^m}{s_\perp} \right] \quad (4.15)
\]

where \( \sigma_{mb(k)}^o = n_{i(k)} \sigma_{ij}^o b_{j(k)} \) is the resolved shear stress to drive slip on path \( k \), due to a unit applied stress \( \sigma_{ij}^o \).
Figure 4.8: Geometry of a Frank-Read source of length \( S \) in the vicinity of a parallel screw dislocation.
Figure 4.9 shows the predicted paths for initial triangular slip as a function of $s_\perp$ and the ratio $R = \sigma_{\text{nb}(c)}/\sigma_{\text{nb}(p)}$ of applied resolved shear stress on paths $c$ and $p$. Here, the boundary between regions $p$ and $c$ is determined by setting $\lambda_{(p)} = \lambda_{(c)}$ with $\rho = 0.1 \, b$ and $L = 7.5 \sqrt{2} \, b$. Inserting $\lambda_{(p)}$ and $\lambda_{(c)}$ from Equation (4.15), the expression for this boundary is

$$R = \frac{b}{L \sin(60^\circ)} \left[ \frac{\ln \left( \frac{16L}{81\rho} \right) + \frac{b}{s_\perp}}{\frac{b}{L \sin(60^\circ)} \ln \left( \frac{16L}{81\rho} \right) + \frac{1}{3} \frac{b}{s_\perp}} \right] \quad (4.16)$$

And similarly, the corresponding construction $\lambda_{(p)} = \lambda_{(-c)}$ is used to determine the boundary between $p$ and $-c$ regions. The expression for this boundary is

$$R = \frac{b}{L \sin(60^\circ)} \left[ \frac{\ln \left( \frac{16L}{81\rho} \right) + \frac{b}{s_\perp}}{\frac{b}{L \sin(60^\circ)} \ln \left( \frac{16L}{81\rho} \right) - \frac{1}{3} \frac{b}{s_\perp}} \right] \quad (4.17)$$

The results indicate that for large $s_\perp$, slip propagation is favored on the path with the largest positive applied resolved shear stress. As $s_\perp$ is decreased, repulsion by the fixed dislocation makes slip on the $-c$ and $c$ paths possible even when path $p$ has the largest applied resolved shear stress (i.e. when $R < 1$). At sufficiently small $s_\perp$, cross slip onto the $-c$ path is preferred even for $R = 0$, due to repulsion from the fixed dislocation.
Figure 4.9: Predicted initial paths of expansion ($p$, $+c$, $-c$) for a Frank-Read source as a function of the ratio $R$ of resolved shear stress on path $c$ to path $p$ and perpendicular distance $s_\perp$ from a parallel, same-sign screw dislocation as shown in Figure 4.8. The number next to each point denotes the Case number listed in Table 4.2
Table 4.2 displays the corresponding numerical results from the CA model using a Frank-Read source length $S = 150 \sqrt{2} b$, and $p$ and $L$ values mentioned above, so that $N_i = 20$. Cases 1, 2, and 3 display the results for $s_\perp = \infty$, 0.17 $S$, and 0.13 $S$, respectively. The components of the applied reference stress state are $\sigma_{11}^o = 1, \sigma_{12}^o = \sigma_{21}^o = 1$, and all other $\sigma_{ij}^o = 0$, so that there is zero resolved shear stress on the cross slip paths ($R = 0$). The prediction in Figure 4.9 is that path $p$ is preferred initially and, indeed, the CA simulations confirm this. For Cases 1 and 2, the source operates without any cross slip but in Case 2, significant distortion occurs as the source pinches through the narrow constriction of dimension $s_\perp$, as shown in Figure 4.10. For Case 3, $s_\perp$ is sufficiently small so that cross slip on the $-c$ path is favored over the pinching process.

The competition between the $p$, $+c$, and $-c$ paths can be manipulated by imposing nonzero values of resolved shear stress on the cross slip planes. Case 4 shows the result for $s_\perp = 0.17 S$ and $R = -0.54$, which is imposed by selecting nonzero components $\sigma_{11}^o = 0.3$ and $\sigma_{12}^o = \sigma_{21}^o = 1$ for the applied stress state. According to Figure 4.9, application of a negative $R$ shifts the prediction toward the $-c$ mode and, indeed, the CA results show that the source expands by a combination of $p$ and $-c$ paths as shown in Figure 4.11. Application of a positive $R = +0.54$ in Case 5 shifts the prediction in Figure 4.9 toward the $c$ mode and, indeed, the CA results shown in Figure 4.12 confirm expansion by a combination of $p$ and $+c$ slip. Thus, Figure 4.9 provides the correct trends as a function of $R$ and $s_\perp$, but it is limited to slip of the first triangle.
Case No.  | $s_\perp$  | $R = \sigma_{\text{rb}(c)}^{\alpha}/\sigma_{\text{rb}(p)}^{\alpha}$ | $(T_{\text{FR}}/\mu)^{\ast}$ | $(T_{\text{FR}}/\mu)$ | Evolution path |
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<tr>
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</tr>
<tr>
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<td>$-0.54$</td>
<td>0.035</td>
<td>$\sim$0.018</td>
<td>$p$ and $-c$</td>
</tr>
<tr>
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<td>0.54</td>
<td>0.035</td>
<td>$\sim$0.018</td>
<td>$p$ and $+c$</td>
</tr>
</tbody>
</table>

Table 4.2: Effect of obstacle distance and applied stress state on Frank-Read source operation‡

‡ $S = 150 \sqrt{2} \, b$, $\rho = 0.1 \, b$ and $N_i = 20$.

* cross slip is excluded from happening.
The results in Table 4.2 support the outcome that cross slip reduces the operating stress for a nearby source. In particular, the CA results for Cases 3, 4, and 5 show that the macroscopic resolved shear stress $T_{\text{FR}}$ to operate the Frank-Read source is larger if the cross slip algorithm in the CA simulations is disabled, so that the loop is constrained to slip in the parent plane. For Cases 1 and 2, parent slip is favored anyway so that disabling the cross slip algorithm does not affect the maximum $T_{\text{FR}}$. 
Figure 4.10: Evolution of the Frank-Read source with applied stress, using parameters listed for (b) Case 2 in Table 4.2
Figure 4.11: Evolution of the Frank-Read source with applied stress, using parameters listed for (c) Case 4 in Table 4.2
Figure 4.12: Evolution of the Frank-Read source with applied stress, using parameters listed for Case 5 in Table 4.2
4.3 Summary

To calibrate this model, nucleation of a triangle onto a straight dislocation segment, and Frank-Read source operations in different kinds of situation are studied. Comparison between the analytic stress and that from our model for the triangular patch nucleation case verifies the divisibility of dislocation line. In addition, from this triangular patch nucleation case, it is observed that the triangular patch side length $L$ normalized by the dislocation cut-off must be at least $81e^2/16 \approx 37$ in order to expand dislocation loops in a stable fashion. This consequence of a Volterra-based dislocation model is well known [29]. Three types of Frank-Read operations are studied in an infinite, elastically isotropic medium. First, an isotropic analysis is considered for which $\nu = 0$, so that dislocation line energy is independent of screw versus edge character. The solution converges with decreasing triangular patch size. Frank-Read sources with different initial length are modeled, and the critical stress for their propagation from simulations is consistent with the analytic values. Second, an anisotropic line energy analysis is considered for which $\nu = 0.1$, so that line energy is a minimum for pure screw character. A non-equiaxed mode of expansion is highlighted in this case. Third, an infinitely long fixed screw dislocation is introduced into the media. This dislocation in the parent plane is parallel to and has the same sign as the Frank-Read source. Frank-Read propagation in front of this dislocation obstacle is studied. The simulations show that the loop will expand by a combination of slip in the parent plane and cross slip, provided the source is sufficiently close to the obstacle or that the applied stress produces a sufficient resolved component on the cross slip system. In such cases, cross slip significantly decreases the stress to operate the source, compared to simulations where cross slip is turned off in the simulations.
CHAPTER 5

MECHANICAL PROPERTIES AND STRUCTURE OF MULTILAYER
– A REVIEW

Since Blum [1] first reported enhanced tensile properties in electrochemically-produced alloys consisting of alternating layers of copper and nickel in 1921, multilayered materials attract great interest of researchers [2-12]. One of the special properties is their extremely high strength, when layer thickness is in nanometer scale. This chapter focuses on reviewing dislocation-based strengthening mechanisms for multilayers, and the interfacial structure evolution due to misfit dislocation behavior in multilayers with lattice parameter mismatch between neighboring layers. Dislocation-based strengthening mechanisms can be grouped into two categories: deformation mode and strengthening source. Interfacial structure will become from coherent to semicoherent to incoherent with increase of layer thickness of multilayers, by deposition of interfacial misfit dislocations on the interfaces. Two main theories for evaluating critical layer thickness corresponding to coherent-semicoherent transition are discussed. They are proposed by Merwe and collaborators (based on energy minimization), and Matthews and Blakeslee (based on force balance) respectively.
5.1 Dislocation-Based Strengthening Mechanisms in Multilayered Materials

By studying the increased hardness, yield and fracture strengths of micromultilayered materials, fundamental advances on the strengthening mechanisms are achieved and several models are built on deformation process due to dislocation motion [58, 59]. These mechanisms can be classified into two categories. One is based on deformation mode, which includes Hall-Petch mechanism [60, 61], and Orowan bowing [62]. The other is based on source of strengthening, which can be image force [63] on dislocations due to the elastic modulus mismatch between the alternative layers, coherency stress [22, 64, 65] due to lattice parameter mismatch between the alternative layers, structural barriers to slip transmission across interfaces caused by misfit dislocations, strength of interfacial bonding [66], and the chemical and structural sharpness of the interfaces [67], and source limited plasticity that stems from the inability of interfaces to provide dislocation content [54].

5.1.1 Strengthening Mechanisms Based on Deformation Mode

Different deformation modes dominate at different layer thickness (h) or grain size (d) regions. Misra [68] developed “deformation mechanism maps” showing strengthening mechanism transitions based on h and d. Hall-Petch mechanism controls at large h or d value. Single Orowan bowing controls at intermediate h or d value. No dislocation behavior exists at extremely small h or d value. **Figure 5.1** gives an example of the map for Cu-Ni, and Cu-Cr system [68]. The map can guide our interpretation of the scale-dependent strengthening mechanisms in multilayers. However, the map does not include
shear moduli difference, interface resistance, and the relationship between lattice mismatch and misfit dislocations.

5.1.1.1 Hall-Petch Mechanism

Early work [69, 70] provided the relation between yield or flow stress and grain size based on dislocation pileup model as

\[ \sigma = \sigma^* + K_{HP} d^{-1/2} \]  \hspace{1cm} (5.1)

where \( \sigma^* \) is a possible frictional stress inside the grain, \( d \) is the diameter of the grain, and \( K_{HP} \) is the Hall–Petch constant.

In multilayered materials, when layer thickness \( h \) is smaller than \( d \), Hall-Petch equation [54] becomes:

\[ \tau = \tau^* + K_{HP} h^{-1/2} \]  \hspace{1cm} (5.2)

where \( \tau^* \) is a resolved shear stress to glide dislocations on the slip plane, which includes lattice resistance, solid solution effects, and precipitation hardening.

Recently, Friedman and Chrzan [71] and Blanckenhagen et al [72] incorporated a threshold stress for dislocation source production and the necessity of a finite-sized dislocation-free region in which a source may operate, which are neglected in the
traditional pileup picture. The flow stress $\tau$ for a double pile-up and a source positioned at the center of the grain was estimated as

$$
\tau = \sqrt{\frac{K_{HP}^2}{d} + \tau_{source}^2}
$$

(5.3)

where $\tau_{source}$ is the source activation stress.

In addition, work are done to try to include different factors in formulating Hall-Patch relation, such as local heterogeneity of strains, stresses and dislocation density [73], temperature[74, 75], annealing twins[76], and work required to eject dislocations from grain boundaries[77, 78].

Nieh [79] and Gryaznov [80] estimated lower-bound value of grain size $d_c$ that can support a dislocation pileup. Assuming that hardness, $H$, is about $3\sigma_{app}$ and $\tau_{app} \approx 0.5\sigma_{app}$, then the approximate equilibrium distance, $d_c$, between two edge dislocations is

$$
d_c = \frac{3\mu b}{\pi(1-\nu)H}
$$

(5.4)

This value is also the critical grain size needed to make Hall-Petch strengthening possible.
Figure 5.1: A “deformation mechanism map” for metallic multilayers with ~2.5% interface misfit strain (e.g., Cu-Ni, Cu-Cr). The map indicates the deformation mechanism for a combination of layer thickness ($h$) and in-plane grain size ($d$) in the multilayer.
5.1.1.2 Orowan Bowing

When the distance \( h \) and \( d \) between obstacles is smaller than \( d_c \), no dislocation pileups will be built up. For multilayers, plastic deformation occurs by the motion of single dislocations rather than piled dislocation arrays, as shown in Figure 5.2 [62] for a structure consisting of lamellar regions \( \alpha \) and \( \beta \), where \( \alpha \) is assumed to be softer. Single dislocations’ moving on closely spaced glide planes from one boundary to the next is illustrated in Figure 5.3[59].

Suppose that the interface dislocations in Figure 5.2(a) are pure edge, and the moving segments in Figure 5.2(b) are screw in character. Orowan stress to move the dislocation segments in Figure 5.2(c) is then

\[
\tau = \left[ \frac{\mu b}{2\pi h} \ln \left( \frac{h}{b} \right) \right] \cos \phi
\]

(5.5)

where core cutoff radius is set equal to \( b \). Angle \( \phi \) is determined by a balance between line tension of the moving screw segment and that of the edge imbedded interface array. Here \( \alpha \) and \( \beta \) layers are assumed to be single crystals. If they are polycrystalline, grain boundaries will need to be considered.
Figure 5.2: Dislocation arrays at interfaces of an imbedded layer. Views parallel to the interface, (a) along dislocation line direction, (b) normal to (a), and (c) detail of end of loop in (b)
Figure 5.3: Schematic illustration of the Orowan mechanism involving single dislocations in nm-scale multilayers, the single dislocations are bowing parallel to the interface and depositing misfit type dislocation at the interface
5.1.2 Strengthening Mechanisms Based on Source of Strengthening

One type of source is image force on a dislocation due to elastic modulus difference between layers. Head [81] first introduced image force concept and gave an expression for stress on a Volterra type screw dislocation at a distance $c'$ from an abrupt interface between pure materials “1” and “2” with shear moduli $\mu_1$ and $\mu_2$, respectively, as shown in Figure 5.4. The line sense and Burgers vector $b$ are assumed to be along $z'$, which is pointing out of the plane in Figure 5.4. The stress on slip plane $y' = 0$ is

$$\tau_{y'z'} = \begin{cases} 
\frac{\mu_1 b}{2\pi} \left( \frac{1}{x' - c'} + \frac{K}{x' + c'} \right) & \text{For } x' > 0, \\
\frac{\mu_1 b}{2\pi} \left( \frac{1 + K}{x' - c'} \right) & \text{For } x' < 0,
\end{cases} \quad (5.6)$$

where $K = (\mu_2 - \mu_1)/(\mu_1 + \mu_2)$. Similarly, the non-zero stress on the slip plane can be obtained when the dislocation is at $x' = -c'$.

Chou[82], and Anderson et al [83] studied image force on a dislocation in three-layered medium. Kamat et al [84] extended the analysis to five-layered medium. Meanwhile, Peierls-Nabarro model was adopted to avoid the singularity with Volterra dislocation model by Pacheco and Mura [85]. Anderson et al [83] further extended Pacheco and Mura’s work. In addition, atomistic simulation [86] is employed in studying image force to avoid this singularity.

Koehler [63] designed a material to study this elastic modulus mismatch effect. Lechezy[87] showed Koehler’s theoretical prediction by vapor deposited multilayered Al-Cu laminates.
Figure 5.4: Screw dislocation near a straight and sharp interfaces between pure materials “1” and “2” with shear moduli $\mu_1$ and $\mu_2$.
Coherency stress due to lattice parameter mismatch between neighboring layers is another strengthening source. If interfaces are coherent in lattice-mismatched multilayers with two types of layers arranged alternatively, there are alternating tensile and compressive stresses in the two kinds of layers. Anderson [88] evaluated this biaxial stress in a multilayer consisting of a periodic arrangement of $N$ distinct types of isotropic layers; each described by a thickness $h_j$, elastic modulus $E_j$, and Poisson’s ratio $\nu_j$. The multilayer is assumed to have 2 equivalent, orthogonal, in-plane directions along which there is equal extension or contraction. Thus an equi-biaxial stress state exists in each layer. Elastic strain and stress in each layer is estimated as

$$
\varepsilon_j = \frac{a - a_j}{a_j}, \quad \sigma_j = M_j \varepsilon_j
$$

(5.7)

where $M_j = E_j / (1 - \nu_j)$, $a$ is an arbitrary dimension along one of the in-plane directions, and $a_j$ is the corresponding stress-free value of $a$ in layer $j$, i.e., when detached from the multilayer. When no macroscopic in-plane loading exists, stress equilibrium is

$$
\sum_{i=1}^{N} \sigma_i h_i = 0
$$

(5.8)

After solving for $a$, and the resulting biaxial stress state in layer $j$ is given by
\[ \sigma_j \frac{M_j}{N} = \frac{\sum_{i=1}^{N} (M_i h_i)}{a_j \sum_{k=1}^{N} M_k h_k / a_k} - 1 \] (5.9)

With increase of layer thickness, dislocation will form to relax the strain due to lattice mismatch. For multilayers with two distinct layer types \( N = 2 \) in Equation (5.9), misfit dislocation along interface, elastic strain in layer type 1 is \( (a_2 / a_1 - 1 - b_1 / S) \), where \( b_1 / S \) is dislocation density. Following the stress equilibrium, the result net in-plane biaxial tensile stress in layer 1 \([64, 71, 89]\) is

\[ \frac{\sigma_{1}}{M_1} = \frac{\Sigma - f_2 M_2 [\ln \frac{a_{1}^0}{a_2^0} + \ln (1 + \frac{b_1}{S_1}) - \ln (1 + \frac{b_2}{S_2})]}{f_1 M_1 + f_2 M_2} \] (5.10)

where \( f_1 \) and \( f_2 \) are volume fraction of layer type (1) and (2) respectively, and \( a_{1}^0 / a_2^0 \) is lattice parameter mismatch. In equation (5.10), only the average effect of misfit dislocations is considered. To get the accurate stress field, misfit dislocations need to be incorporated by superimposing their stress fields.

There are other strengthening sources, such as strength of interfacial bonding [65], and the chemical and structural sharpness of the interfaces [67], and source limited plasticity that stems from the inability of interfaces to provide dislocation content [54].

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Figure 5.5: Epilayer A grown on a thick substrate B. (a) \( h < h_c \), elastic strain only; and (b) \( h > h_c \), a misfit dislocation is introduced to accommodate lattice mismatch.
5.2 Interfacial Structure of Multilayered Materials

Generally, lattice parameter mismatch exists between materials forming multilayers. This lattice mismatch can be accommodated by elastic strain or interfacial dislocations, where elastic strain takes up lattice mismatch until layer thickness reaches a critical value whereupon elastic strain is partially relieved by the appearance of interfacial dislocations as shown schematically in Figure 5.5. The structure changes from coherent to semicoherent or incoherent. The division of mismatch between dislocations and elastic strain depends upon the difference between bulk lattice parameters, and layer thickness [90-99]. For a specific lattice mismatch, misfit dislocations form at some critical layer thickness \( h_c \). With good prediction of \( h_c \), we can know the possible interface structure and understand mechanical property according to strengthening mechanisms mentioned before. This section reviews the process of interface misfit dislocation formation, and the derivation for critical misfit or critical layer thickness.

5.2.1 Interfacial Misfit Dislocation Formation

Several misfit dislocation formation mechanisms are [97]: (1) Multiplication mechanisms arising from dislocation pinning and/or interaction; (2) Heterogeneous nucleation at specific local stress concentrations due, for example, to growth artifacts or preexisting substrate defects, and film surface roughness [100]; and (3) Homogeneous or spontaneous nucleation of dislocation loop or half-loops.

Matthews and Blakeslee [101] proposed two different processes to explain interfacial dislocation formation. One is dislocation-arrays. As shown in Figure 5.6, a substrate dislocation with suitable Burgers vector is replicated in the deposit. Under the influence
of coherency strain, the threading dislocation glides back and forth and generates interfacial misfit dislocations. This process gives arrays with the geometry of those observed, but it can only account for less than 1% of the observed arrays. Then Matthews and Blakeslee proposed that many threading dislocations are created during layer growth. Freund [102] illustrated the formation of a misfit dislocation from a threading dislocation as the increase of $h$ in Figure 5.7.

The other is paired-dislocations as illustrated in Figure 5.8. During the growth of the next layer, portions of the loop labeled P and Q move towards one another and annihilate.

### 5.2.2 Critical Misfit $f_c$ and Critical Layer Thickness $h_c$

Critical misfit $f_c$ is the limiting misfit below which a layer of fixed thickness is homogeneously strained into registry with the substrate. Critical layer thickness $h_c$ is the layer thickness above which an interface of given natural misfit loses registry by the introduction of misfit dislocations. For epilayer growth [96] of thin film with lattice constant $a_{\text{film}}$ on a thick substrate with lattice constant $a_{\text{sub}}$, lattice misfit parameter $f_m$ is

$$f_m = \frac{a_{\text{film}} - a_{\text{sub}}}{a_{\text{sub}}} \quad (5.14)$$

When $f_m$ and layer thickness $h$ are small, the misfit is accommodated by homogeneous strain (misfit strain). The elastic energy $e$ per unit area in the epilayer due to homogeneous strain is [103, 104]
where elastic constant $B$ is given by $B = 2\mu(1+\nu)/(1-\nu)$, $\nu$ is Poisson’s ratio, and $\mu$ is shear modulus of elasticity.

At $h > h_c$, misfit dislocations will appear to relax the homogeneous strain. To predict $f_c$ or $h_c$, two major theories are developed. The first theory, introduced by Merwe and collaborators [96, 105, 106], is based on the principle of energy minimization. The second is force balance theory proposed by Matthews and Blakeslee [101, 107, 108]. Both theories begin the analysis with two-layer configuration, and extend to multilayer configuration.

The theory postulates that the introduction of dislocations relaxes a proportion of misfit strain between layer to uniform relaxed misfit strain and introduce the energy associated with a set of well separated, and so non-interacting, dislocations, which is estimated from the solution for a single dislocation. Using Frenkel and Kontorowa (FK) model in Figure 5.9[109], and a Fourier series truncated at first-order harmonic, energy of the system is

\[
E(x_1, x_2, \ldots) = \frac{1}{2} \sum_n \left\{ \mu(x_{n+1} - x_n + a - b)^2 + W \left[ 1 - \cos\left(\frac{2\pi x_n}{a}\right) \right] \right\}
\]

where $W$ is the overall amplitude of $V$ and $x_n$ is the displacement of the nth particle from the nth potential trough. $(x_{n+1} - x_n + a - b)$ is the homogeneous misfit strain.
Figure 5.6: An array of misfit dislocations in multilayer system of B/C formed on the top of substrate A
Figure 5.7: Schematic of bowed dislocation configuration for increasing layer thickness
Figure 5.8: Mechanism for formation of paired misfit dislocations in multilayer system B/C on the top of substrate A
\[ \frac{\partial E}{\partial x_n} = 0 \] is employed to determine the structure of the chain. With the displacement function \( \zeta_n = x_n / a \), Figure 5.10 shows the displacement curve \( \zeta_n \) as computed from the relation in [110]. It indicates very localized disr egistries, centered on regularly spaced points, as defined by \( \zeta_n = \pm (1/2), \pm (3/2), \text{ etc.} \) The critical misfit for commencement of misfit strain relief by misfit dislocations:

\[
f_c = \frac{2}{\pi} \left( \frac{W}{\mu a^2 / 2} \right)^{1/2}
\]  (5.17)

Merwe also extended this model to multilayers [111, 112, 113]. In the case of a superlattice of alternating layers of materials (with the same elastic constants and layer thickness), for a given misfit \( f \), the critical thickness for epitaxial superlattices, free from their substrate, is more than 4 times that for a single epilayer on a thick substrate. This difference is due to the fact that, in the superlattice, each layer takes up only half of the misfit, that the misfit strain energy varies quadratically with strain, and that the variation of energy with misfit is somewhat different in the two cases.

The model by Frank and Merwe[96, 110, 114], which attempted to obtain critical layer thickness by minimizing the energy of a misfit dislocation array at the interface, is rigorous, but mathematically complex and analytical solution to the equations constructed exist only in the limits of very thin or very thick films [97]. Meanwhile, the approximation of atomic potential needs to be improved for different materials.
Figure 5.9: The FK model comprises a chain of particles (“atoms”) connected by springs of natural length $b$, strained length $\tilde{b}$, and force constant $\mu$. The particles are otherwise acted on by a periodic (interfacial) potential $V(x)$ of wavelength $a$ and overall amplitude $W$, emanating from a “rigid substrate”. Particles and troughs are numbered alike and particle displacements are specified with respect to corresponding troughs, e.g. $\alpha \zeta_2$. 
Figure 5.10: The curve is a plot of the displacement function $\zeta(n) = x_n / a$ of particles $n$ from trough $n$ in the FK model. Note that the misfit dislocations (centered within the short intervals of poor matching) are at $\zeta(0) = 0.5, \zeta = 1.5$, etc, where particles would be furthest away from trough (matching) positions $\zeta = 0$, and $\zeta = 1.0$. $P$ is the number of atoms per misfit dislocation and $\alpha \zeta_0$ is the displacement of the particle at the free end.
In force balance theory \cite{101, 107, 108}, a grown-in dislocation line extends from crystal B through interface and into crystal A and bows under the influence of the misfit strain as shown in Figure 5.11. A segment of misfit dislocation is deposited on the interface by migration of the bowed dislocation.

Misfit strain imposes force $F_a$ on the grow-in dislocation. Misfit dislocation generated from dislocation bowing produces a restoring force $F_T$ on the propagating threading arm. This restoring stress is often loosely referred to as being due to a “line tension”.

Assume that the elastic constants of A and B are equal and isotropic, and $h_A = h_B$, force $F_a$ \cite{101, 107, 108} is

$$F_a = \frac{2\mu(1+\nu)}{(1-\nu)}bh\varepsilon\cos\lambda$$

(5.18)

where $\mu$ is shear modulus of A and B, and $\lambda$ is the angle between the slip direction and the direction in the film plane which is perpendicular to the intersection line of the slip plane and the interface.

The restoring force acting upon the threading dislocation, $F_T$, may be calculated from the energy required to create a segment of interfacial misfit dislocation of length $dx$: $dE = E_s dx$, where $E_s$ \cite{52} is

$$E_s = \frac{\mu b^2 (1-\nu \cos^2 \theta)}{4\pi (1-\nu)} \ln \left( \frac{aR}{b} \right)$$

with $\theta$ is the angle between Burgers vector and line sense, and $\alpha$ is a factor intended to account for the dislocation core energy, generally estimated to be form 0.5 to 1.0 in metals and from 1 to 4 in semiconductors.
Using the relation that the total force acting on the threading dislocation is given by $dE/dx$, we have

\[
F_T = \frac{\mu b^2 (1 - \nu \cos^2 \theta)}{4\pi (1 - \nu)} \ln\left(\frac{a h}{b}\right)
\]  \hspace{1cm} (5.19)

If $F_a > F_T$, threading dislocation will propagate and a misfit dislocation is generated. Matthews and Blakeslee defined layer thickness at $F_a = F_T$ as critical layer thickness. Energetically, this is equivalent to saying that misfit dislocations form when their self-energy is less than the elastic strain energy they relax.

For epilayer, equating $F_a$ and $F_T$ yields the critical thickness for the Matthews and Blakeslee definition:

\[
h_c = \frac{b}{8\pi \varepsilon} \left(\frac{1 - \nu \cos^2 \theta}{1 + \nu \cos \lambda}\right) \left(\ln \frac{c h_c}{b}\right)
\]  \hspace{1cm} (5.20)

For a multilayer system [101, 115], the maximum strain is half of that in epilayer system and $F_a = 2F_T$ gives the critical layer thickness. Therefore, $h_c$ for multilayer systems is 4 times that of epilayers.

This method is very simple mathematically, and the extension from single layer to multilayers is very obvious. Figure 5.12 compared the Matthews and Blakeslee result with experimental result [101].
Figure 5.11: Schematic illustration of the Matthews and Blakeslee model of critical thickness for growth of film A on top of substrate B
People [116, 117] showed that the two theories gave different numerical values of the critical thickness for the same epilayer. However, Hirth and Feng [118] suggested that volterra and atomistic models should agree fairly well until the dislocation spacing approaches core dimensions. They pointed out the difference between the results of the two theories is because they used a single-dipole result to estimate a dislocation array. Hirth and Feng studied different misfit dislocation configurations. Their result showed that volterra dislocation result agrees very well with that for a discrete parabolic potential model when the same multiple dislocation configuration is treated, provided that a specific core parameter is selected. Willis and Jain [96, 119] also demonstrated that the two competing theories in fact should make identical predictions for the critical thickness. The result showed that the original formulation would yield precisely the correct value for $h_c$, when using the correct expression for the energy of a single dislocation.

More factors are studied in predicting $h_c$. Fisher [120, 121] included elastic interaction between straight misfit dislocations in Volterra dislocation approach, and introduced “image dislocation” [100], and predicted a higher value for $h_c$ than Matthews and Blakeslee. Recently, Ogasawara et al [122] pointed out the influence of net strain, strain type and temperature on the critical thickness. Huang et al [123] calculated critical layer thickness in Si$_{1-x}$Ge$_x$/Si strained-layer heterostructures with considering thermal strain. To get a more accurate prediction of $h_c$, all these factors need to be considered.
Figure 5.12: Critical thickness $h_c$ for the formation of misfit dislocations, compared with the present experimental results for single nitride layers, plotted versus the mismatch between film and underlayaer. The symbol indicates an essentially fully relaxed film, $\theta$ indicates a partly relaxed film, and $\bigcirc$ indicates an essentially unrelaxed film. Also shown is the prediction for superlattices along with data for the TiN/NbN superlattice that was only slightly relaxed.
CHAPTER 6

MECHANICAL PROPERTY OF MULTILAYERS
—MODEL APPLICATION

In this chapter, 3D Cellular Automaton Dislocation Model is employed to study mechanical behavior and structure development during deformation in fine-scale metallic multilayers. Multilayers studied in this chapter are composed of alternating (1) and (2) phases with no elastic modulus mismatch. First, geometry and discretization of multilayer structure in the simulations is described. After that, theory on deformation and structure evolution is developed. Dislocation can propagate in confined layer slip mode or transmit through interfaces to multiple layer slip mode. The analytic formulas for the stresses to drive confined layer slip and interfacial transmission are derived. Then, an ideal multilayer structure is studied. This ideal multilayer has no lattice parameter mismatch, same volume fraction of phases (1) and (2), and intransmissible interfaces. Both interfacial and threading dislocation configurations are simulated. The stress needed for confined layer slip is obtained for different layer thickness. The results for threading dislocation agree with theory developed in the former section. The results for interfacial dislocation show the competition between layer thickness and dislocation source length, and the stress is controlled by the smaller one. Next, multilayers with lattice parameter
mismatch are studied. Multilayers with threading dislocation through several layers are modeled. For small lattice parameter mismatch and small layer thickness condition, strength of material is controlled by dislocation source length. For large lattice parameter mismatch and large layer thickness condition, initial confined layer slip will deposit interfacial misfit dislocations on the interfaces, and strength of material is controlled by the propagation of interfacial dislocation and threading dislocation through one layer. So, the motion of interfacial dislocation and threading dislocation through one layer is studied. The simulation and analytic results predict that two regimes exist for multilayers with fine layer thickness. At larger layer thickness, strength depends primarily on layer thickness. This occurs since slip is confined to individual layers, prior to macroscopic yield. At sufficiently small layer thickness, strength depends primarily on lattice parameter mismatch and the dislocation source length scale, rather than layer thickness. This occurs since slip is not confined to individual layers, even during the initial stage of plastic deformation. Last, simulation results are compared with experimental data. The model results capture experimental trends of multilayer yield strength versus layer thickness.

6.1 Description and Discretization of Multilayer Structure

The geometry of multilayer structure needs to be specified in the model. Figure 6.1 depicts a multilayer thin film consisting of alternating (1) and (2) phases with respective individual layer thicknesses $h_1$ and $h_2$; stress-free lattice parameters $a_1^0$ and $a_2^0$; and isotropic elastic properties described by shear moduli $\mu_1$ and $\mu_2$, and Poisson's ratios $\nu_1$ and $\nu_2$. Each phase is assumed to have an FCC crystal structure and a cube-on-cube
epitaxial orientation between these phases is adopted, so that \{111\} crystallographic slip planes traverse through the multilayer thin film as shown. Each of the layers may deform elastically and also plastically via the propagation of perfect dislocations with \(<110>\) Burgers vectors on \{111\} slip planes. Geometrically, there are two types of dislocations in multilayered materials: threading dislocations (such as segment A-A’) and interfacial dislocations (such as B-B’). For threading dislocation configuration, dislocations can span over one layer or many layers.

Variables should also be identified. Here, multilayers are assumed to have lattice parameter mismatch and no elastic parameter mismatch. The variables used are stress-free lattice parameter ratio \(a_2^0/a_1^0\), layer thickness \(h_1\) and \(h_2\), elastic modulus \(\mu = \mu_1 = \mu_2\), Poisson’s ratio \(\nu = \nu_1 = \nu_2\), dislocation core cut-off \(\rho\), and interface structure represented by misfit dislocation density \(b/S\), where \(S\) is the in-plane distance between two neighboring misfit dislocations in the arrays.

For multilayer thin films with coherent interfaces, the mismatch in stress-free lattice parameter will produce an in-plane biaxial stress state \(\sigma_{xx} = \sigma_{yy}\) in each phase which alternates in sign from tension in the phase with the smaller stress-free lattice parameter to a compression in the phase with the larger lattice parameter. According to symmetry, \(a_1^0 < a_2^0\) will be adopted for multilayer systems with lattice parameter mismatch throughout the chapter. The magnitudes \(\bar{\sigma}_1\), \(\bar{\sigma}_2\) of the average biaxial stress in the respective layers may be sufficiently large so that it is energetically favorable to form semi-coherent interfaces that are described by uniform arrays of misfit dislocations with line directions along \[110\] and \([\text{110}]\), pure edge character, and in-plane spacing \(S\).
Application of a macroscopic biaxial tension $\Sigma$ will serve to drive additional dislocation slip, via the bowing out of interfacial dislocation segments (A-A') into adjoining layers or via the propagation of threading segments (B-B') that may or may not extend across multiple layers.

To represent multilayered structure in the CA model, discretization scheme in chapter 3 is employed, and interfaces are expressed as cube cell surfaces. Since gliding dislocations are assumed in $\{111\}$ slip planes, Figure 6.2 illustrates a 2-dimensional discretized (111) plane through the multilayered structure. Only three layers are shown in Figure 6.2, and different shadings are used to represent different types of layers.
Figure 6.1 (a) Schematic geometry of multilayer thin film of alternating (1) and (2) phases with respective layer thicknesses $h_1$ and $h_2$, and cube-on-cube epitaxial orientation between phases. A-A' and B-B' are interfacial and threading dislocations in (111) plane. (b) Misfit dislocation arrays along [1\bar{1}0] and [110] and with spacing $S$ on the interfaces.
Figure 6.2: Illustration of discretization of (111) plane into triangles in a multilayered composite consisting of alternating (1) and (2) phases; AB is a threading dislocation; CD is an interfacial dislocation
Figure 6.3 Illustration of dislocation expansion modes along $\pm 1'$ and $\pm 2'$ directions in (111) slip plane of multilayers with alternating phases (1) and (2), using initial dislocation A-A' with Burgers vector $\mathbf{b}$ and line sense $\xi$ as an example.
6.2 Theory of Deformation and Structure Evolution

Due to the special structure of multilayers, materials can be deformed with confined layer slip of dislocations [54], where dislocations propagate within one layer instead of expand through many layers. Confined layer slip via motion of these segments, such as A-A’ and B-B’, deposits 60° dislocations with the same line directions noted for misfit dislocations, but with slip direction along four possible directions of the type [10\(\overline{1}\)], [\(\overline{1}0\overline{1}\)], [01\(\overline{1}\)], and [0\(\overline{1}\)\(\overline{1}\)]. Thus, the dislocation content at interfaces may evolve as the thin film is deformed. If layer thickness of multilayers is very small or interfacial misfit dislocation density is high enough, dislocation will transmit through the interfaces and propagate through several layers and take multiple layer slip mode. Therefore, as shown in Figure 6.3, dislocation expands along ±1’ direction or transmits in ±2’ direction.

Some critical stress is needed to drive dislocations in confined layer slip mode (\(\Sigma_{CLS}\)) or dislocation transmission through interface (\(\Sigma_{trans}\)). For confined layer slip along 1’ direction as shown in Figure 6.3, the incremental advance of the loop by \(d_w\) along the 1’ direction increases the stored energy of interfacial dislocations by \(2e_w\ dw\), where \(e_w\) is the line energy per unit length of dislocation along the \(w\) dimension. The supply of energy for this process is derived from the work, \(\overline{\tau} b h’\ dw\), where \(\overline{\tau}\) is the shear stress acting on the slip plane in the slip direction, averaged over the incremental area of advance. According to energy conservation, equating these two incremental energies furnishes the critical condition to drive confined layer slip,

\[
\pm \overline{\tau}_{cls} = \frac{2e_w}{bh} \tag{6.1}
\]
The convention adopted here is that a (+) sign denotes confined layer slip that induces a positive in-plane plastic strain and a (-) sign denotes slip that induces a negative in-plane plastic strain.

A corresponding analysis for an incremental advance $dh'$ of the loop along the 2' direction, so that it extends into the adjoining layer (2) requires an energy $\partial e_w/\partial x_2, wdh' + 2e_h dh'$, where the partial derivative denotes the change in line energy of a dislocation as it emerges from the interface into layer (2). The second term accounts for the increase in dislocation line length along the 2' direction ($h'$ axis), where $e_h$ is the line energy per unit length along the $h'$ axis. Equating this to the corresponding supply of energy, $\tau b w dh'$ furnishes the critical condition to drive slip transmission,

$$\pm \tau_{trans} = \frac{\partial e_w/\partial x_2}{b} + 2e_h \left( \approx \frac{\partial e/\partial x_2}{b} - \text{for } L >> h \right)$$  \hspace{1cm} (6.2)

The same ± sign convention for Equation (6.1) is adopted here.

Despite the idealized geometry of expansion along the 1' and 2' directions assumed here, additional simplifications are required to relate $\tau_{cls}$ and $\tau_{trans}$ to corresponding values of applied biaxial tension $\Sigma_{cls}$ and $\Sigma_{trans}$, for confined layer slip and transmission, respectively. Further, the functions $e$ and $\partial e/\partial x_2'$ are dependent on the detailed interaction of dislocations with interfaces. The resolved shear stress in layer (1), averaged over the entire layer, is obtained by partitioning the total biaxial strain in each layer into elastic
plus plastic components and introducing the volume fractions $f_1, f_2$ and biaxial moduli $M_1, M_2$ for the respective phases [64]

$$\tau_1 = s \frac{M_1}{f_1 M_1 + f_2 M_2} \left( \Sigma - f_2 M_2 \left[ \ln \frac{a_1^0}{a_2^0} + \ln \left( 1 + \frac{b_1}{S_1} \right) - \ln \left( 1 + \frac{b_2}{S_2} \right) \right] \right)$$ \hspace{1cm} (6.3)

The Schmid factor $s$ is defined by $\tau_1 = s \bar{\sigma}$, where $\bar{\sigma}$ is the average value of biaxial tension in layer 1 and $\bar{\tau}_1$ is the average resolved shear stress on a candidate slip system. In particular, $s = n_x u_x + n_y u_y$, where $\mathbf{n}$, a unit normal to the slip plane, and $\mathbf{u}$, a unit Burgers vector indicating the slip induced following expansion of the loop, are chosen so that $s > 0$. For the geometry described in Section 6.1 and Figure 6.3, $s = 1/\sqrt{6}$. The terms in the square $[ \ ]$ brackets in eqn. (3) highlight the contributions from mismatch in stress-free lattice parameter, average positive in-plane biaxial plastic strain $\ln(1 + (b/S)_1)$ induced by a square grid of misfit dislocations of Burgers vector magnitude $b_1$ and spacing $S_1$ in phase (1), and the corresponding plastic strain induced by misfit dislocations in phase (2).

Combining eqns. (1) and (3) provides an estimate of the critical macroscopic biaxial tension to induce confined layer slip in phase (1),

$$\Sigma_{cls(1)} = \frac{f_1 M_1 + f_2 M_2}{s M_1} \frac{\pm 2e}{bh'_1} - f_2 M_2 \left[ \ln \frac{a_2^0}{a_1^0} - \ln \left( 1 + \frac{b_1}{S_1} \right) + \ln \left( 1 + \frac{b_2}{S_2} \right) \right]$$ \hspace{1cm} (6.4)
Consistent with eqn. (1), the (+/−) option in eqn. (6.4) is used to compute expansion of loops that produce positive/negative in-plane plastic strain in layer (1). A corresponding expression for the applied biaxial tension to cause transmission from phase (1) to (2) is obtained by setting \( \tau_{\text{trans}} \) in eqn. (6.2) to \( \tau_2 \), obtained by interchanging indices (1) and (2) in eqn. (6.3),

\[
\Sigma_{\text{trans}(1\rightarrow2)} = \frac{f_1 M_1 + f_2 M_2}{s M_2} \pm \frac{\partial e}{\partial x_2} \cdot b + f_1 M_1 \ln \left( \frac{a_2^0}{a_1^0} \right) - \ln \left( 1 + \frac{b_1}{S_1} \right) + \ln \left( 1 + \frac{b_2}{S_2} \right) \]

(6.5)

where the (+/−) convention has the same meaning as for eqn. (6.4). Corresponding expressions for \( \Sigma_{\text{cls}(2)} \) and \( \Sigma_{\text{trans}(2\rightarrow1)} \) are obtained by interchanging indices (1) and (2) in eqns. (6.4) and (6.5).

A final task in the development of critical conditions for confined layer slip and transmission is to estimate values of dislocation line energy \( e \) and the variation \( \partial e / \partial x_2 \) during motion across the interface from phases (1) to (2). An approximate formulation is obtained by considering the expansion of a 2D configuration of a screw dislocation dipole in a layer of phase (1), which is embedded in an infinite body of phase (2) with non-slipping interfaces as shown in Figure 6.4. The work to move dislocation (2) from an initial position \( x_2 = r_0 / 2 \) to a final position \( x_2 = h / 2 \) is used to define the energy per unit length \( e \) of an infinitely long straight screw dislocation that resides at an interface. Thus,

\[
e = - \int_{r_0 / 2}^{h / 2} \left( \tau^{1\rightarrow2} + \tau^{1'\rightarrow2} + \tau^{1''\rightarrow2} + \tau^{2'\rightarrow2} + \tau^{2''\rightarrow2} \right) b \, dx_2 \]

(6.6)
where the superscript notation $1 \rightarrow 2$ denotes the resolved shear stress produced by dislocation 1 at the site of dislocation 2, such that $\tau_{1 \rightarrow 2} b$ is the force exerted by dislocation 1 on a unit length of dislocation 2, as to produce a positive in-plane plastic strain in phase (1). Terms $1' \rightarrow 2$ and $1'' \rightarrow 2$ denote the corresponding resolved shear stress produced by the first order image constructions for dislocation 1 about the ' and '' interfaces, respectively. In a similar manner, $2' \rightarrow 2$ and $2'' \rightarrow 2$ represent the first order image contributions from dislocation 2.

The first four terms are identified as the real and image terms for Volterra dislocations and may be obtained from Hirth and Lothe [52] and Head [81]. However, the last term representing $2'' \rightarrow 2$ becomes singular as the real and image dislocations approach the sharp " interface at the upper limit of integration. Thus, the last term is replaced by a solution by Pacheco and Mura [85] for a Peierls screw dislocation approaching a single, sharp interface. Accordingly,

$$e = -\frac{\mu_1 b^2}{2\pi} \int_{r_0/2}^{h/2} \left( -\frac{1}{2x_2} - \frac{k\mu}{h} + \frac{k\mu}{h + 2x_2} - \frac{2k\mu}{\pi b} \left[ \frac{1}{1 + u^2} + \tan^{-1} \frac{u}{u} \right] \right) dx_2 \quad (6.7)$$

where $\kappa\mu = (\mu_2 - \mu_1)(\mu_2 \mu_1)$, $u = (h - 2x_2)/b$, and $\mu' = \mu$ for a screw dislocation. Further, the Pacheco and Mura solution assumes an unstable stacking fault energy $\gamma_{us}/\mu b = 1/2\pi^2$ for the participating slip planes in phases (1) and (2), although Xin and Anderson [124] have extended the formulation to include a large range of other stacking fault energy
values. Integration of eqn. (6.7) and application of the limit \( h \gg r_0 \) furnishes the line energy for a dislocation residing at the interface

\[
e = \frac{\mu \mid b^2}{2\pi} \left[ \frac{1}{2} \ln \frac{h}{r_0} + \kappa \mu \left\{ \frac{1}{2} \ln 2 + \frac{1}{\pi} \left( \tan^{-1} u' + \frac{\mu}{2 \pi} \ln u' + \frac{1}{u'} - \frac{1}{25u'^3} - ... \right) \right\} \right]
\]

(6.8)

where \( u' = h/b \). The corresponding value of \( \frac{\partial e}{\partial x_2} \) for this geometry is obtained by evaluating the integrand of eqn. (6.6) at \( x_2 = h/2 \), so that

\[
\frac{\partial e}{\partial x_2} = \frac{\mu \mid b^2}{2\pi} \left[ \frac{1}{h} + \kappa \mu \left\{ \frac{1}{2h} + \frac{2}{\pi b} \right\} \right]
\]

(6.9)

Thus, elementary dislocation theory permits estimates of dislocation line energy and first derivatives of it, so that eqns. (6.4) and (6.5) may be used to estimate the critical applied biaxial tension for confined layer slip and slip transmission. However, the estimates for \( e \) and \( \frac{\partial e}{\partial x_2} \) are idealized, in that the effects of chemically diffuse interfaces, dislocation interaction with interfacial dislocation content [125], or dislocation core spreading into the interface are not considered. Recent work by Shen and Anderson [66] and Hoagland et al [65] suggests that the last effect can significantly decrease \( e \) but increase \( \frac{\partial e}{\partial x_2} \), so that confined layer slip is relatively easy compared to transmission. Hoagland [65] also provides evidence that coherency stress can significantly alter \( \kappa \mu \) from bulk values and, further, application of a biaxial stress may reconfigure misfit dislocation content and thus change the nature of \( e \) and \( \frac{\partial e}{\partial x_2} \).
Figure 6.4: 2D screw dislocation dipole in phase (1), which is embedded in an infinite body of phase (2). $h$ is the layer thickness of the embedded phase (1).
6.3 Property of Multilayers with $a_2^0/a_1^0 = 1$ and Intransmissible Interfaces

An ideal multilayer is assumed, who has alternating (1) and (2) phases of equal elastic modulus ($M_1 = M_2$) and volume fractions ($f_1 = f_2$), intransmissible interfaces, and no lattice parameter mismatch. Dislocations are restricted to propagate in layer type of $\ell = (1)$ here. Deformation happens via confined layer slip of dislocations. Two elementary dislocation geometries are employed. One is a threading geometry in which a dislocation spans across a layer and is pinned at the interfaces (e.g., dislocation AB in Figure 6.2); the other is an interfacial geometry such as dislocation CD in Figure 6.2, with the end points pinned as well.

From the theory developed in Section 6.2, the relation between $\Sigma_{\text{cls}}$ and layer thickness $h$ is obtained by inserting $a_2^0/a_1^0 = 1$, $b_1/S_1 = 0$, and $b_2/S_2 = 0$ into Equation (6.4).

$$
\Sigma_{\text{cls}}(1) = \frac{f_1 M_1 + f_2 M_2 \pm 2e}{s M_1} \frac{bh_1'}{b h_1'}
$$

(6.10)

where $h' = h_{[112]} = \sqrt{3/2} h_{[001]}$ and $s = 1/\sqrt{6}$.

Since there is no elastic modulus mismatch, $\kappa_1$ in Equation (6.4) is zero, and $e$ is

$$
e = \frac{\mu' h^2}{2\pi} \frac{1}{2} \ln \frac{h}{r_0}
$$

(6.11)
Inserting Equation (6.11) into Equation (6.10), the analytic critical stress for CLS is

\[ \Sigma_{\text{cls}(1)} = \frac{f_1 M_1 + f_2 M_2}{sM_1} \pm \frac{2e}{bh_1'} \text{ or } \pm \tau_{\text{cls}} = \frac{\mu' b}{2\pi h'} \ln \frac{h'}{r_0} \]  

(6.12)

Our simulations are employed to obtain critical stress for CLS of threading and interfacial dislocation configurations shown in Figure 6.2. For both configurations, different layer thickness is studied. The critical stress from the code is gained by using the window averaging method. The results are compared with theoretical predictions.

6.3.1 Threading Dislocation Configuration

Figure 6.5 presents the comparison of the critical stress \( \tau_{\text{cls}} \) from the simulation and the theoretical value; the inset shows the propagation configuration of a threading dislocation for the case \( h = 200b \). In all cases, the cutoff \( \rho = 0.3b \), \( \mu_1 = \mu_2 = \mu \), \( \nu_1 = \nu_2 = 0 \), and 10 initial segments are used to model the line AB in Figure 6.2. The two results compare well over a large range of layer thickness. The results from our simulations agree very well with the corresponding theoretical results, and strength increases with layer thickness decrease.
Figure 6.5: Comparison of the critical stress for confined layer slip from the code and the analytic value; $\rho = 0.3b$
6.3.2 Interfacial Dislocation Configuration

For the interfacial case, the length, \( L \), of the initial dislocation line CD in Figure 6.2 enters as an additional length scale. Again, \( \rho = 0.3b \), \( \mu_1 = \mu_2 = \mu \), \( \nu_1 = \nu_2 = 0 \), and 10 segments are used to simulate the initial interfacial dislocation. From the simulation result, when \( L \) is greater than \( h' \), confined layer slip mode intervenes before the loop forms a critical bow out typical at an isolated Frank-Read source. Thus, the critical shear stress is determined by \( h' \) and the corresponding circles for \( L > h' \) in Figure 6.6 is the same as for the threading case shown in Figure 6.5. When \( L \) is less than \( h' \), the loop must first overcome a critical stress to form a Frank-Read bow out before expanding by confined layer slip. In such cases, the critical stress is dictated by \( L \) rather than \( h' \). Figure 6.6 shows that for a fixed interfacial pinning distance \( L = 100b \), the critical stress to expand the loop is controlled by \( h' \), provided \( h < 150b \); for \( h > 150b \), the critical stress is controlled by \( L \) and is independent of \( h' \). Simulation results indicate that the smaller scale is the controlling factor in determining the strength of multilayers here.
Figure 6.6: Critical stress for confined layer slip for the interfacial dislocation; $\rho = 0.3b$
6.4 Multilayers with Lattice Parameter Mismatch

Generally, lattice parameter mismatch exists between different types of layers. The following part studies the effect of lattice parameter mismatch. Interfaces are transmissible, and misfit dislocation content deposits on the interfaces to relieve elastic strain due to non-one lattice parameter ratio. In this section, theoretical prediction of different deformation regimes is given first; next, simulation procedure in our modeling is described; after that, the propagation of threading dislocation through several layers is studied; then, yield strength of multilayers based on interfacial dislocation and threading dislocation through one layer is analyzed.

6.4.1 deformation regimes

Regimes of deformation can be defined based on whether the applied biaxial stress is sufficient to reach $\Sigma_{\text{cls}}$ or $\Sigma_{\text{trans}}$. Figure 6.7 shows the anticipated results for a multilayer with equal volume fraction of phases (1) and (2) and with zero elastic modulus mismatch, so that $\kappa_\mu = 0$ in eqns. (6.8) and (6.9). In this limit, $\mu' = c(\phi) = \mu[\cos^2\phi + \sin^2\phi(1 - \nu)]$ may be used to reflect the pure screw ($\phi = 0$) versus pure edge ($\phi = 90^\circ$) character of dislocations deposited at the interface, where $\phi$ is the angle subtended by the Burgers vector and line direction [52]. $\phi = 60^\circ$ is chosen here with $\nu = 1/3$. Further, eqns. (6.8) and (6.9) are generalized to the case where the slip plane is inclined to the interfaces as shown in Figure 6.3, so that $h$ is replaced by the distance $h'$ measured along the $[\overline{1} \overline{1} 2]$ direction, where $h' = \sqrt{3}/2 \ h$ and $s = 1/\sqrt{6}$. Finally, the core cutoff parameter $r_0 = 0.16b$. 

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Figure 6.7: Deformation regimes for multilayers predicted from eqns. (6.13) and (6.14), with equal volume fraction of phases (1) and (2), zero elastic modulus mismatch, $\nu = 1/3$, $\phi = 60^\circ$, and $r_0 = 0.16b$. Single slip (non pile-up) deformation regimes are defined as: I = coherent macroyield; II = semicoherent macroyield. Regime II is subdivided into IIa = initially coherent and IIb = initially semicoherent. Regime III = macroyield due to pile-up rather than single slip. Circles are simulation results corresponding to series A to D in Table I, with open circles = Regime I, gray circles = Regime IIa, and black circles = Regime IIb.
Three distinct regimes of deformation are identified in Figure 6.7, based on the nature of interfaces prior to and during loading. The coherent macro-yield regime (Regime I) signifies that at smaller layer thickness and lattice parameter mismatch, interfaces are predicted to be coherent initially at $\Sigma = 0$ and also remain coherent as the biaxial stress $\Sigma$ is increased up to macroyield, at which $\Sigma = \Sigma_{\text{trans}}$. Thus, no confined layer slip in individual layers occurs prior to macroyield. Rather, expanding dislocation loops are predicted to transmit across interfaces prior to reaching conditions for confined layer slip. In order to have coherent interfaces initially, the first term in eqn. (6.4) must have a larger magnitude than the second term, evaluated with $b_1/S_1 = b_2/S_2 = 0$. This is equivalent to imposing that the required biaxial tension for confined layer slip (first term) must be larger in magnitude than the magnitude of biaxial tension developed from coherency (second term). Further, coherent interfaces are maintained during biaxial tension only if the biaxial stress required for transmission is reached before that for confined layer slip, or equivalently, if $|\Sigma_{\text{trans}}| < |\Sigma_{\text{cls}}|$ with $b_1/S_1 = b_2/S_2 = 0$. The latter condition may be restated as

$$\left| \ln \frac{a_2^0}{a_1^0} \right| < \frac{11}{32 \pi h / b} \ln \frac{\sqrt{3/2} h}{eb} \quad \text{(Regime I)} \quad (6.13)$$

The boundaries of Regime I in Figure 6.7 are obtained using eqn. (6.13) with an equality between the terms.

The semi-coherent macro-yield regime (Regime II) signifies that at larger layer thickness and lattice parameter mismatch, eqn. (6.13) is not satisfied and thus interfaces
are semi-coherent at the onset of macro-yield. The semi-coherent state may occur in two ways. In Regime IIa, interfaces are predicted to be coherent initially but become semi-coherent during loading, due to deposition of dislocation content via confined layer slip. In Regime IIb, interfaces are semi-coherent prior to loading and typically acquire additional dislocation content during loading due to confined layer slip. The boundary between Regimes IIa and IIb occurs when the magnitude of biaxial tension in phase (1) of a coherent multilayer just equals the critical magnitude required for confined layer slip. This is implemented by rearranging eqn. (6.4) so that the magnitudes of the first and second terms are equal when \( b_1/S_1 = b_2/S_2 = 0 \),

\[
\ln \frac{a_2^0}{a_1^0} = \frac{11}{16\pi h/b} \ln \frac{3/2}{h/b} \quad \text{(Boundary: Regimes IIa and IIb)} \tag{6.14}
\]

The boundaries between Regimes IIa and IIb in Figure 6.7 are obtained from eqn. (6.14). Corresponding expressions to address confined layer slip in phase (2) and transmission from phase (2) to (1) furnish the same expressions in eqns. (6.13) and (6.14) since, in this case, the elastic modulus mismatch is 0 and the volume fractions of phases are equal.

6.4.2 Simulation Procedure

The simulations adopt the same parameters used to construct the map in Figure 6.7. A ratio \( a_2^0 / a_1^0 \) in stress-free lattice parameter and layer thickness \( h_1/b = h_2/b = h/b \) is selected. Initially, a coherent state is adopted so that the biaxial stress state in phase (1) is given by \( \tau_1/s \) in eqn. (6.3), with \( b_1/S_1 = b_2/S_2 = 0 \). The corresponding biaxial stress in
phase (2) is given by $\tau_2 / s$ using the same procedure but with indices 1 and 2 interchanged in eqn. (6.3). The cellular automaton model follows the evolution of a threading dislocation segment such as B-B' or an interfacial segment A-A' as depicted in Figure 6.1. This is achieved by discretizing a (111) crystallographic plane into equilateral triangles with edge length $l = x b$, where $x$ is chosen so that a straight threading segment such as B-B' in Figure 6.1 is represented by at least 5 triangular edge lengths. As described in chapter 3, any triangle on a (111) plane may slip along any of the <110> slip directions within that plane. The progression of slip is dictated by a path of steepest decent in system energy. Although the model permits cross slip of dislocations onto other {111} slip planes, that feature is suppressed in this study as to model slip on the candidate (111) plane only.

Three steps are followed to determine the deformation mode and the applied biaxial tension $\Sigma_{\text{macroyield}}$ needed to propagate dislocation loops across interfaces and thus induce macroyield. The Relaxation Step involves inserting into a coherent, unloaded ($\Sigma = 0$) multilayer a straight threading segment B-B' of length $L_{BB'} = \sqrt{2} h$, with both line sense $\xi$ and Burgers vector $b$ along the [10 $\overline{1}$] direction. The FS/RH convention as described in Hirth and Lothe [52] dictates that bowing out of the loop along $[\overline{1} 10]$ as shown in Figure 6.1 displaces material above the (111) plane by $b$, relative to that below the plane. Since $a_2^0 / a_1^0 > 1$ is used, the tensile biaxial coherency stress in layer (1) will bow out loop B-B' as shown in Figure 6.1, but the compressive state in layer (2) will suppress transmission of it across the interface. If the bow out is stable, then no significant content is deposited
and interfaces remain coherent, with \((b/S)_1 = (b/S)_2 = 0\). If B-B' expands by confined layer slip, dislocation content is deposited at interfaces.

It is assumed that this process, if modeled on the other \{111\}/<110> slip systems, would produce a grid of 60° dislocations with a net Burgers vector content equivalent to a square grid of misfit edge dislocations as shown in Figure 6.1. The grid would alternate in sign as shown from a "positive grid" bounding the bottom of a phase (1) layer to a "negative grid" bounding the top of a phase (1) layer. These grids effectively impart extra vertical planes of matter into phase (1), as to produce a positive, in-plane, biaxial plastic strain. Thus, interfaces would become semi-coherent with nonzero \((b/S)_1\) prior to any macroscopic loading. In this case, the stress state in the multilayer thin film is modified by the superposition of the stress field from these interfacial misfit arrays.

The response of an initially straight threading segment is studied with successively larger values of \((b/S)_1\). The threading segment is positioned relative to the grid such that the center of the initially straight segment has a vertical projection onto the center of dislocation-free squares in the grids above and below. Ultimately, a critical \((b/S)_1\) is identified which is large enough to make the bow-out stable, so that confined layer slip is suppressed and no additional content is added to interfaces. The relaxation process described here is also repeated for an interfacial dislocation segment A-A' with length \(L_{AA'} = 2 \sqrt{2} \, h\), positioned such that the center of the segment is in the center of a dislocation-free square in the misfit grid. The larger initial segment length ensures that formation of a bow-out requires a smaller stress than the confined layer slip process.

The subsequent Macroyield Step models the response of a threading or misfit segment during application of \(\Sigma\), with the initial value of \((b/S)_1\) provided by the relaxation step. If
confined layer slip is observed, it is assumed that more content is deposited at interfaces during loading. Thus, the calculation is repeated using successively larger values of \((b/S)_1\) until the deformation mode changes from confined layer slip to transmission. Macroyield is defined as the onset of slip propagation across interfaces. Following transmission, loops typically expand via confined *multiple-layer* slip, such that the loop propagates parallel to the interface but with a projected height \(h'_{\text{multiple}} = m_1 h'_1 + m_2 h'_2\). Thus, a feature of macroyield is that dislocation content is not deposited at every interface as with confined *single*-layer slip.

### 6.4.3 Simulation results for threading dislocation source

As shown in Figure 6.1, there is biaxial tension in layers (1) and biaxial compression in layers (2), when \(a_2^0\) is greater than \(a_1^0\). This coherency stress affects the deformation mode of the multilayered structures. When the lattice parameter difference is small and thus the coherency stress in each layer is small, co-deformation will occur in which a threading dislocation AB in Figure 6.9(a) propagates as to deform both types of layers. At the other extreme, if the lattice mismatch is sufficiently large, then the coherency stress will be sufficient to confine slip to individual layers.

For a fixed layer thickness, this concluding study will consider three cases of small, medium and large lattice mismatch. For all the cases, \(h_1 = h_2 = 75b\), \(\rho = 0.66b\), \(\mu_1 = \mu_2 = \mu\), \(SB = 15b\), and no misfit dislocation arrays at the interfaces. The initial threading dislocation is represented with 40 segments. For reference, \(\tau_{\text{CLS}} = 0.01022\mu\). Our choice of a critical value of \(a_2^0/a_1^0\) for confined layer slip is guided by a simple analysis. The
force balance in Figure 6.8 indicates that confined layer slip in phase (1) requires

\[ \tau^{(1)} = \tau_a + \tau_a^{(1)} \geq \tau_{CLS}, \]

where \( \tau_a \) and \( \tau_a^{(1)} \) are the resolved shear stress contributions from the applied stress and lattice parameter mismatch, respectively. For the simple analysis here where \( h_1 = h_2 = h \) and \( \mu_1 = \mu_2 = \mu \), the net energetic force to drive the threading dislocation in \( \ell = (2) \) in a co-deformation mode is

\[ F_{co-def}^{(2)} = (\tau_{CLS} + \tau_a + \tau_a^{(2)})bh \tag{6.15} \]

The contribution \( \tau_{CLS} \) enters into the force balance due to the line energy of trailing dislocation line that attempt to pull the loop along in a co-deformation mode. The condition \( F_{co-def}^{(2)} < 0 \) to ensure CLS in phase (1) only is obtained by replacing \( \tau_a = \tau_{CLS} - \tau_a^{(1)} \) in equation (6.15), so that

\[ \tau_a^{(1)} - \tau_a^{(2)} > 2\tau_{CLS} \tag{6.16} \]

is necessary for CLS.
Figure 6.8: Stress balance illustration for confined layer slip. $\tau_{a_0}^{(1)}$ and $\tau_{a_0}^{(2)}$ are the resolved shear stress due to lattice mismatch, and $\tau_a$ is the resolved shear stress due to applied stress.
Figure 6.9: Deformation modes with respect to the magnitude of lattice mismatch; (a) small $a_2^0/a_1^0 = 1.002$, (b) moderate $a_2^0/a_1^0 = 1.005$, (c) large $a_2^0/a_1^0 = 1.015$
The ratio $a_2^0/a_1^0 = 1.002$ is considered for small lattice mismatch. The resolved shear stresses in $\ell = (1)$ and (2) due to the lattice mismatch are 0.001515$\mu$ and -0.001515$\mu$, according to equation (3.18), with $\tau = \sigma_{11}/\sqrt{6}$. This stress is much smaller than the corresponding $\tau_{CLS}$. As the applied stress is increased, the total resolved shear stress in $\ell = (2)$ becomes positive long before the stress in $\ell = (1)$ reaches $\tau_{CLS}$. Thus, co-deformation in $\ell = (1)$ and (2) dominates and the corresponding propagation path is shown in Figure 6.9(a).

The ratio $a_2^0/a_1^0 = 1.005$ is considered for medium lattice mismatch. For reference, the resolved shear stresses in $\ell = (1)$ and (2) due to the lattice mismatch are 0.00378$\mu$ and -0.00378$\mu$. An applied stress is necessary to increase the resolved shear stress in $\ell = (1)$ to $\tau_{CLS}$, but prior to that event, the resolved shear stress in $\ell = (2)$ becomes positive and co-deformation intervenes as shown in Figure 6.9(b). A notable difference, however, is that the threading dislocation has an oscillating front, compared to the small mismatch case. The stress difference in $\ell = (1)$ and (2) is a little smaller than $\tau_{CLS}$. From the propagation route in Figure 6.9(b), confined deformation in $\ell = (1)$ starts, but co-deformation intervenes.

For large lattice mismatch, we select $a_2^0/a_1^0 = 1.015$ so that the resolved shear stresses in $\ell = (1)$ and (2) due to the lattice mismatch are 0.0113$\mu$ and -0.0113$\mu$, and accordingly, the condition equation (6.9) for confined layer slip is satisfied. In fact, the stress magnitude in each layer is larger than $\tau_{CLS}$, so that the dislocation can propagate in opposite directions in each layer type without any applied stress. The corresponding
model prediction in Figure 6.9(c) confirms confined layer slip propagation of the threading dislocation in both kinds of layers.

For the case of $a_2^0/a_1^0 = 1.005$, simulations are performed for different layer thickness. When $h$ is big ($h = 500b$), dislocation propagates in confined layer slip mode; while when $h$ is small ($h = 40b$), codeformation appears. Therefore, increasing $a_2^0/a_1^0$ with fixed $h$ has the similar effect as increasing $h$ with fixed $a_2^0/a_1^0$.

For the cases with confined slip mode, multilayer structure is still not stable. Interfacial dislocation deposition needs to be studied. For the case of $a_2^0/a_1^0 = 1.015$ and $h = 75$, the process of confined layer slip in Figure 6.9(c) deposits dislocation content along interfaces. This dislocation content decreases the oscillation in average biaxial stress caused by lattice parameter mismatch. If the net dislocation content of the arrays can be approximated by orthogonal arrays of dislocations as depicted in Figure 6.1, then equation (3.18) reflects that the coherency stress is annihilated when $\frac{b}{S} = \frac{a_2^0}{a_1^0} - 1$.

Thus, a critical dislocation density is anticipated at which the difference in stress between layer types no longer exceeds $2\tau_{CLS}$, and co-deformation will intervene. Three misfit dislocation densities, $b/S = 0.004714$, 0.006286 and 0.009428 are considered here, and the corresponding propagation configurations are given in Figure 6.10. Even for $b/S = 0.009428$, co-deformation is not observed completely, even though the misfit arrays have reduced the difference in average resolved shear stress across layers to the equivalent of a multilayer with an effective $a_2^0/a_1^0 = 1.015 - 0.0094 = 1.0054$. It is apparent that the highly inhomogeneous stress state generated by the misfit arrays serves
to locally pin the threading dislocation. The net result is that confined layer slip and thus extraordinary strength is preserved here, even though the difference in average stress between layers is comparable to that considered in Figure 6.9(b).
Figure 6.10: Deformation modes with respect to the density of interfacial misfit dislocations for $a_2^0/a_1^0 = 1.015$; (a) low $b/S = 0.004714$ or $S = 212b$, (b) moderate $b/S = 0.006286$ or $S = 159b$, (c) high $b/S = 0.009428$ or $S=106b$; layer thickness is $75b$
6.4.4 Strength of Multilayers via interfacial dislocation simulation

Table 6.1 reports the numerical results from several cellular automaton dislocation simulations, each corresponding to a discrete value of lattice parameter ratio \(a_2^0/a_1^0\) and individual layer thickness \(h_1 = h_2 = h\). In all cases, the mismatch in elastic shear modulus \(\mu\) is zero, Poisson's ratio \(\nu = 1/3\) for each phase, and the core cutoff parameter \(\rho = r_0/2 = 0.08\). The simulations are based on a discretization of a (111) slip plane into triangular patches of side length \(l = x b\), where \(x\) is chosen to ensure that the distance B-B' \(\geq 5 l\) in Figure 6.1. A threading dislocation B-B' with slip direction/line direction equal to [10 \(\bar{T}\)]/[10 \(\bar{T}\)] or an interfacial dislocation A-A' with slip direction/line direction [10\(\bar{T}\)]/[\(\bar{T}\)10] is introduced as shown in Figure 6.1, so that the loops bow out as shown schematically in Figure 6.1, due to a tensile coherency stress in phase (1) layers. For each case in Table 6.1, the mode of expansion \((m_1, m_2)\), dislocation density \((b/S)_1\), and macroscopic stress \(\Sigma\) are reported at the onset of loop expansion and at macroyield. All cases listed in Table 6.1 are indicated by circular symbols in Figure 6.7. Series A to D are organized according to increasing \(a_2^0/a_1^0\) and Cases 1, 2, 3... in each series are correspond to increasing values of \(h\). Also for these series, the length \(L_{AA'} = 2\sqrt{2} h\) is used to ensure that the stress to operate the source via loop bow-out is less than the corresponding stress to propagate the loop in a confined layer mode. The last Case AA1 at the bottom of Table 6.1 adopts the same conditions as Case A1, except that \(L_{AA'} \neq 2\sqrt{2} h\).
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<th>$\Sigma_{\text{macro-yield}}$</th>
<th>$\Delta \Sigma_{\text{hardening}}$</th>
<th>Regime</th>
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</tr>
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<td></td>
<td>B3</td>
<td>(1, 0)</td>
<td>0.027 (2, 1)</td>
<td>10^{-8}</td>
<td>0.027</td>
<td>0/0</td>
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<tr>
<td></td>
<td>B4</td>
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<td>0.004</td>
<td>0.020</td>
<td>.010/.003</td>
</tr>
<tr>
<td></td>
<td>B5</td>
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<tr>
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<td>C1</td>
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<td>0.100 (2, 1)</td>
<td>0.100</td>
<td>0/0</td>
<td>I</td>
</tr>
<tr>
<td></td>
<td>C2</td>
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<td>0.061 (1, 0.13)</td>
<td>0.061</td>
<td>0/0</td>
<td>I</td>
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<tr>
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<td>10^{-8}</td>
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<td>0/0</td>
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<tr>
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<td>0.027</td>
<td>.013/.004</td>
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<td>0.135</td>
<td>0/0</td>
<td>I</td>
</tr>
<tr>
<td></td>
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<td>10^{-8}</td>
<td>0.059</td>
<td>.007/0</td>
</tr>
<tr>
<td></td>
<td>D3</td>
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<td>0.026 (2, 1)</td>
<td>0.01</td>
<td>0.049</td>
<td>.023/.007</td>
</tr>
<tr>
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<td>AA1</td>
<td>(2, 1)</td>
<td>0.027 (2, 1)</td>
<td>0.027</td>
<td>0/0</td>
<td>I</td>
</tr>
</tbody>
</table>

Table 6.1: Results from cellular automaton dislocation simulations.

Note: Interfacial source length $L = 2 \sqrt{2} h$ except for Case AA1, where $L = 160 \sqrt{2} b$.

Also, $h_1 = h_2 = h$. Hardening is defined by eqn. (6.18).
6.4.4.1 Effect of threading vs interfacial sources

The cases in Series A were simulated for both threading and interfacial sources. All quantities reported in Series A in Table I were identical for threading versus interfacial geometries, to within the significant figures reported. Thus, all remaining studies were conducted using an interfacial source geometry only.

6.4.4.2 Regimes of plastic response

A primary conclusion from the Series A study is that the non pile-up regimes postulated in the theoretical development are also observed in the simulations. Regime I behavior is observed for sufficiently small \( h/b \) \((= 30, 80)\). Here, interfaces remain coherent up to macroyield. This is confirmed by noting that for Cases A1 and A2 in Table 6.1, \( (b/S)_1 = 0 \) at macroyield. Figure 6.11a shows that for Case A1 \( (h = 30b) \), an interfacial source operating in a coherent system bows out across interfaces and then expands in a \( (m_1, m_2) = (2, 1) \) multiple-layer mode. Thus, the same loop that generates initial yield in layer 1 also precipitates macroscopic yield. For Case A2, \( (m_1, m_2) = (1, 0.13 \text{ or } 1/8) \) is reported, suggesting the onset of multiple-layer slip in an otherwise coherent system, but with a non-integral number of multiple layers.

Cases A3 and A4 display Regime I1a behavior, whereby the layer thickness \( h/b \) \((= 150 \text{ and } 400)\) is sufficiently small so that interfaces are coherent initially. However, at the onset of initial slip, a \( (m_1, m_2) = (1, 0) \) single-layer mode prevails so that dislocation content is deposited at each interface. At macroyield, numerical values in Table 6.1 indicate an increase in dislocation density to \( (b/S)_1 \sim 10^{-8} \) and 0.0012 for the respective cases, and a transition to a \( (m_1, m_2) = (2, 1) \) multiple-layer mode. The approximately
zero value of \((b/S)_1\) at macroyield for Case A3 suggests that it is near the Regime I/IIa border. For case A4, the corresponding succession of geometries leading to macroyield is shown in Figure 6.11b. Here, the expanding 60° loop interacts with a grid of misfit dislocations, so that the loop takes on an irregular shape.

Case A5 displays Regime IIb behavior, whereby the layer thickness \(h/b (= 800)\) is sufficiently large so that interfaces are initially semi-coherent, with \((b/S)_1 = 0.0006\). During loading, initial slip occurs via a \((m_1, m_2) = (1, 0)\) mode, so that dislocation content is deposited at each interface. The deposition increases interfacial content to \((b/S)_1 = 0.0018\), at which an interfacial dislocation source is able to bow out and expand via a \((m_1, m_2) = (1, 1)\) multiple-layer mode, as depicted in Figure 6.11c. This mode is an outcome of the interaction with a denser misfit grid, which suppresses formation of the \((m_1, m_2) = (2, 1)\) expansion mode observed for Case A4.

The shaded and unshaded regions in Figure 6.7 that are based on eqns. (6.13) and (6.14) approximately describe the deformation behavior trends observed in the simulations. Data from remaining series are also included to study the trend with increasing lattice parameter ratio. The similar trends between the theoretical boundaries and the simulation observations suggests that the regime is controlled by a combination of lattice parameter ratio and individual layer thickness as dictated in eqns. (6.13) and (6.14).
Figure 6.11: Expansion of an interfacial dislocation source A-A' for $a_2^0/a_1^0=1.002$, as predicted from the cellular automaton simulations, for $h$ equals (a) $30b$ (Case A1); (b) $400b$ (Case A4); and (c) $800b$ (Case A5). The critical macroyield configuration is the innermost expansion state shown and the outer states depict the subsequent evolution to a multiple-layer mode. The projection axis normal to the page is [111]. Other material and geometric parameters are reported in Table 6.1.
6.4.4.3 Evolution of interfacial dislocation density with applied stress

Table 6.1 indicates that each regime has a characteristic evolution of interfacial dislocation density with imposed deformation. The cases labeled Regime I remain coherent throughout the deformation process and thus do not incur any interfacial dislocation content up to the macroyield point. This is indicated by \((b/S)_I = 0\) entries in Table 6.1 at initial slip and also at macroyield. In Regime IIa, interfaces are initially coherent but since \(\Sigma_{\text{cls}} < \Sigma_{\text{trans}}\), confined layer slip occurs first, so that dislocations are deposited at interfaces prior to macroyield. Eqns. (6.4) and (6.5) indicate that a positive \((b/S)_I\) will increase \(\Sigma_{\text{cls}}(1)\) and decrease \(\Sigma_{\text{trans}}(1 \to 2)\) so that ultimately, a critical \((b/S)_I\) is reached at which \(\Sigma_{\text{cls}}(1) = \Sigma_{\text{trans}}(1 \to 2)\). Implementing this condition using eqns. (6.4) and (6.5) gives

\[
\left(\frac{b_1}{S_1}\right)_{\text{macroyield}} = \max \left\{ \frac{a_2^0}{a_1^0} \exp \left[ \frac{1}{sM_2} \left( \frac{\partial e_w}{b} \right) + \frac{e_h}{bw} \right] - 1 \right\}, \quad \frac{a_2^0}{a_1^0} > 1
\]

(6.17)

The first expression indicates that the critical density of interfacial dislocations at macroyield is 0, unless the lattice parameter ratio \(a_2^0 / a_1^0\) is sufficiently large and/or the terms \(\partial e_w / \partial x^2 + e_h / w\) which confine dislocations to individual layers are sufficiently large compared to the required driving force \(e_w / h^1\) for confined layer slip. The second expression is valid in the 2D limit of \(w >> h\) and \(L\), so that \(e_h / bw \to 0\) and \(e_w\) and \(\partial e_w / \partial x^2\)
are determined from eqns. (6.9) and (6.10), respectively, with $M_1 = M_2$. An identical construction holds for Regime IIb.

**Figure 6.12** shows contours of constant interfacial dislocation density as a function of lattice parameter ratio and layer thickness, predicted from the second version of eqn. (6.17). The discrete points show the cases reported in Table I, with numerical values of $(b/S)_1$ at which macroyield is observed. In the majority of cases, the simulation values are modestly larger than those predicted by eqn. (6.17). The underestimate may be due to the idealization of the 2D limit in which $e_h/w \rightarrow 0$, or it may stem from the inability of the theory to capture the suppression of transmission caused by the discrete misfit dislocation arrays.

**6.4.4.4 Work hardening leading up to macroscopic yield**

The evolution of interfacial dislocation content serves to increase the macroscopic applied stress needed to deform the film. This can be understood by studying the effect of confined layer slip on $\Sigma_{cls(1)}$ and $\Sigma_{trans(1\rightarrow2)}$. Eqn. (6.4) suggests that $\Sigma_{cls(1)}$ increases with deformation for two reasons. First, the line energy $e_w$ of dislocations deposited at interfaces may increase with interfacial dislocation density. In particular, Anderson and Kreidler [126] computed $e_w$ for misfit dislocations via the work to separate dislocation dipoles in multilayers containing an existing grid of misfit dislocations and zero modulus mismatch. A principal observation is that $e_w$ is expected to remain relatively uniform up to $(b/S)_1 \approx b/10h$ but then increase due to the proximity of nearby array elements. A second source of hardening in eqn. (6.4) stems from the logarithmic dependence of $\Sigma_{cls(1)}$.
on \( (b/S)_1 \). This dependence reflects that plastic deformation in phase (1) relieves stress in that phase via load shedding to phase (2). The corresponding effect of confined layer slip on \( \Sigma_{\text{trans}(1 \rightarrow 2)} \) is mixed. The logarithmic dependence of \( \Sigma_{\text{trans}(1 \rightarrow 2)} \) on \( (b/S)_1 \) in eqn. (6.5) reflects that plastic deformation in phase (1) reduces the magnitude of alternating biaxial tension/compression that serves to confine slip to phase (1). However, the interfacial content may serve to pin slip at interfaces \([125]\) and thus enhance confinement. In fact, the bow out dimensions observed in Fig. 6 of Anderson, Focke, and Hazzledine \([54]\) are in agreement with misfit dislocation spacing inferred from transmission electron microscopy images.

**Figure 6.13a** displays the evolution in \( \Sigma/\mu \) with \( (b/S)_1 \) up to the point of macroyield, for \( h/b = 400 \) and 800, with \( a_2^0 / a_1^0 = 1.002 \). The thick gray curves show results from the simulations and the black lines show corresponding theoretical predictions using eqn. (6.4) with \( \Sigma = \Sigma_{\text{cls}} \) and \( e_w \) given by eqn. (6.9). The similar trend between theory and simulation suggests that load shedding contributes to hardening; the additional hardening displayed in the simulation results is attributed to the role of interfacial dislocation content interacting with confined layer slip and transmission processes.

The overall hardening is defined as the increase in macroscopic stress between initial slip and macroyield,

\[
\Delta \Sigma_{\text{hardening}} = \Sigma_{\text{macroyield}} - \Sigma_{\text{initial slip}}
\]  

(6.18)
The column $\Delta \Sigma_{\text{hardening}}$ in Table 6.1 indicates zero hardening for simulations in Regime I, where both phases in the multilayer are predicted to deform elastically up to macroyield. Large amounts of hardening are predicted for simulations in Region II, where dislocation content is deposited at interfaces prior to macroyield. A comparison of Cases A4 and A5 suggests that for a given $a_2^0 / a_1^0$, hardening is larger in Region IIa, where interfaces are initially coherent, compared to Region IIb, where interfaces are initially semi-coherent.

A theoretical estimate of hardening in biaxial tension can be made using eqn. (6.18), with macroyield defined as the onset of transmission from phase (1) to (2),

\begin{equation}
\Sigma_{\text{macroyield}} = \Sigma_{\text{trans}(1\rightarrow2)} \left( \frac{b_1}{S_1} \right)_{\text{macroyield}}, \quad b_2 = 0
\end{equation}

and initial slip defined as the non-negative stress required to plastically deform phase (1),

\begin{equation}
\Sigma_{\text{initial slip}} = \max \left( 0, \Sigma_{\text{cls}(1)} \left( \frac{b_1}{S_1} = 0, \frac{b_2}{S_2} = 0 \right) \right)
\end{equation}

Here, it is assumed that slip initiates in phase (1) during loading and that $a_2^0 / a_1^0 > 1$, consistent with the simulations. The theoretical values of $\Delta \Sigma_{\text{hardening}}$ in Table 6.1 underestimate the hardening observed in simulations in Region II. The discrepancy is
attributed to the inability of the theory to capture discrete interaction between dislocations propagating by confined layer slip and existing interfacial dislocation arrays.

Figure 6.13b displays the evolution in $\Sigma/\mu$ with macroscopic biaxial strain $\varepsilon_{\text{macro}}$ for the same multilayer systems, up to the point of macroyield. The thick gray lines are the simulation results and the black lines are obtained for biaxial stretching using

$$
\Sigma = \begin{cases} 
(M_1 f_1 + M_2 f_2) \varepsilon_{\text{macro}} & \Sigma \leq \Sigma_{\text{initial slip}} \\
\Sigma_{\text{initial slip}} + M_2 f_2 \varepsilon_{\text{macro}} & \Sigma_{\text{initial slip}} \leq \Sigma \leq \Sigma_{\text{macroyield}} 
\end{cases}
$$

(6.21)

Provided that $\Sigma < \Sigma_{\text{initial slip}}$, both phases respond elastically, so that the macroscopic response is elastic with an effective biaxial modulus approximated by an isostrain approach. For $\Sigma_{\text{initial slip}} < \Sigma < \Sigma_{\text{macroyield}}$, phase (1) deforms by confined layer slip (cls) while phase (2) deforms elastically. Provided the line energy $e_w$ of interfacial dislocation content remains uniform during deformation, eqn. (6.1) indicates that phase (1) will be perfectly plastic and not sustain additional load during deformation. Thus, the approximation in eqn. (6.21) leads to linear response here, but with a reduced slope given by $M_2 f_2$. The results in Figure 6.13b indicate that eqn. (6.21) captures the trends from the simulation, but underestimates strength during the cls portion of the response, where hardening is generated via interaction between cls segments and misfit arrays. The simulations also show a nonlinear behavior in the cls regime that is not captured by eqn. (6.21).
Figure 6.12: Contours of constant interfacial dislocation density \((b/S)_1\) at macroyield as a function of lattice parameter ratio and layer thickness, as predicted from eqn. (6.17). Circles depict simulation cases in Table 6.1, with numbers beside circles showing the predicted \((b/S)_1\) at macroyield from simulations. The shading of circles and the material/geometric parameters are identical to those used in Figure 6.7.
Figure 6.13 Macroscopic biaxial stress $\Sigma$ versus (a) average biaxial plastic strain in phase (1) and (b) macroscopic biaxial strain, for $h/b = 400$ (Case A4) and 800 (Case A5), with $a_2^0 / a_1^0 = 1.002$. Gray lines show results from the cellular automaton simulations and black lines show predictions from eqns. (6.4) and (6.21), with average biaxial plastic strain in phase (1) $= \ln[1 + (b/S_1)]$. $\Sigma$ is normalized by elastic shear modulus $\mu = \mu_1 = \mu_2$; other geometric and material parameters are the same as for Figure 6.7.
6.4.4.5 Macroyield Strength, $\Sigma_{\text{macroyield}}$

Figure 6.14 shows the variation in biaxial macroyield strength $\Sigma_{\text{macroyield}}$ with layer thickness $h$, for discrete values of lattice parameter ratio $a_2^0 / a_1^0$. The gray circular points in Figure 6.14(a) show the simulation results for $a_2^0 / a_1^0 = 1.002$, based on Cases A1-A5 and AA1. Cases A1-A5 have the common feature that the interfacial source length $L = 2\sqrt{2} h$. There, the macroyield strength monotonically increases with decreasing layer thickness (and source length). This occurs even in Regime I, where layers are sufficiently thin so that confined layer slip is not possible.

An alternate approach to model Regime I is to impose a constant source length. This assumption is plausible since interfaces in Regime I are predicted to remain coherent and thus constant in structure all the way to macroyield. Cases A2 and AA1 show the outcome if $L = 160 \sqrt{2} b$ for $h = 80 b$ and $30 b$, respectively. Here, macroyield strength is more uniform with layer thickness, similar to the experimental observations discussed earlier. Thus, a plateau is possible at small $h$, provided the source length is constant with layer thickness.

A theoretical approximation to the simulation results is proposed for each regime, based on the prior analytic development and on observations from simulations. For Regime I, the simulations suggest a critical configuration as shown in Figure 6.3, with the critical event corresponding to the transmission of the segment C-C’ across the interface. Thus, the macroyield strength is evaluated as $\Sigma_{\text{trans}(1 \rightarrow 2)}$ in eqn. (6.5), with $(b/S)_1 = (b/S)_2 = 0$ and also $M_1 = M_2$, $a_2^0 / a_1^0 > 1$ as assumed in the simulations,
\[
\frac{\sum_{\text{macroyield}}}{\mu} \bigg|_I = \frac{1}{s\mu} \left( \frac{\partial e_w}{\partial x_2'} + \frac{2e_h}{bw} \right) + \frac{M}{2\mu} \ln \frac{a_2^0}{a_1^0} \left( \text{for } M_1 = M_2; a_2^0 \geq a_1^0 \right)
\approx \frac{c(90^\circ - \phi)}{2\pi sL/b} \ln \left( \frac{2h'}{e\rho} \right) + \frac{M}{2\mu} \ln \frac{a_2^0}{a_1^0} \left( \text{for } w = L > h \text{ also} \right)
\]

(6.22)

The first expression shows that macroyield strength is controlled by the barrier $\partial e_w/\partial x_2'$ to dislocation transmission provided by the interface, the line energy $e_h$ of segments created during the advance across the interface, and the ratio $a_2^0/a_1^0$ of stress-free lattice parameters. The second expression imposes an important geometrical observation made from the simulations that in Regime I, the critical width $w \approx L$ at least when $L > 2\sqrt{2}h$. In that case, Figure 6.3 shows that the segment C-C' has a negligible length of dipole on the opposing interface, so that the leading $1/h$ term in eqn. (6.10) vanishes. Further, zero elastic modulus mismatch is adopted here, so that $\kappa \mu = 0$ in eqn. (6.10). Thus, $\partial e_w/\partial x_2' \sim 0$. Since $w \approx L$, the term $2e_h/bw \approx 2e_h/bL$, where $e_h = (\mu b^2/4\pi)\ln(h'/e\rho)$ is adopted from Hirth and Lothe [52] for an isolated segment of length $h'$. Thus, this treatment suggests that macroyield strength in Regime I is controlled primarily by the source length scale and lattice parameter ratio, with a weaker logarithmic dependence on projected layer thickness. The short black segment labeled "I" in Figure 6.14(a) is the corresponding prediction from the second form of eqn. (6.22), with $s = 1/\sqrt{6}$, $\phi = 60^\circ$, $h'_1 = \sqrt{3}/2h$, $\nu_1 = \nu_2 = 1/3$, and $r_0 = 0.16b$.

The corresponding theoretical value of macroyield strength for Regime II is achieved when confined layer slip increases interfacial dislocation density $(b/S)_1$ to a critical value.
This occurs when $\Sigma_{\text{cls}(1)} = \Sigma_{\text{trans}(1 \to 2)}$. Imposing this condition using eqns. (6.4, 6.5) and applying the assumptions $M_1 = M_2$ and $a_2^0 / a_1^0 > 1$ furnishes

$$
\frac{\Sigma_{\text{macroyield}}}{\mu} = \frac{1}{s \mu} \left( \frac{e_w}{bh'_1} + \frac{\partial e_w / \partial x_2}{b} \right) \left( \text{for } M_1 = M_2, a_2^0 \geq a_1^0 \right)
$$

(6.23)

$$
\approx \frac{c(\phi)}{4 \pi h'_1 / b} \left[ \ln \frac{h'}{r_0} + 2 \right] \quad \text{(for } w \gg L > h \text{ also)}
$$

The first expression shows that macroyield in this regime depends on both the height and width of the critical loop, as well as line energies $e_w$, $e_h$ and interfacial barrier strength $\partial e_w / \partial x_2$. The second form of eqn. (6.23) adopts the limit $w \gg L$, so that the term $e_h / bw \to 0$. This is motivated by observations of critical configurations in the simulations, which suggest that candidate loops for transmission across interfaces are those which have already expanded via confined layer slip into a 2D configuration. The longer black curve labeled "II" in Figure 6.14(a) is the corresponding prediction from the second form of eqn. (6.23), with $s = 1 / \sqrt{6}$, $\phi = 60^\circ$, $h' = \sqrt{3} / 2 h$, $v_1 = v_2 = 1 / 3$, and $r_0 = 0.16 b$.

The results in Figures 6.14 (a, b) suggest that the analytic expressions in eqns. (6.22, 6.23) capture the basic trends observed in the simulations but underestimate macroyield strength. A principal trend for Regime II is that macroyield strength increases monotonically with decreasing layer thickness, at least for $L > 2 \sqrt{2} h$ as assumed here. This observation holds for the $a_2^0 / a_1^0 = 1.002$ and 1.006 series considered in Figure 6.14(a) and (b), respectively. A second principal trend is that in Regime I, macroyield strength is controlled primarily by lattice parameter ratio and source length scale. The
former trend is supported by a comparison of Cases B1, C1, and D1, which document the increase in macroyield strength due to an increase in $a_2^0 / a_1^0$ at fixed $h$. The latter trend is supported by a comparison of Cases AA1 and A1, which demonstrate a large increase in macroyield strength when the source length $L$ is decreased from $160 \sqrt{2} b$ to $60 \sqrt{2} b$ at constant $h (= 30b)$. Finally, a comparison of Cases A2 and AA1 supports the concept that in Regime I, macroyield strength is relatively constant with decreasing $h$, provided other variables such as source length scale and lattice parameter ratio are held constant.

A final observation consistent with eqns. (6.22, 6.23) is that increasing the lattice parameter ratio decreases the range of layer thickness over which Regime I dominates. This is most easily observed by comparing the domain of Region I response in Figure 6.14(a) and (b).

There are some important features in the simulations that are not rigorously captured by the analytic results. The first is that eqn. (6.22) predicts macroyield strength to decrease logarithmically with decreasing $h$ in Regime I, yet a comparison of Cases A2 and AA1 shows a modest increase. The principal reason for this is idealization of the critical configuration according to a near rectangular shape in Figure 6.3, with a segment C-C’ of length $w = L$ transmitting from phase (1) to (2). In reality, simulations show that decreasing $h$ will shift the critical configuration from a large, more fully-formed bow-out with a small amount of segment C-C’ located at the interface to a more shallow bow-out with a longer length of segment at the interface. A second discrepancy is that the analytic result for Regime II suggests macroyield strength should not depend on lattice parameter ratio. The simulations, however, show approximately a 10% increase in macroyield strength when $a_2^0 / a_1^0$ is increased from 1.002 in Figure 6.14(a) to 1.006 in Figure 6.14.
(b). Presumably, this is due to the larger density of interfacial dislocations for \( \frac{a_2^0}{a_1^0} = 1.006 \) and the discrete pinning role they play. That feature is not adequately captured in the analytic expressions.
Figure 6.14: Macroscopic biaxial stress at macroyield versus individual layer thickness $h$ in a multilayer thin film, for $a_2^0/a_1^0 = \text{(a)} 1.002$ and (b) 1.006. Gray lines show results from the cellular automaton simulations and black lines show predictions from eqns. (6.22, 6.23), with geometric and material parameters identical to those used in Figure 6.7. Labels AA1, A2, etc. denote simulations referred to in Table 6.1. $\Sigma_{\text{macroyield}}$ is normalized by elastic shear modulus $\mu = \mu_1 = \mu_2$. 

\[ \Sigma_{\text{macroyield}}/\mu \]
6.5 Comparison to experimental data

The effectiveness of the model is assessed by comparing simulation predictions of macroyield strength for the Ag/Al system to experimentally measured values of hardness as a function of layer thickness provided by Kim et al [127]. This system is chosen since the bulk values of elastic shear moduli are relatively similar, with \( \mu_{\text{Ag}} = 30 \text{ GPa} \) and \( \mu_{\text{Al}} = 26 \text{ GPa} \), compared to other systems for which experimental measurements are available. Thus, the simulation adopts an elastically homogeneous multilayer with \( \mu = 28 \text{ GPa} \). Bulk values of stress-free lattice parameter \( a_{\text{Ag}}^0 = 0.40853 \text{ nm} \) and \( a_{\text{Al}}^0 = 0.40495 \text{ nm} \) are used [128], so that \( a_{\text{Ag}}^0 / a_{\text{Al}}^0 = 1.009 \). For a <001> epitaxy, the Al layers are expected to be in tension, with macroyield in biaxial tension defined by the propagation of slip from tensile Al layers into adjoining Ag layers. The sputtered thin films show a well-defined multilayer structure with a layer thickness ratio \( h_{\text{Ag}}/h_{\text{Al}} = 2.7 \), so that \( f_{\text{Al}} = 0.27 \). Since the simulation geometry uses \( h_1 = h_2 \), the experimental system is modeled using \( h_1 = h_2 = (h_{\text{Al}} + h_{\text{Ag}})/2 \) as to capture approximately the physical dimensions of the layers and the trends with decreasing layer thickness. Further, \( b_{\text{Al}} = b_{\text{Ag}} = 0.3 \text{ nm} \), \( L = 2\sqrt{2} h \), and \( \rho = 0.08 b \) is used. Values of macroyield in biaxial tension are converted to hardness using \( H = 3 \Sigma_{\text{macroyield}} [129] \).

Figure 6.15 shows that the simulation results capture the trend of experimental data over the range, \( \Lambda = 1.35 \) to 21.3 nm. The simulations predict that all response over this bilayer thickness range is in Regime I. This is consistent with experimental observations that interfaces are coherent prior to indentation, although there is not adequate experimental information to determine the state of interfaces at or following yield. The
analytic map in Figure 6.7 indicates that the transition from Regime I to II occurs at $h \sim 63b \ (= 19 \text{ nm here})$ for $a_{Ag}^0 / a_{Al}^0 = 1.009$, so that the analytic expressions predict Regime I behavior over the majority of the experimental range. The simulations furnish the combination of $(m_1, m_2)$ associated with the multiple layer slip. It is revealing that the effective height, $h_{\text{eff}} = h_1m_1 + h_2m_2$, remains relatively constant over the range of bilayer thickness studied. This is consistent with the concept that in Regime I, the expanding dislocation loop seeks out an effective height such that the critical stress to drive the $(m_1, m_2)$ mode becomes less than the corresponding value for slip transmission. Since interfacial structure and thus conditions for slip transmission do not vary significantly over the range of $\Lambda$ studied here, $h_{\text{eff}}$ does not vary substantially either.
Figure 6.15: Macroscopic biaxial stress at macroyield versus bilayer period $\Lambda = h_{Ag} + h_{Al}$ for Ag/Al multilayer thin films. The dark vertical lines denote experimental results [127] based on hardness measurements ($H$) with $\Sigma_{\text{macroyield}} = H/3$. Gray circles denote cellular automaton results using $a_2^0/a_1^0 = 1.009$, $h = h_1 = h_2 = \Lambda/2$, $b_{Al} = b_{Ag} = 0.3\text{nm}$, $\mu = 28$ GPa, and initial interfacial segment length $L = 2\sqrt{2}h$. 
6.6 Summary

The strength of multilayers is owed to the ability to confine slip to small individual layers. The ability to confine slip to individual layers can stem from the large alternating coherency stress generated by mismatch in stress-free lattice parameters of the phases, oscillation in dislocation line energy caused by mismatch in the elastic moduli or core cutoff parameters of the parent phases, source limited plasticity that stems from the inability of interfaces to provide dislocation content, and structural barriers to slip transmission across interfaces caused by misfit dislocations, variation in interfacial bond strength, and chemical and structural sharpness of interfaces.

The numerical model demonstrates that the critical stress for confined layer slip scales as \( \ln(h')/h' \), where \( h' \) is the distance between dislocation segments that are deposited along neighboring interfaces in a layer (projected layer thickness). In cases where a pinned interfacial dislocation segment serves a source for confined layer slip, the critical stress for slip may be higher than that predicted for confined layer slip, if the interfacial pinning distance is less than the projected layer thickness. Modeling gives the same predication as theory that smaller dimension controls the process.

Several computer simulations are performed for the simple case of a multilayer with equal thickness and elastic properties of both layer types, in which an oscillating coherency stress serves as the primary source of confinement. The coherency stress in two types of layers has the same magnitude and opposite sign. When the coherency stress magnitude is greater than \( \tau_{CLS} \), dislocation propagates in both types of layers in CLS mode spontaneously. It is clear that in this spontaneous CLS case, the difference in coherency stress between layer types is greater than or equal to twice the critical stress.
required for confined layer slip ($\tau_{CLS}$). On the other hand, a threading dislocation is predicted to propagate by co-deformation as long as the difference in coherency stress between layer types is less than twice the critical stress required for confined layer slip ($\tau_{CLS}$). Corresponding simulations are in agreement with this prediction.

For the case with large lattice mismatch, the difference in coherency stress exceeds $2\tau_{CLS}$, confined layer slip deposits dislocation content along interfaces. Although this content serves to decrease the difference in average stress between layer types to equal to $2\tau_{CLS}$, the misfit content acts to pin dislocation transmission through the interfaces and preserve the confined layer slip mode and to obtain extraordinary multilayer strength.

A formalism for hardening and bulk yield under biaxial tension is developed for multilayer thin films of alternating (1) and (2) phases. This formalism is developed by numerically simulating the response of threading and interfacial dislocation loops using a Volterra dislocation model and by analyzing the energetics of depositing dislocation content at interfaces and transmitting dislocation content across interfaces. An outcome is that three regimes of slip are identified at small bi-layer thickness, where single rather than multiple or pile-up slip predominates. In Regime I, layer thickness and mismatch in stress-free lattice parameter are sufficiently small so that interfaces are coherent initially and remain so until macroyield is reached. At this critical condition, an interfacial loop bows out in a relatively equi-axed manner as to cross multiple layers, and then it expands parallel to interfaces in a confined multiple-layer slip mode. In Regime II, the layer thickness and/or lattice parameter mismatch is increased so that interfaces are semi-coherent at macroyield. Thus, a critical biaxial tension is identified at which interfacial loops bow out over multiple layers, but across interfaces that contain dislocation content.
Two subregimes are identified: one in which interfaces are coherent initially but develop content due to confined layer slip during loading (Regime IIa); the other in which interfaces are semi-coherent initially and develop further content due to confined layer slip during loading (Regime IIb).

The predictions of an analytic formalism indicate that in Regime II, the biaxial macroyield stress increases as \((\ln h)/h\), where \(h\) is individual layer thickness, with no dependence on the mismatch in stress-free lattice parameter. Further, there is substantial hardening via deposition of dislocation content at interfaces. In Regime I, the analytic results suggest that hardening is negligible, and that macroyield strength depends on lattice parameter mismatch, with a weaker \(1/h\) dependence than in Regime II.

The simulations confirm the basic trend predicted by the analytic model, but the detailed loop geometry in the simulation and the discrete interaction between interfacial content and gliding dislocation loops introduce important differences. In Regime I, a sharp plateau is observed rather than a weaker dependence on \(h\). The simulations show relatively equi-axed loop expansions across multiple layers, leading to a multiple-layer slip mode that is independent of layer thickness. In Regime II, deposition of interfacial dislocation content generates inhomogeneous stress states that can impede confined layer slip and slip transmission. However, the net effect of such deposition is to shed load to alternating compressive layers in the structure, reducing the ability of alternating stress to confine loops to individual layers. The decrease in alternating stress overwhelms any increase in confinement due to increased interfacial content so that ultimately, the multilayer yields by multiple-layer slip.
Hardness data for the Ag/Al system for bi-layer thickness ranging from 1.35 to 21.3 nm is selected to assess model predictions. The outcome is that both experimental observations and simulations predict interfaces to be coherent initially, and hardness values inferred from biaxial yield simulations agree well with experimental measurements.
CHAPTER 7

CONCLUSIONS AND FUTURE WORK

In this chapter, conclusions of this research are reported first; then, future work is described.

7.1 Summary

This work is composed of three major parts: 3D dislocation cellular automaton model development, model calibration, and model application in the study of multilayer thin film systems.

A 3D discrete dislocation cellular automaton (CA) model is developed. The discretization in this model follows the symmetry of crystal structure. Simulated systems evolve along a path of steepest decent in Gibbs free energy, where energy change includes elastic energy change due to dislocation configuration variation and work done by applied stress and microstructural stress. This model provides the raw instantaneous applied stress for each evolution step. Different averaging methods can be used to return the data to be comparable to macroscopic phenomenon. Two averaging methods are employed. One is kink pair averaging, which is on microscopic level. The other is window averaging, which is on macroscopic level.
This model is calibrated by studying nucleation of a triangle onto a straight dislocation segment, and Frank-Read source operations in different situations. This triangular patch nucleation case provides a criterion for choosing discretization size. Three types of Frank-Read operations are studied in an infinite, elastically isotropic medium. The first type of Frank-Read source is assumed to be isotropic with $\nu = 0$. The expansion is equiaxed and the critical Frank-Read stress is consistent with and converges to the analytic value for an expanding semi-hexagonal loop with decreasing triangular patch size. Second, an anisotropic line energy analysis is considered for which $\nu = 0.1$, so that line energy is a minimum for pure screw character. A non-equiaxed mode of expansion is highlighted in this case. Third, an infinitely long fixed screw dislocation is introduced into the media as an obstacle to source operation. This dislocation is in the parent plane, and is parallel to and of the same sign as the Frank-Read source. Frank-Read propagation near this dislocation obstacle is studied. The simulations show that the loop will expand by a combination of slip in the parent plane and cross slip, provided the source is sufficiently close to the obstacle or that the applied stress produces a sufficient resolved component on the cross slip system. In such cases, cross slip significantly decreases the stress to operate the source, compared to simulations where cross slip is turned off in the simulations.

Next, our 3D dislocation cellular automaton model is applied to study the mechanical properties of multilayer thin films. Dislocations propagate by choosing between a confined layer slip mode and multiple layer slip mode by transmitting through interfaces in multilayers. First, an ideal multilayer is studied, which has no elastic modulus mismatch or lattice parameter mismatch, and intransmissible interfaces. Second, lattice
parameter mismatch and interfacial misfit dislocations are introduced into multilayer systems. Threading and interfacial dislocation sources are studied. For all simulation cases, multilayer thin films are consisted of alternating two types of phases with equal thickness and elastic properties.

For the cases of ideal multilayers with no lattice parameter mismatch and intransmissible interfaces, the simulation results for threading dislocation source demonstrate that the critical stress for confined layer slip scales as \( \ln(h')/h' \), where \( h' \) is the distance between dislocation segments that are deposited along neighboring interfaces in a layer (projected layer thickness); the corresponding results for interfacial dislocation sources propose that the critical propagation stress is controlled by the smaller dimension of source length and projected layer thickness.

For the cases of multilayers with lattice parameter mismatch and transmissible interfaces, the simulations and theory suggested by simulations provide a deformation map for multilayers with varying layer thickness and lattice parameter mismatch. Two regimes of slip are identified at small bi-layer thickness, where single rather than multiple or pile-up slip predominates. In Regime I, layer thickness and mismatch in stress-free lattice parameter are sufficiently small so that interfaces are coherent initially and remain so until macroyield is reached. At this critical condition, an interfacial loop bows out in a relatively equi-axed manner as to cross multiple layers, and then it expands parallel to interfaces in a confined \textit{multiple-layer} slip mode. In Regime II, the layer thickness and/or lattice parameter mismatch is increased so that interfaces are semi-coherent at macroyield. Thus, a critical biaxial tension is identified at which interfacial loops bow out over multiple layers, but across interfaces that contain dislocation content. Two
subregimes are identified: one in which interfaces are coherent initially but develop content due to confined layer slip during loading (Regime IIa); the other in which interfaces are semi-coherent initially and develop further content due to confined layer slip during loading (Regime IIb). Theoretical models are developed to explain simulation results for both regimes. In regime I, strength is controlled by lattice parameter mismatch and initial dislocation source length. Strength increase, plateau, or decrease can be explained by the dependence on dislocation source length. In regime II, strength follows the trend of \( \frac{\ln h}{h} \). The strengthening is due to confined layer slip mode, the alternating compressive and tensile coherency stress, and the pinning effect from interfacial misfit dislocations.

Hardness data for the Ag/Al system for bi-layer thickness ranging from 1.35 to 21.3 nm is selected to assess model predictions. The outcome is that both experimental observations and simulations predict interfaces to be coherent initially, and hardness values inferred from biaxial yield simulations agree well with experimental measurements.

7.2 Assessment of the CA Model

Like all other models, this CA model has its special advantages and limitations. This section focuses on summarizing the benefits and limitations of this model.

The primary benefit to a CA approach is that complicated evolution of dislocation loops, including cross slip, can be modeled in a geometrically simple manner. Computational complexities associated with the singular interaction between Volterra dislocation segments are avoided using a discrete system. The approach has a
microstructural appeal since, in the limit of decreasing patch size, the discretization mimics the nucleation and growth of kink or jog pairs. Thus, the model lends itself to a Monte-Carlo approach for system evolution. This model also catches internal symmetry of study structure. The 3D space filling discretization permits kink and jog formation at arbitrary locations along a dislocation line, and even loop formation at arbitrary volume sites. This model can be easily adapted to study BCC structures and partial dislocations. Dislocation reactions can also be incorporated. The evolution process allows the equilibrium state for a given stress to be obtained. This model can also capture post critical events. Due to the discretization and report of local stress for each evolution step, the information allows the analysis of different length scales. This model tries to nucleate and slip a small triangular region along the whole dislocation. This provides detailed information and can be analyzed after collecting all the data. Post-processing of these data connects the results to macroscopic parameters by studying the behavior of a collection of triangles. Slipping of a single triangle may be artificial, however, this allows us to use different types of clusters in post processing.

The limitations are that a uniform 3D array of triangular patches requires that the smallest features of the analysis control the overall scale of the discretization. For example, a long straight dislocation line with a small bow out is modeled with triangles dictated by the size of the bow out. Further, slip of triangular patches produces systematic fluctuations in line length, so that smoothening via averaging over clusters of slipped triangles is necessary to mimic a continuum response. Thus, in geometries with disparate length scale and in cases where a continuum response is desired, the CA approach is not as computationally efficient as those using arbitrary grid-free motion of frontal tracking.
nodes. When there is $N$ dislocation segments and $s$ propagation steps are needed, the number of computation steps is on the order of $N^2s$. The number of computation steps can be lowered by introducing a window in total energy change calculation. This is reasonable because dislocation segments outside the window will not feel the change in the middle of the window by nucleating a new triangle, due to its dipole-like effect. With a window size of $w$, the number of computation steps becomes $Nws$. The discretization of dislocation line sense makes the model unable to study dislocations with arbitrary character.

7.3 The Nature of Hardening in Multilayer Thin Films

From this study, we know that Regime I has coherent interfaces and Regime II has semicoherent interfaces. Dislocation density increases with loading in Regime II and hardening behavior is shown in this regime. With increase of interfacial dislocation density, hardening will happen if dislocation line energy increases, and softening will happen if dislocation line energy decreases. In addition, there is hardening from local pinning.

Regime II shows hardening behavior during loading. With the assumption that initial interfaces are coherent, $\Sigma_{\text{cls}(1)}$ is initially smaller than $\Sigma_{\text{trans}(1 \rightarrow 2)}$, and dislocations propagate in a confined layer slip mode and deposit interfacial misfit dislocations. With the deposition of misfit dislocation and increase of the density $(b/S)_1$, the magnitude of coherency stress from lattice parameter mismatch is reduced. This process increases $\Sigma_{\text{cls}(1)}$ for further deformation, and decreases the barrier for dislocation transmission through the interfaces. Equations (6.4) and (6.5) include this effect from misfit
dislocations. With the increase of \((b/S)_1\), \(\Sigma_{\text{cls}(1)}\) will become equal to \(\Sigma_{\text{trans}(1\rightarrow2)}\), and the corresponding misfit dislocation density can be obtained by equating equations (6.4) and (6.5). The hardening theory proposed by equations (6.4) and (6.5) only represents the average effect of misfit dislocation arrays. However, the modeling code includes the real stress field of misfit dislocation arrays. The local pinning effect makes the transmission process harder and equation (6.5) underestimates \(\Sigma_{\text{trans}(1\rightarrow2)}\). Similarly, equation (6.4) underestimates \(\Sigma_{\text{cls}(1)}\). Therefore, simulations give higher prediction of hardening than the theory.

7.4 Implication for the Strength Plateau in Multilayer Thin Films

For the cases A1 and AA1 in Table 6.1, the difference is that they have different dislocation source length \(L\). \(L\) is 60\(\sqrt{2}\) b in case A1, and 160\(\sqrt{2}\) b in case AA1. There is a big decrease in yield stress from case A1 to AA1. The yield stress for case AA1 is almost equal to that for case A2, and the dislocation source length is also the same in cases AA1 and A2. This suggests that the strength behavior (plateau, increase, or decrease with layer thickness decrease) is due to dislocation source length. Another simulation run assumes \(L = 480\sqrt{2}\) b and the other parameters are the same as those for cases A1. The corresponding yield stress is 0.023\(\mu\), which is smaller than that for case A2; and the dislocation source length is much larger than that for case A2. From these simulation results, a proposal is made that multilayer thin film strength can increase, plateau, or decrease as layer thickness decreases in Regime I by varying dislocation source length. When dislocation source length \(L\) is approximately constant with layer
thickness, a strength plateau will be obtained in Regime I. When \( L \) decreases or increases with layer thickness decrease, strength increases or decreases accordingly.

\[
\frac{\Sigma_{\text{macro yield}}}{\mu} = \left. \frac{\Sigma_{\text{trans}(1 \rightarrow 2)}}{\mu} \right| = \frac{f_1M_1 + f_2M_2}{sM_2\mu} \left( \frac{\partial \epsilon_w}{\partial x_2} \frac{2e_h}{bw} + \frac{2e_h}{bw} \right) + \frac{f_1M_1}{\mu} \left[ \ln \frac{a_0^3}{a_1^3} \right] \quad (7.1)
\]

where \( \frac{\partial \epsilon_w}{\partial x_2} = \frac{\mu b^2}{2\pi} \left[ \kappa_{\mu} \left( -\frac{1}{2h} + \frac{2}{\pi b} \right) \right], \ w \approx L. \)

Equation (6.22) is generalized to incorporate the difference in elastic modulus to get Equation (7.1) and used to get dislocation source length for the experimental data of Regime I shown in Figure 1.1. Table 7.1 shows the lattice parameter and elastic property of components in the multilayer thin film systems studied. Hardness data are converted to yield strength using \( H = 3\Sigma_{\text{macro yield}} \) [129]. Burger’s vector is obtained from lattice parameter data.

Table 7.2 reports the bilayer period and hardness for two points in Regime I of multilayer thin films systems, and the corresponding dislocation source length given by Equation (7.1). The parameters used are \( \phi = (0^\circ, 60^\circ, 90^\circ), \ \nu = 0.3, \ s = 1/\sqrt{6}, \) and \( \rho = (0.05~0.5)b. \) When there is a strength plateau, the dislocation source length is almost constant. When strength decreases/increases in Regime I, dislocation source length increases/decreases. There are some negative predictions of source length; this may due to microstructure of materials because those systems have components with BCC structure.
<table>
<thead>
<tr>
<th>Component</th>
<th>a(nm)</th>
<th>E(GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NbN</td>
<td>0.439</td>
<td>480</td>
</tr>
<tr>
<td>TiN</td>
<td>0.424</td>
<td>590</td>
</tr>
<tr>
<td>Fe</td>
<td>0.287</td>
<td>211</td>
</tr>
<tr>
<td>Cu</td>
<td>0.362</td>
<td>130</td>
</tr>
<tr>
<td>Cr</td>
<td>0.289</td>
<td>279</td>
</tr>
<tr>
<td>Ni</td>
<td>0.352</td>
<td>200</td>
</tr>
<tr>
<td>Mo</td>
<td>0.315</td>
<td>329</td>
</tr>
<tr>
<td>W</td>
<td>0.317</td>
<td>411</td>
</tr>
<tr>
<td>Pt</td>
<td>0.392</td>
<td>168</td>
</tr>
<tr>
<td>Nb</td>
<td>0.330</td>
<td>105</td>
</tr>
<tr>
<td>Ag</td>
<td>0.409</td>
<td>83</td>
</tr>
</tbody>
</table>

Table 7.1: Lattice parameter and Yong’s modulus of components [13] of multilayers thin film systems
<table>
<thead>
<tr>
<th>Multilayer system</th>
<th>$\Lambda$(nm)</th>
<th>$H$(GPa)</th>
<th>$L/b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>e-TiN/ NbN</td>
<td>22</td>
<td>42</td>
<td>52 ~ 88</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>42</td>
<td>41 ~ 78</td>
</tr>
<tr>
<td>e-Mo/NbN</td>
<td>12</td>
<td>22</td>
<td>15 ~ 27</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>23</td>
<td>11 ~ 24</td>
</tr>
<tr>
<td>e-W/NbN</td>
<td>6</td>
<td>27</td>
<td>31 ~ 62</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>28</td>
<td>23 ~ 56</td>
</tr>
<tr>
<td>e-Cu/Ni</td>
<td>5</td>
<td>5</td>
<td>16 ~ 38</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>4</td>
<td>14 ~ 41</td>
</tr>
<tr>
<td>e-Fe/Cr</td>
<td>3</td>
<td>8</td>
<td>-65 ~ -343</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>7</td>
<td>-44 ~ -209</td>
</tr>
</tbody>
</table>

Table 7.2: Experimental bilayer period and hardness [13] in Regime I, and corresponding dislocation source length predicted from theory in Equation (7.1)
7.5 Future work

7.5.1 Computation aspect in CA model

In this 3D dislocation cellular automaton (CA) model, interaction energy between all dislocation segments is calculated to get energy change for each evolution step. This is computationally intensive. A moving window can be introduced to reduce the number of dislocation segments, which interact with the studying segment. Things need to be considered are: what size the window should be, and how to incorporate the long-range force from the dislocation segments outside the moving window.

7.5.2 Extension of this study

This research did not study dislocation pileup. To extend the study region to large layer thickness, dislocation pileup needs to be studied. This extension will make the study cover the whole range of layer thickness and provide the complete information of multilayer thin film systems.

FCC structure and perfect dislocation is the focus of this study. Other structures (BCC, HCP) and partial dislocations can be incorporated into the model in the future.

When there are misfit dislocation arrays on the interfaces, the location of dislocation sources will affect the strength. Using case A4 as an example, moving the middle of dislocation source to the position of about (0.25S, 0.5S) in the square with neighboring misfit dislocation as the sides, the critical misfit dislocation density and yield strength is 0.0015 and 0.008, compared to 0.0012 and 0.007 in case A4. This result shows that the location of dislocation source has an effect on both critical misfit dislocation density and yield strength. The case with dislocation middle at about (0.5S, 0.5S) in the square
formed by misfit dislocation arrays gives lower values than that for the case with dislocation middle at about (0.25S, 0.5S). Further study can be done to get a clearer and more comprehensive picture on the effect of dislocation source location.
BIBLIOGRAPHY


