Mechanics of dislocations in multilayered materials

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MECHANICS OF DISLOCATIONS
IN MULTILAYERED MATERIALS

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MULTILAYERED MATERIALS**

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SCHOOL OF MECHANICAL & AEROSPACE ENGINEERING

2007

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**Mechanics of Dislocations
in
Multilayered Materials**

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School of Mechanical & Aerospace Engineering

A thesis submitted to the Nanyang Technological University
in fulfilment of the requirement for the degree of
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SUMMARY

Multilayer materials have been used in many engineering systems and adapted to fulfill a variety of functions. However, defects (e.g., dislocations) are often inevitable in these systems. Since the stability and durability of multilayer materials are strongly influenced by the generation and evolution of defects, the study of defects in multilayer materials is crucially important for the performance of many engineering systems.

The current thesis research aims to conduct an in-depth investigation into the mechanics of anisotropic multilayered materials embedded with dislocations. The major components of the research are to develop (1) solutions for two-layer systems, (2) solutions for general N -layer systems, and (3) a discrete dislocation pile-up model for predicting multilayer shear strengths. The details are described below.

The image dislocation method is utilized to obtain the solutions for two-layer systems, which include infinite bi-layer systems and film-substrate systems. The infinite bi-layer systems consist of two semi-infinite layers bonded along the interface, and the film-substrate systems consist of a semi-infinite substrate layer bonded to a film layer with a free surface. The exact solutions for an infinite bi-layer problem are obtained by decomposing the problem into two homogeneous subproblems, and dislocation densities as unknowns are distributed along the interface in each subproblem to satisfy the boundary conditions. The resulting singular Cauchy integral equations are solved by the superposition of appropriate functions. The film-substrate problem is solved by distributing image dislocations on the free surface of an infinite bi-layer, where the interfacial conditions are exactly satisfied *a priori*. The singular Cauchy integral equations

are transformed into non-singular Fredholm integral equations by using certain H and I transforms, and numerical solutions are obtained via the Neumann series or Nyström method. The numerical results demonstrate the importance of elastic anisotropy, film-substrate inhomogeneity and the free surface in determining the various stress components and the image forces.

A generalized image decomposition method is developed and used to solve the problem of a general N -layer system. The N -layer problem is decomposed into N homogeneous subproblems with strategically placed image dislocations which satisfy the consistency conditions for degenerate $N-M$ ($M < N$) layer problems. All singular integrals in governing Cauchy integral equations are eliminated through H and I transforms. Numerical investigations reveal that elastic anisotropy, layer inhomogeneity, layer thicknesses, dislocation mixity and dislocation position all influence the image forces in a complex manner and the actual values of the forces can be determined only through a computational model capable of simultaneously handling all these factors.

Finally, a discrete dislocation pileup model is developed and used to predict shear strength (in yield) of three-layer systems with a free surface. Dislocations are assumed to be generated at a source at the lower interface if the threshold stress and back stress are overcome by the applied shear stress, and pile up against the upper interface. The system is considered to yield if the leading dislocation is forced to within a distance of $1b$ from the upper interface, where b is the Burgers vector magnitude. Numerical results demonstrate that the shear strength versus layer thickness predictions obey the Hall-Petch relation very well for sufficiently thick layers. If the layer thickness is less than a critical value (around 40 nm), image forces from the free surface and the lower interface result in a breakdown of the Hall-Petch relation. Furthermore, experimental data for the

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LIST OF SYMBOLS

Symbol	Definition
a	Normalized position of dislocation
a_f	Stress-free lattice dimensions of the film material
a_s	Stress-free lattice dimensions of the substrate material
$A_{\alpha k}, L_{\alpha t}$	The k – th and t – th components of normalized eigenvector
b	Burgers vector
c_{ii}, c'_{ii}	Coefficients specifying the image dislocations
C_{ij}	Material constants in the global coordinate system of $x_1 - x_2 - x_3$
C'_{ij}	Material constants in the local system of $x'_1 - x'_2 - x'_3$
C_{ijkl}	The components of the elasticity tensor
C_R	Semi-circle of radius R in the upper half of the complex plane
$\mathbf{C}$	Constant matrix
d	Distance from leading dislocation to the upper interface
D_{ij}^t	Constants specifying stress σ_{ij}
E_{ij}^t	Constants specifying displacement gradient $\frac{\partial u_i}{\partial x_1}$
F_2	Image force on the dislocation in the $x_2 -$ direction
F	Face number
h	Thickness of film
H, I	General integral transform
$\mathbf{H}(0,0)$	Hilbert transform matrix

H, I	H, I transform matrix
I	Identity matrix
J	Layer number
K	Subproblem number
K	Operating matrix
N	Number of layer
P, Q	Polynomial functions
p_α	The α – th eigenvalue
p_α^R, p_α^I	Real and imaginary parts of eigenvalue p_α
r_{ai}^t	Constant specifying $\xi_{aij}^t, \zeta_{aij}^t$
R	Radius in the upper half of the complex plane
R	P and Q rational function matrix
u_i	Displacement
x_1^o, x_2^o	Position of source dislocation
x_r, y_r	x –, y – coordinate of certain dislocation source
σ_y	Yield strength
σ_{ij}	Stress
$\delta(.)$	Dirac delta function
α	Angle of source edge dislocation oriented to the x_1 – axis
ρ	Image dislocation density
δ_{ij}	Kronecker delta
$\xi_{aij}^t, \zeta_{akl}^t$	Values specifying stress and displacement gradient in Stroh's formalism

η_{AB}	Constant specifying whether two neighboring materials are the same or not in two-layer problem
$\Psi_{ij}^{\alpha\beta}, \chi_{ij}^{\alpha\beta}$	Constants specifying stress σ_{ij} in film-substrate system
ρ_{JK}^l	Partial solutions in Layer J of Subproblem K
ρ	Image dislocation density matrix
μ	Shear modulus
γ	Material inhomogeneity parameter
θ	Angle between the c -axis and the x_1 -axis
τ^*	Critical shear stress

CHAPTER ONE

INTRODUCTION

The present thesis is to develop the mechanics of multilayer materials embedded with dislocations. This introductory chapter presents the research background and the objectives in several subsections as follows. First, Section 1.1 outlines the research background, from which the motivation of current research is explained in Section 1.2. Following that, the objectives are presented in Section 1.3 and the structure of the thesis is described in Section 1.4.

1.1 Research background

Multilayer materials are widely used and play critical roles in contemporary technologies because they often exhibit superior properties compared to bulk materials, such as higher hardness, greater resistance to corrosion and improved stability under severe conditions (e.g., Tixier et al., 1999; Verdier et al., 2001; Schweitz et al., 2001; Kim et al., 2004). However, defects such as dislocations and cracks are inevitable in these materials and they can induce a variety of undesirable effects. Consequently, the studies of defects in multilayer materials are critical from the viewpoint of material integrity and hence the performance and reliability of devices incorporating such materials.

1.1.1 The applications of multilayer materials

Multilayer materials have been used in many types of engineering systems and have been adapted to fulfill a variety of functions. They play critical roles in many contemporary technological systems, e.g., electronics, optoelectronics, protective coatings, and micro-electro-mechanical systems. The uses of multilayer materials in these systems are briefly discussed below.

Great strides in thin film technology have resulted in the rapid development of miniature, highly integrated electronic circuits. In these devices, the interfaces between materials with dissimilar electronic properties largely affect the confinement of electric charge. The performances of these systems highly depend on the materials synthesis, characterization and modeling. In fact, the need for thin materials of exceptionally high quality and reliability has driven film growth technology through a rapid succession of significant achievements.

The using of surface coating or surface treatments can substantially extend the lifetimes of components subjected to hostile environments such as high temperature, severe friction and wear. Among the technologies that rely on the use of multilayer materials in this way are internal combustion engines, artificial hip and knee implants, and computer hard disks for magnetic data storage. The use of surface coatings to protect structural materials in high temperature environments is of enormous commercial significance. For example, in gas turbine engines, thin surface films of materials chosen for their chemical inertness, stability at elevated temperatures and low thermal conductivity are used to increase engine efficiency and to extend significantly the useful lifetimes of the structural materials that they protect. Multilayer materials or continuously graded coatings offer the potential for further progress in this effort.

Multilayer materials are also main parts of many micro-electro-mechanical systems such as sensors or actuators. For example, a piezoelectric or piezoresistive thin film deposited on a silicon membrane can be used to electronically detect a deflection of the membrane, which is caused by the surface pressure, or by an acceleration of its supports. Multilayer materials can be used on instruments such as microphones in hearing aids, blood pressure monitor on exercising machines, thin film mirrors on flexible supports in sensitive optical display systems.

1.1.2 The defects in multilayer materials

The performance and reliability of multilayer devices are compromised by defects, especially dislocations and cracks. The stresses caused by defects can induce a variety of undesirable consequences in most circumstances – excessive deformation, fracture, delamination and microstructural changes in the systems. Nonetheless, such structures have been inserted into engineering systems in order to accomplish a wide range of practical service functions. The stability of both the structure and the properties of multilayer materials are strongly influenced by the generation and the evolution of dislocations and cracks.

Many related phenomena were recognized as early as in the nineteenth century. For example, an antimony film deposited on a substrate was found to be prone to crack as a result of vibration or local application of heat (Gore, 1858, 1862). Gore ascribed the bending of the deposited layers to the development of ‘unequal states of cohesive tension’ through the thickness of the deposit. The state of tension is most manifest in thin deposits, and especially in the first-formed layer. Stoney (1909) found that copper electrodeposited

as a protective layer on silver films in searchlight reflectors easily ‘peeled off’ when the thickness of the copper layer was in excess of 10 μm .

The presence of defects, such as dislocations and cracks in multilayer materials, is now well-documented (Freund and Suresh, 2003). For instance, observations of misfit dislocations in experiments have been made by high resolution transmission electron microscopy. Figure 1.1 shows an example of misfit dislocations in the $\text{Si}_{0.9}\text{Ge}_{0.1}/\text{Si}$ film-substrate system.

Fig. 1.1. A plan-view, bright-field transmission electron microscopy image of misfit dislocations within the interface between a 200 nm thick $\text{Si}_{0.9}\text{Ge}_{0.1}$ film and a much thicker (001) Si substrate. The dislocations form a crossed-grid pattern which is oriented along two $\langle 110 \rangle$ directions on the (001) interface plane (Freund, L.B. and Suresh. S., 2003).

Theoretically, the formation of misfit dislocations in heteroepitaxial film growth can be described as follows. The substrate crystal structure provides a template for positioning

the first arriving atoms of the film material. Each atomic layer of the film material serves the same function for the next layer to be formed. Figure 1.2 illustrates heteroepitaxial film growth with lattice mismatch. In general, the stress-free lattice dimensions of the film material a_f and the substrate material a_s are different. In order to maintain the film-substrate system, mismatch strain is necessary along the interface. Among the most common mechanisms of relaxation of the elastic mismatch strain in epitaxial films is the formation of misfit dislocations.

Fig. 1.2. Schematic illustration of heteroepitaxial film growth with lattice mismatch. The symbol a_f and a_s denote the stress-free lattice dimension of the film material and substrate materials in a direction parallel to the interface, respectively (Freund, L.B. and Suresh. S., 2003).

Under an applied stress, dislocations can be generated from sources located on grain boundaries or interfaces, or from sources within grains. The external stress drives the dislocations against obstacles located on the other side of the sources, such as grain boundaries or interfaces, forming a pileup. A transmission electron micrograph of a dislocation pileup against a grain boundary is shown in fig. 1.3. Observations of dislocation pileups and Orowan bowing in single crystal Cu/Ni nanolaminates have also been made via transmission electron microscopy (Foecke and vanHeerden, 1997).

Fig. 1.3. Electron-transmission micrograph of dislocation pileup at a grain boundary. The system is Cu-4.5% Al alloy (Hirth and Lothe, 1982).

Theoretically, the process of forming a pileup which causes yielding of the material may be described as follows. When the threshold stress to generate a dislocation at the source is overcome by the applied stress, the first or leading dislocation emerges. The source then suffers from a back stress produced by the first dislocation. The back stress

suppresses the generation of new dislocations. The second dislocation will emerge from the source after the threshold stress and the back stress acting on the source are both overcome by an increasing applied stress. In this manner, more dislocations can be generated after the threshold stress and the back stress produced by all the existing dislocations are overcome. Also, the largest force bears on the leading dislocation, which may eventually penetrate the obstacle, causing the material to yield. Two criteria have been used to predict such failure: (1) the force on the leading dislocation reaches the maximum repelling force from the obstacle (Pande et al., 1993), and (2) the leading dislocation moves to within a critical distance of the obstacle (Koehler, 1970).

1.2 Motivation

Since dislocations are ubiquitous in multilayer materials, their investigation is of critical importance for the fundamental understanding of strain relaxation, damage, yielding and other properties of thin solid film materials, all of which affect systems functionality and reliability. With the increasing trend to miniaturize devices and to employ them in severe environments or critical systems, it becomes an urgent task to understand the fundamental mechanisms leading to material deterioration and to develop a methodology for analyzing multiple dislocations in multilayer materials. Furthermore, a crack in an elastic solid can be considered as distributed dislocations on the crack plane. The mechanics of dislocations in multilayered composites can thus be usefully employed to investigate the problem of cracks in such materials.

Many previous studies have investigated dislocations in homogeneous media, e.g., straight dislocations in infinite, continuous, isotropic media (Hirth and Lothe, 1982; Mura,

1987), and dislocations in isotropic and anisotropic half spaces (Head, 1953; Dundurs and Sendeckyj, 1965; Barnett and Lothe, 1974). For infinite bimetals, researchers have similarly made significant contributions, e.g., dislocations in isotropic and anisotropic bimetals (Head, 1953; Weertman, 1996; Suo, 1990; Ting, 1992, 1996; Wu, et al., 2003). Also, screw dislocations in the periodic *B-A-B* type of multilayer systems have been studied (Chou, 1966; Koehler, 1970; Kamat et al., 1987). However, the problem of dislocations in general multilayer systems is the most difficult and relatively fewer researchers have investigated this topic. Some recent investigations include mixed dislocations (with both edge and screw components) in trilayers (Choi and Earmme, 2002, 2003) and dislocations in general anisotropic multilayer systems (Alshits and Kirchner, 1995a, b). However, although theoretical solutions can be obtained in principle for general multilayered solids it is difficult to obtain actual numerical results, as pointed out by Alshits and Kirchner (1995a, b).

To summarize, the study of dislocations in homogeneous and infinite bimaterial solids is well-developed. In contrast, the problem of general anisotropic multilayer systems with free surfaces, dissimilar layer thicknesses and arbitrarily located mixed dislocations can be further investigated, since comparatively fewer solution methodologies have appeared in the literature and numerical results for such complex multilayer systems may be difficult to obtain using existing methods. The development of an efficient method for analyzing dislocations in general multilayer systems is of great relevance for contemporary thin film technologies since devices often contain films of more than two layers.

1.3 Objectives

The proposed research aims to conduct an in-depth investigation into the elastic mechanics of two-dimensional multilayer systems embedded with dislocations, which are infinitely long and straight under the plane strain condition. The dislocations are of the general mixed type and can be located anywhere in the system, which may be finite, semi-infinite or infinite in extent. The various layers can be of various thicknesses. The solution methodology will be based on a further development of the image method, i.e., the consistent use of image dislocations (or virtual dislocations) to satisfy all the boundary conditions of the problem.

The specific objectives are to:

- 1) Establish the elastic solutions for a pure edge and a pure screw dislocation in a two-layer system, i.e., an infinite bimaterial and a semi-infinite film-substrate. The stress field caused by the dislocation and the dependence of the image force on the dislocation will be investigated;
- 2) Develop an efficient image method for solving the problem of a general N -layer system embedded a mixed dislocation. The dependence of the image force on dislocation position, layer thickness, dislocation mixity, and material anisotropy will be studied;
- 3) Apply the developed method to the study of discrete dislocation pileups in multilayered systems, including nanolayered composites. The prediction of the yield stress will be attempted, and its dependence on the size (thickness) will be investigated. The predicted results will be compared to previous theoretical and experimental results for metallic multilayer materials.

The current work generalizes the image decomposition technique for solving general N -layer systems embedded with mixed dislocations. The method satisfies the consistency requirement when N -layer systems, with $N-M$ materially identical neighboring layers, reduce to M -layer systems ($M < N$). Solution accuracy and efficiency are improved by removing all singular terms in the governing equations. Two-layer systems are first investigated as special cases to test the workability of the generalized image method. The study is then extended to N -layer systems. As an important application, the shear strengths of anisotropic multilayer systems are investigated via a discrete dislocation pile-up model. It is shown that the Hall-Petch relation and its deviation are successfully simulated with the pile-up model alone, whereas most previous works explain the deviation from Hall-Petch relation by a combination of physical mechanisms.

1.4 The structure of this thesis

This thesis is organized as follows.

Chapter 1 (the current chapter) introduces the research background, motivation, and research objectives.

Chapter 2 contains the literature review, including the concept of a dislocation and related previous research on dislocations. Following that, the differences between the proposed research and previous works are discussed.

Chapter 3 presents the mathematical preliminaries, which are crucial for both the formulation and solution of the governing integral equations to be developed.

Chapter 4 covers in detail the problems of a pure edge and a pure screw dislocation in anisotropic two-layer systems, including bimaterials, film-substrates and strips. The effect

of elastic anisotropy, inhomogeneity and the free surface on the stress components and the image forces is studied in this chapter.

Chapter 5 presents the solutions of mixed dislocations in general N -layer systems. A new image decomposition method is developed; the key features being the decomposition of an N -layer system into N homogeneous systems with predetermined partial image solutions, and the removal of all singular kernels in the governing integral equations.

Chapter 6 studies the yield stress of multilayer systems by employing the discrete dislocation pileup model. This is achieved by using a simple failure criterion and the solution methodology for discrete dislocations developed in Chapter 5.

Finally, Chapter 7 summarizes the major findings of this thesis and presents some recommendations for future research.

CHAPTER TWO

LITERATURE REVIEW

This chapter is organized as follows. Section 2.1 briefly introduces the concept of dislocations. Section 2.2 reviews the previous research on discrete straight dislocations in multilayer materials. Following that, works on the pileup of dislocations in multilayer systems are reviewed in Section 2.3. Finally, Section 2.4 provides an overview of the reviewed literature, highlights the advances that can be gained in further work, and presents the scope of the proposed research.

2.1 Introduction of dislocations

Volterra and other researchers investigated the elastic behavior of homogeneous, isotropic media containing line defects by using the model of cylinder deformation, as shown in fig. 2.1. The original cylinder fig. 2.1 (a) is imagined to be cut along a line parallel to the cylinder axis. If the deformation operations are to slip the faces of the cut with respect to each other, the resulting configurations are dislocations. They are edge dislocations if the slips are perpendicular to the cylinder axis (figs. 2.1 (b) and (c)) and screw dislocation if the slip is parallel to it (fig. 2.1 (d)). The rotation operations result in disclinations (figs. 2.1 (e) and (f)), which are not considered in this thesis.

Fig. 2.1. The illustration of the physical basis of Volterra dislocations. (a) The original cylinder; (b) and (c) edge dislocation; (d) screw dislocation; (e), (f), and (g) disclinations. (Hirth and Lothe, 1982).

The above represents the continuum viewpoint of dislocations. In crystals, dislocations are line defects of the lattices. The Burgers vector of such a line defect is defined using a Burgers circuit which encloses the line. In a perfect crystal with no dislocation, the Burgers vector is zero. In a dislocated solid, the Burgers vector is the displacement vector necessary to close the Burgers circuit. In general, the Burgers vector

is at an angle to the dislocation line, which is then said to be mixed. If the Burgers vector is parallel to the line, the dislocation is pure screw in character; if perpendicular to it, it is pure edge. These are illustrated in fig. 2.2. In this thesis, straight dislocations (which may be pure edge, pure screw or mixed) with infinitely long lines in the third direction (perpendicular to the plane of view) are studied under the plain strain condition.

Fig. 2.2. A dislocation defect in a crystal lattice, showing Burgers vectors parallel, at an angle, and perpendicular to the line direction. Burgers circuits around the pure screw and pure edge dislocation lines are also shown.

2.2 Previous research on dislocations

Generally speaking, the problems can be categorized into three types: dislocations in homogeneous systems, dislocations in two-layer systems, including infinite bimetals and semi-infinite film-substrate systems, and dislocations in general N -layer systems.

2.2.1 Dislocations in homogeneous systems

Investigation of the elasticity of dislocations in homogeneous materials has a long history. The stress and displacement fields, the dislocation line energy and the image forces have all been derived and investigated in detail. The classic books of Hirth and Lothe (1982) and Mura (1982) provide an excellent summary. The review here focuses on dislocations in infinite homogeneous media, half spaces, plates and strips.

Eshelby et al. (1953) used anisotropic elastic theory to study the three-dimensional state of stress caused by a single dislocation, in which the stress does not vary with one of the Cartesian coordinates. By assuming a displacement vector that satisfies the compatibility equations, the equilibrium equations become a set of second order differential equations. On the other hand, Lekhnitskii (1957) assumed the existence of a stress function which satisfies the equilibrium equations. The compatibility equations then assume the form of second order differential equations. Combining these two strategies, Stroh (1958) proposed a mixed formalism (now called the Stroh formalism) in which a stress function vector and a displacement vector satisfy the equilibrium equations and compatibility equations respectively. Hooke's law then turns into a set of first order differential equations.

A half space is a semi-infinite medium with a surface, where it is usually taken to be traction free. Head (1953) derived an expression for the image force on a screw

dislocation in an isotropic half space. Image forces on dislocations arise as a result of boundaries and surfaces. Subsequently, Dundurs and Sendeckyj (1965) obtained image force expressions for an edge dislocation in an isotropic half space. Almost a decade later, Barnett and Lothe (1974) studied a dislocation near the free surface in an anisotropic half space. The effect of elastic anisotropy was thus considered, and the solutions for a mixed dislocation in an anisotropic half space were obtained. Later, many solutions for singularities and cracks in anisotropic half-spaces were given in Kirchner and Lothe (1987) and Ting (1992, 1996). More recently, Pan et al. (1997) obtained the Green's function for a homogeneous, generally anisotropic half space.

Dislocations in homogeneous plates and strips have also received attention. Nabarro and Kostlan (1978) studied the stress field of a dislocation lying in an infinite isotropic plate. Specifically, the stress field of an edge dislocation lying in the mid-plane of the plate with two free surfaces was calculated. Later, the problem of an edge dislocation in an infinite isotropic strip was studied by Wu and Chiu (1995). The Stroh formalism and Fourier transforms were used to obtain the elastic field.

2.2.2 Dislocations in two-layer systems

An infinite bimaterial is made up of two different materials joined along an interface. The boundary conditions across the interface need to be satisfied. A film-substrate is a bimaterial system with a finite film thickness. It has an interface and a free surface (if the substrate is semi-infinite in the thickness direction) or two free surfaces (if the substrate is finite). Traction free conditions need to be satisfied in addition to the interface conditions. Because of the boundaries (interfaces and surfaces) and the inhomogeneity arising from

the bonding of dissimilar materials, the problem of dislocations is naturally more difficult in bimaterial and film-substrate systems than in homogeneous solids.

Attempts on the solutions for bimaterials have been made first for isotropic media and later for anisotropic media. Head (1953) derived the stresses for an edge dislocation in an isotropic bimaterial by reducing the original problem into two potential type problems. Miller (1989) derived certain jump potentials for edge dislocations in anisotropic bimaterials. Suo (1990) investigated the problems of dislocations and other singularities in anisotropic bimaterials by using the method of analytic continuation. The dislocation in bimaterial systems was also studied in the work of Kirchner and Lothe (1987) and Ting (1992, 1996). Weertman (1996) summarized the use of the image method to solve the problem of a dislocation in isotropic bimaterials. On the related problem of disclinations, Wu (2000) constructed exact continuously distributed image solutions for a wedge disclination dipole in hexagonal bimaterials. Subsequently, Wu (2002) found the stress and strain energy of interfacial wedge disclination dipoles in transversely isotropic bicrystals with special c -axis orientations, and Wu et al. (2003) obtained the closed-form solutions for interfacial dislocations in dissimilar anisotropic bimaterials.

In the investigation of anisotropic film-substrates, Abbudi (1990) reduced the dislocation problem to a traction type problem, which in turn was solved by a Fourier expansion method. The results were expressed as Fourier integrals. More recently, Choi and Earmme (2002) studied anisotropic film-substrate systems using the alternating method, in which the boundary conditions on the various interfaces/surfaces are alternately, but not concurrently, satisfied.

All the problems above are considered to have perfect interfaces. The problems of an imperfect interface have also been considered by some researchers. For example, the

problems of screw and edge dislocations interacting with a slightly wavy interface in a bimaterial have been investigated by Fan and Xiao (1996) and Xiao et al. (2002), respectively. Xiao et al. (2001) further studied the problem of an edge dislocation interacting with a wedge-shaped bimaterial interface, and Fan and Wang (2003) studied the screw dislocation interacting with an imperfect interface, where the displacement across the interface suffers from a jump.

2.2.3 Dislocations in general N -layer systems

Multilayer systems with alternating layers have been studied since the 1960s. Based on isotropic theory, Chou (1966) presented the elastic solution for a screw dislocation in a B - A - B multilayer system consisting of a B layer bounded by two semi-infinite A layers. Koehler (1970) investigated the problem of a screw dislocation in a multilayer system comprising alternate isotropic A and B layers. Kamat et al. (1987) further investigated the N -layer system consisting of alternate isotropic A and B layers with equal layer thickness for N up to 5. They found that an infinite number of images are required for $N > 2$, and the images can be interpreted as reflections and transmissions at the interfaces. Gosling et al. (1993) investigated dislocation formation in a strained layer sandwiched between two unstrained layers. Their calculations were also based on isotropic theory, but material inhomogeneity was not taken into account explicitly. Hence, the multilayer system studies reviewed here essentially deal with one or in two isotropic layers.

The problem of dislocations in the general anisotropic multilayer system is rather complicated, and few researchers have investigated it. Alshits and Kirchner (1995a, b) obtained solutions for singular sources in a multilayer system by combining Stroh's method and the Fourier transform technique. This requires the inversion of the transform.

Choi and Earmme (2002, 2003) studied an anisotropic trimaterial (consisting of three layers A , B and C with different thicknesses and elastic constants) using the method of analytic continuation and the Schwarz-Neumann alternating technique. The solution is expressed in terms of infinite series for the analytic functions from which the elastic field can be derived. Also, Han and Ghoniem (2002) investigated dislocation loops in anisotropic multilayer systems by using Stroh's method and the Fourier transform technique. This requires inverse Fourier transforms to obtain the physical solutions, with the consequence that intensive computations are often needed.

2.3 Previous research on dislocation pileups in general multilayer systems

The literature review thus far focuses on the elastic solutions for a single dislocation. Dislocations, however, often occur in groups, e.g., dipoles, quadrupoles and arrays. Of particular interest is the pileup of a number of dislocations, which has been accepted as a possible explanation for the size effect of the yield strength or hardness of materials. As a matter of fact, a very large number of experiments to determine the hardness or yield strength in homogenous and multilayer materials have been carried out (e.g., Hall (1951), Petch (1953), Ju (1996), and Misra, et al. (2005)). It was found that the hardness or yield strength increases with the inverse square root of the structural size (grain size or layer thickness) for sizes larger than about 100 nm (the Hall-Petch relation). Deviations from this relation occur for sizes less than about 100 nm and an inverse relation may exist for sizes less than about 20 nm. Several models have been used to explain the Hall-Petch relation, the deviations from it, and the inverse relation. The first is the dislocation pileup model in which dislocations are generated from sources within the material and pileup against an obstacle or an interface. This gives rise to the classical Hall-Petch relation.

Various types of pileup configurations for both continuously distributed and discrete dislocations have been considered, see for instance the monograph of Hirth and Lothe (1982). The second is the Koehler model. Koehler (1970) investigated the problem of a dislocation in an isotropic multilayer consisting of alternating materials. The dislocation located in the softer layer needs to overcome the repulsive image force from the interface. The third is the Orowan model by Embury and Hirth (1994) and Nix (1997). They studied systems with layer thicknesses in the tens of nanometers, with only one dislocation lying in the softer layer. During deformation, the dislocation is bowed between the layers, and the dislocation loop interacts with the dislocations deposited along the interfaces. Some refinements were made by Misra et al. (2005) by including details such as the cores of the deposited interface dislocations, interface stresses, and dislocation interactions. The fourth is the coherency stress model by Shinn et al. (1992) and Rao and Hazzledine (2000). In the system of very thin lattice matched multilayers, there exist large in-plane coherency stresses which alternate from tension to compression between layers. These alternating stresses offer a periodic resistance to dislocation motion across interfaces. The latter three models may explain the deviations from the classical relation.

In the next section, the literature on dislocation pileup is reviewed as it pertains to the present study. The considered problems are categorized into three types: dislocation pileup in homogeneous systems, two-layer systems, and general multilayer systems. This categorization is based on the theoretical idealization that the materials under study can be considered as homogeneous, two-layer and multilayer.

2.3.1 Dislocation pileup in homogeneous systems

It is known that the grain boundaries behave like barriers to dislocations. Dislocations pile up along their glide plane and experience repulsion near the grain boundary until the stress concentrated at the head of the pileup causes yielding. Based on many experiments, Hall (1951) and Petch (1953) proposed the relation $\sigma_y \propto d^{-1/2}$, where σ_y denotes the yield strength and d the grain size. Further theoretical investigations were carried out in the 1990s. Pande et al. (1993) studied the effect of a small number of single-ended dislocations. The single-ended model refers to a pileup at one end with the dislocation source at the other end, whereas the double-ended model admits pileup at both ends with the source in between. Applying the single-ended pileup model, Sun (1997) investigated fully lamellar microstructures and found that the yield stress is increased by decreasing the lamellar thickness, and obeys the Hall-Petch relation if thickness is larger than a certain value. Subsequently, the Hall-Petch relation was modified by Friedman and Chrzan (1998). Different sources of dislocations, i.e. single-ended or double-ended dislocation pileup were studied. In particular, threshold stress for dislocation generation was considered for the calculations. Also, results obtained by using discrete and continuum pileup models were compared. At the same time, many experiments were carried out; for instance Nieh and Wadsworth (1991) found that the Hall-Petch relation is obeyed for nanocrystalline materials with grain sizes over a critical value. However, a breakdown of the relation or even an inverse relation has also been observed. Chokshi et al. (1989) studied the variation of hardness with grain size in nanocrystalline copper (Cu) and palladium (Pd) and showed that there is a decrease of hardness with a decrease in grain size.

2.3.2 Dislocation pileup in two-layer systems

As the simplest model for dislocation pileup in general multilayer systems, bilayer systems have attracted considerable attention. Armstrong and Head (1965) studied dislocation pileup against the interface in an anisotropic bimaterial under an applied shear stress. Yielding was considered to occur when the distance between the locked dislocation and the preceding one was less than one Burgers vector. Based on this model, Pande et al. (1993) investigated the effect of elastic anisotropy in bimaterial systems. It was found that the grain size exponent varies from 0 to 1 depending on the anisotropy. In order to apply the Hall-Petch relation for homogeneous materials to lamellar systems, Friedman and Chrzan (1998) proposed the scaling theory for isotropic bimaterial systems. It is based on the assumption that the yielding caused by dislocation pileup is local to the head of pileup. If the total stress on the leading dislocation overcomes the pinning stress, the system yields. Four parameters are employed: the pileup length, the exponent characterizing the divergence of the dislocation density at the interface, a critical distance between the leading dislocation and the interface, and the pinning stress at the interface. Recently, Friedman (2004) developed the generalized the Hall-Petch relation for bimaterial systems, assuming that the source activation stress is zero.

2.3.3 Dislocation pileup in general multilayer systems

Lehoczky (1978) investigated thin-layer metal laminates based on isotropic theory, and established that strength enhancement was caused by repulsive dislocation image forces. Chu and Barnett (1994) used a model of dislocation glide across layers to explain superlattice hardening. The stress for dislocation gliding across layers was calculated by considering the core effects and all interfaces in trapezoidal or sawtooth composition

modulations. The theoretical results coincided quite well with experimental data. Anderson and Li (1995) investigated the infinite isotropic three-layer *A-B-A* system by using the double-ended pileup model. They predicted the critical shear stress necessary to produce slip transmission across the interface. Was and Foecke (1996) reviewed the deformation and fracture in microlaminates. The deviation from Hall-Petch relation could occur if the layer was thin enough to contain only one or two dislocations. Misra and Kung (2001) used dislocation based models to explain the various deformation mechanisms in metallic multilayers with alternating materials. From the micro- to the nano-scale, the deformation mechanism changes from dislocation pileup to Orowan bowing of single dislocations. Also, Phillips (2003) used the confined thread dislocation model to study the deformation behavior of Al/Al₃Sc metallic multilayers, and Friedman (2004) studied the generalized Hall-Petch relation for a multilayer based on the solutions for homogeneous materials and bi-layer systems. Zhang et al. (2004) used the nanoscale twinning model to explain the enhanced hardening in Cu/330 stainless steel multilayers. Misra et al. (1998, 2002, 2005) investigated the breakdown of the Hall-Petch relation by employing different deformation mechanisms for different layer thicknesses. If the layer was sufficiently thick, the Hall-Petch relation was obeyed well. For thicknesses of a few nanometers, the confined layer slip of single dislocation loops was used to explain the increase of strength with decrease of thickness. If the layer thickness was reduced to about 1 nm, interface cutting was considered to be the dominant mechanism. Also, Li and Anderson (2005) investigated the multilayer system of alternating materials using a three-dimensional dislocation cellular automation model, and found that if the layer thickness was small enough the dislocation loops could not be confined to individual layers. The

strength of the system was mainly dependent on the internal dislocation source length rather than the layer thickness.

2.4 Overview, further advances and proposed work

2.4.1 Overview and further advances

On the basis of previous contributions, further advances in the mechanics of defects in inhomogeneous multilayer materials can be made. First, more complex and yet application-relevant problems should be addressed. In particular, the problem of defects in finite anisotropic multilayer materials requires urgent attention because many engineering devices such as actuators are finite in dimensions and typically consist of more than three layers of dissimilar anisotropic materials. Previous works have largely focused on infinite isotropic multilayered systems. Indeed, there is an increasing trend to miniaturize engineering devices and to employ newly developed materials in the device construction. The influence of defects on both the short- and long-term behavior of innovative structural-material configurations is often unknown, but the issue must be addressed if the new devices are to be successfully commercialized. For these reasons, advances in the analysis of finite anisotropic multilayered solids are critical for the new generation of devices incorporating multilayers. The semi-infinite dissimilar anisotropic film-substrate system, which consists of a free surface and a bimaterial interface, is a two-layered system. Investigation of the film-substrate is an important first step towards the future investigation of multilayered solids. Examples of film-substrate systems abound: ceramic coating on gears and bearings to reduce wear, paint film on steel plates to reduce corrosion, and piezoelectric film on metal electrodes. For the general N -layer systems, the many boundary conditions of the free surfaces and interfaces increase the difficulty in

solving the problems. Up to now, very few works have been done and even lesser numerical results have been obtained in this area.

In the previous studies on the relation between yield strength and grain size or layer thickness, homogeneous, bi-layer, tri-layer, and N -layer systems have been considered. However, screw dislocation pileup was mostly studied and edge dislocation pileup was rarely studied because of the additional complexity. Also, many studies were based on the isotropic theory. For inhomogeneous and anisotropic systems, such as ceramic-metal, metal-intermetallic, ceramic-ceramic systems, the error introduced by the homogeneous and isotropic simplification is uncertain. For the general N -layer system, the common approach is to consider alternating layer materials of equal thickness. Scaling theory for the N -layer system requires an exact solution for the pileup density, which is usually very difficult to obtain. To avoid this, scaling function in homogeneous media has been adopted as solution. Consequently, it is useful to develop an efficient methodology for directly solving the general case of an N -layer system with arbitrary layer thicknesses and elastic anisotropies, dislocations of various degree of mixity, and multiple boundaries including free surfaces (the solid is thus not infinite in all three directions).

Further advances may also be made in the solution methodology. Currently, at least three methods have been employed to solve the problems of dislocations in film-substrate systems and three-layer systems: Fourier transform method, alternating technique and image method. For instance, Zhang (1995) investigated the effect of elastic constants on the critical thickness of film-substrate systems using superposition and Fourier transformation. Alshits and Kirchner (1995a, b) studied multilayered materials by using Stroh's formalism (Stroh, 1958) in conjunction with the Fourier transform technique. In order to obtain the numerical results, inverse transforms should be calculated. To date,

such numerical results have not been obtained. Choi and Earmme (2001) used the alternating technique to study the infinite three-layer A - B - C system. For the general N -layer systems with or without free surfaces, the efficiency and accuracy of the alternating technique are not known. Huang and Kardomateas (2001) studied dislocation in a bimaterial with a free surface. A stress potential function was chosen to satisfy the interfacial conditions, and a dislocation array was distributed along the traction free boundary.

In this thesis, we employ and further develop the image dislocation method to study two-layer, three-layer, and general N -layer systems. The related contents will be presented in the next. Efficient and accurate methods of solving integral equations are also developed in the course of the investigation.

Finally, a detailed investigation into image forces on dislocations and the stress field will contribute significantly to the understanding of defects in multilayer materials. Parametric studies on the influence of various parameters such as layer thicknesses, layer inhomogeneity, material anisotropy and dislocation position are also lacking. As mentioned above, although the problems of dislocations in multilayered solids have been attempted, the solutions are often very complicated and numerical results are very difficult to obtain and thus very few parametric studies have been carried out.

2.4.2 Proposed work

In light of the above discussion, the objective of this thesis is to make further progress in the three aspects identified: problems of increasing complexity, improved solution techniques and parametric studies. The specific tasks are to:

- 1) Establish the solutions for edge and screw dislocations in the film-substrate (two-layer) systems;
- 2) Develop solutions for mixed dislocations in general anisotropic multilayered (N -layer) composites and conduct parametric studies;
- 3) Investigate discrete dislocation pileups in anisotropic three-layer systems and predict the yield strength of composites.

CHAPTER THREE

MATHEMATICAL PRELIMINARIES

In this chapter, certain integral transforms are developed. The equations to manipulate these transforms are critical elements in both the formulation and the solution. The organization of the chapter is as follows: the general H and I transforms are introduced in Section 3.1, and the proof of these equations is illustrated by an example in Section 3.2.

3.1 Integral transforms with rational kernels: the general H and I transforms

The stress components of a mixed dislocation with edge and screw components in an anisotropic homogeneous solid can be written in the form of a rational function of first-order to second-order polynomials, as shown in Wu et al. (2003). The rational function is of two types, designated as functions of P and Q :

$$P(x - x_r, a(y - y_r), b(y - y_r)) = \frac{x - x_r + a(y - y_r)}{[x - x_r + a(y - y_r)]^2 + [b(y - y_r)]^2}, \quad (3.1)$$

$$Q(x - x_r, a(y - y_r), b(y - y_r)) = \frac{b(y - y_r)}{[x - x_r + a(y - y_r)]^2 + [b(y - y_r)]^2}, \quad (3.2)$$

where x, y denote the rectangular coordinates of the destination point of interest, x_r, y_r the position of a certain dislocation source, and a, b some material parameters. The limits of P and Q as $y \rightarrow y_r$ can be deduced by first noting the results of integrating Eqs. (3.1) and (3.2):

$$\int_{-\infty}^{\infty} P(x - x_r, a(y - y_r), b(y - y_r)) dx_r = 0, \quad (3.3)$$

$$\int_{-\infty}^{\infty} Q(x - x_r, a(y - y_r), b(y - y_r)) dx_r = \pi \operatorname{sgn}(b(y - y_r)), \quad (3.4)$$

where $\operatorname{sgn}(\cdot)$ is the signum function. By insisting that

$$\lim_{y \rightarrow y_r} \int_{-\infty}^{\infty} P(x - x_r, a(y - y_r), b(y - y_r)) dx_r = \int_{-\infty}^{\infty} \lim_{y \rightarrow y_r} P(x - x_r, a(y - y_r), b(y - y_r)) dx_r, \quad (3.5)$$

$$\lim_{y \rightarrow y_r} \int_{-\infty}^{\infty} Q(x - x_r, a(y - y_r), b(y - y_r)) dx_r = \int_{-\infty}^{\infty} \lim_{y \rightarrow y_r} Q(x - x_r, a(y - y_r), b(y - y_r)) dx_r, \quad (3.6)$$

it can be deduced that:

$$\lim_{y \rightarrow y_r} P(x - x_r, a(y - y_r), b(y - y_r)) = P(x - x_r, 0, 0) = \frac{1}{x - x_r}, \quad (3.7)$$

$$\lim_{y \rightarrow y_r} Q(x - x_r, a(y - y_r), b(y - y_r)) = Q(x - x_r, 0, 0) = \pi \operatorname{sgn}(b(y - y_r)) \delta(x - x_r), \quad (3.8)$$

where $\delta(\cdot)$ is the Dirac delta function and Eq. (3.8) is independent of $a(y - y_r)$ and $b(y - y_r)$, except for the sign of the latter.

As shown subsequently, it is necessary to consider integrals of the form:

$$H(a(y - y_r), b(y - y_r))[\rho(x)] = \frac{1}{\pi} \int_{-\infty}^{\infty} P(x - x_r, a(y - y_r), b(y - y_r)) \cdot \rho(x_r) dx_r, \quad (3.9)$$

$$I(a(y - y_r), b(y - y_r))[\rho(x)] = \frac{1}{\pi} \int_{-\infty}^{\infty} Q(x - x_r, a(y - y_r), b(y - y_r)) \cdot \rho(x_r) dx_r, \quad (3.10)$$

where $\rho(x)$ is an image dislocation density function and the integrals represent the integral transforms H and I of ρ with the rational kernels P and Q .

Important special cases are now presented. If $y \rightarrow y_r$, then by Eqs. (3.7) and (3.9):

$$H(0, 0)[\rho(x)] = \frac{1}{\pi} \int_{-\infty}^{\infty} P(x - x_r, 0, 0) \rho(x_r) dx_r = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\rho(x_r)}{x - x_r} dx_r \quad (3.11)$$

yields the classical Hilbert transform, and by Eqs. (3.8) and (3.10):

$$\begin{aligned} I(0, 0)[\rho(x)] &= \frac{1}{\pi} \int_{-\infty}^{\infty} Q(x - x_r, 0, 0) \rho(x_r) dx_r \\ &= \frac{1}{\pi} \int_{-\infty}^{\infty} \pi \operatorname{sgn}(b(y - y_r)) \delta(x - x_r) \rho(x_r) dx_r = \operatorname{sgn}(b(y - y_r)) \rho(x), \end{aligned} \quad (3.12)$$

which establishes that $I(0, 0)$ is an identity transform with the Dirac delta as the kernel.

Thus, the H and I transforms include the Hilbert and identity transforms as special cases.

Note however that in the general I transform does not leave the operand $\rho(x)$ invariant.

The following iterative properties of the H and I transforms, which are crucial to the formulation and solution, can be proved, i.e.:

$$\begin{aligned} & H(a(y_1 - y_r), b(y_1 - y_r)) \cdot H(\alpha(y_2 - y_s), \beta(y_2 - y_s)) \\ &= -I(a(y_1 - y_r) + \alpha(y_2 - y_s), |b(y_1 - y_r)| + |\beta(y_2 - y_s)|), \end{aligned} \quad (3.13)$$

$$\begin{aligned} & H(a(y_1 - y_r), b(y_1 - y_r)) \cdot I(\alpha(y_2 - y_s), \beta(y_2 - y_s)) \\ &= \text{sgn}(\beta(y_2 - y_s)) \cdot H(a(y_1 - y_r) + \alpha(y_2 - y_s), |b(y_1 - y_r)| + |\beta(y_2 - y_s)|), \end{aligned} \quad (3.14)$$

$$\begin{aligned} & I(a(y_1 - y_r), b(y_1 - y_r)) \cdot H(\alpha(y_2 - y_s), \beta(y_2 - y_s)) \\ &= \text{sgn}(b(y_1 - y_r)) \cdot H(a(y_1 - y_r) + \alpha(y_2 - y_s), |b(y_1 - y_r)| + |\beta(y_2 - y_s)|), \end{aligned} \quad (3.15)$$

$$\begin{aligned} & I(a(y_1 - y_r), b(y_1 - y_r)) \cdot I(\alpha(y_2 - y_s), \beta(y_2 - y_s)) \\ &= \text{sgn}(b(y_1 - y_r)) \cdot \text{sgn}(\beta(y_2 - y_s)) \cdot I(a(y_1 - y_r) + \alpha(y_2 - y_s), |b(y_1 - y_r)| + |\beta(y_2 - y_s)|), \end{aligned} \quad (3.16)$$

where y_1, y_2 denote the y -coordinates of different destination points, y_r, y_s those of different source points, and α, β material parameters which may be different from a, b . These integrals, which appear in the explicit evaluation of the iterative transforms, are important in identifying the kernels of integral equations to be developed later. As an

example, a proof is conducted in Section 3.2. The iterative transforms of Eqs. (3.13)-(3.16) essentially state that H operating on H (in general with different arguments) equals $-I$, H operating on I or vice versa equals H , and I on I equals I . In all cases, the result must be multiplied by the signum function of the second argument of any I on the left-hand side of the equation. Most importantly, the first argument of the result equals the sum of the first arguments in the two operating transforms, while the second argument of the result equals the sum of the absolute values of the second arguments. The iterative transforms are communicative. This is easily verified in the case of Eq. (3.13) or Eq. (3.16) since the result is determined by the simple addition of the respective arguments and addition is communicative. Equations (3.14) and (3.15) together also prove that each is communicative.

The H and I transforms on the rational functions P and Q can be formalized as follows:

$$\begin{aligned} & H(a(y_1 - y_r), b(y_1 - y_r)) [P(x - x_s, \alpha(y_2 - y_s), \beta(y_2 - y_s))] \\ &= \frac{1}{\pi} \int_{-\infty}^{\infty} P(x - x_r, a(y_1 - y_r), b(y_1 - y_r)) \cdot P(x_r - x_s, \alpha(y_2 - y_s), \beta(y_2 - y_s)) dx_r \quad (3.17) \\ &= -Q(x - x_s, a(y_1 - y_r) + \alpha(y_2 - y_s), |b(y_1 - y_r)| + |\beta(y_2 - y_s)|), \end{aligned}$$

$$\begin{aligned} & H(a(y_1 - y_r), b(y_1 - y_r)) [Q(x - x_s, \alpha(y_2 - y_s), \beta(y_2 - y_s))] \\ &= \frac{1}{\pi} \int_{-\infty}^{\infty} P(x - x_r, a(y_1 - y_r), b(y_1 - y_r)) \cdot Q(x_r - x_s, \alpha(y_2 - y_s), \beta(y_2 - y_s)) dx_r \quad (3.18) \\ &= \text{sgn}(\beta(y_2 - y_s)) \cdot P(x - x_s, a(y_1 - y_r) + \alpha(y_2 - y_s), |b(y_1 - y_r)| + |\beta(y_2 - y_s)|), \end{aligned}$$

$$\begin{aligned}
& I(a(y_1 - y_r), b(y_1 - y_r)) \left[P(x - x_s, \alpha(y_2 - y_s), \beta(y_2 - y_s)) \right] \\
&= \frac{1}{\pi} \int_{-\infty}^{\infty} Q(x - x_r, a(y_1 - y_r), b(y_1 - y_r)) \cdot P(x_r - x_s, \alpha(y_2 - y_s), \beta(y_2 - y_s)) dx_r \quad (3.19) \\
&= \operatorname{sgn}(b(y_1 - y_r)) \cdot P(x - x_s, a(y_1 - y_r) + \alpha(y_2 - y_s), |b(y_1 - y_r)| + |\beta(y_2 - y_s)|),
\end{aligned}$$

$$\begin{aligned}
& I(a(y_1 - y_r), b(y_1 - y_r)) \left[Q(x - x_s, \alpha(y_2 - y_s), \beta(y_2 - y_s)) \right] \\
&= \frac{1}{\pi} \int_{-\infty}^{\infty} Q(x - x_r, a(y_1 - y_r), b(y_1 - y_r)) \cdot Q(x_r - x_s, \alpha(y_2 - y_s), \beta(y_2 - y_s)) dx_r \\
&= \operatorname{sgn}(b(y_1 - y_r)) \cdot \operatorname{sgn}(\beta(y_2 - y_s)) \cdot Q(x - x_s, a(y_1 - y_r) + \alpha(y_2 - y_s), |b(y_1 - y_r)| + |\beta(y_2 - y_s)|). \quad (3.20)
\end{aligned}$$

Consider next the useful identities obtained from Eqs. (3.13)-(3.16) for the limit

$y_1 \rightarrow y_r$:

$$H(0, 0) \cdot H(\alpha(y_2 - y_s), \beta(y_2 - y_s)) = -I(\alpha(y_2 - y_s), |\beta(y_2 - y_s)|), \quad (3.21)$$

$$H(0, 0) \cdot I(\alpha(y_2 - y_s), \beta(y_2 - y_s)) = \operatorname{sgn}(\beta(y_2 - y_s)) \cdot H(\alpha(y_2 - y_s), |\beta(y_2 - y_s)|), \quad (3.22)$$

$$I(0, 0) \cdot H(\alpha(y_2 - y_s), \beta(y_2 - y_s)) = \operatorname{sgn}(b(y_1 - y_r)) \cdot H(\alpha(y_2 - y_s), |\beta(y_2 - y_s)|), \quad (3.23)$$

$$I(0, 0) \cdot I(\alpha(y_2 - y_s), \beta(y_2 - y_s)) = \operatorname{sgn}(b(y_1 - y_r)) \cdot \operatorname{sgn}(\beta(y_2 - y_s)) \cdot I(\alpha(y_2 - y_s), |\beta(y_2 - y_s)|), \quad (3.24)$$

where the signum functions are retained to correctly capture the direction of approach to zero, i.e., whether $b(y_1 - y_r) \rightarrow 0^+$ or $b(y_1 - y_r) \rightarrow 0^-$. Note that $I(0,0)$ is taken to mean either $I(0,0^+)$ or $I(0,0^-)$.

If both $y_1 \rightarrow y_r$ and $y_2 \rightarrow y_s$, the above four equations reduce to:

$$H(0,0) \cdot H(0,0) = -I(0,0^+), \quad (3.25)$$

$$H(0,0) \cdot I(0,0) = \text{sgn}(\beta(y_2 - y_s)) H(0,0), \quad (3.26)$$

$$I(0,0) \cdot H(0,0) = \text{sgn}(b(y_1 - y_r)) H(0,0), \quad (3.27)$$

$$I(0,0) \cdot I(0,0) = \text{sgn}(b(y_1 - y_r)) \text{sgn}(\beta(y_2 - y_s)) I(0,0^+), \quad (3.28)$$

where the second argument in $I(0,0^+)$ on the right-hand side of Eqs. (3.25) and (3.28) emphasizes the addition of absolute values.

Equation (3.25) establishes that the inverse of the Hilbert transform is the negative of itself. This fact allows exact closed-form solutions to be obtained for the problem of disclination dipoles and dislocations in an infinitely extended anisotropic bimaterial (Wu, 2000; Wu et al., 2003), since the Hilbert transform is the only integral transform appearing in the governing equations. In the problem of a dislocation in a film-substrate or a general multilayer solid, however, the Hilbert transform as well as the H and I transforms appear simultaneously in the governing integral equations, as shown

subsequently. Unlike Eq. (3.25), Eqs. (3.13)-(3.16) do not suggest that the H transform has a closed-form inverse since the I transform is in general not an identity integral operator. This is the fundamental reason why exact closed-form solutions for a dislocation in multilayer systems have not yet been found.

In this thesis, the formulation, although conceptually simple, is mathematically complicated and would be quite difficult to handle without using the properties of the iterative transforms developed in this section. It will also be shown that exact solutions for either the dislocation image density or the stress field exist at least formally. For instance, for the film-substrate problem the solutions are expressed in the form of infinite series. Each term of the series involves the H and I transforms, which can be evaluated exactly in closed-form. Thus, the solutions presented can be as accurate as required. Moreover, the solution accuracy can be verified not only in the sense of convergence by comparing the answers obtained using different numbers of terms in the series, but directly by back-substituting the answers into the governing equation.

3.2 Proof for the equation (3.13)

The iterative transform in Eq. (3.13), when operating on $\rho(x)$, can be expanded in full as:

$$\begin{aligned}
 & H(a(y_1 - y_r), b(y_1 - y_r)) \cdot H(\alpha(y_2 - y_s), \beta(y_2 - y_s)) [\rho(x)] = \\
 & \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{x - x_r + a(y_1 - y_r)}{[x - x_r + a(y_1 - y_r)]^2 + [b(y_1 - y_r)]^2} \cdot \left\{ \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{x_r - x_s + \alpha(y_2 - y_s)}{[x_r - x_s + \alpha(y_2 - y_s)]^2 + [\beta(y_2 - y_s)]^2} \rho(x_s) dx_s \right\} dx_r \\
 & = \frac{1}{\pi^2} \int_{-\infty}^{\infty} \rho(x_s) dx_s \int_{-\infty}^{\infty} \frac{x - x_r + a(y_1 - y_r)}{[x - x_r + a(y_1 - y_r)]^2 + [b(y_1 - y_r)]^2} \frac{x_r - x_s + \alpha(y_2 - y_s)}{[x_r - x_s + \alpha(y_2 - y_s)]^2 + [\beta(y_2 - y_s)]^2} dx_r.
 \end{aligned} \tag{3.29}$$

The integral with respect to x_r can be evaluated exactly by residue calculus as follows.

Consider the integral of the complex function:

$$S(z) = \frac{x - z + a(y_1 - y_r)}{[x - z + a(y_1 - y_r)]^2 + [b(y_1 - y_r)]^2} \frac{z - x_s + \alpha(y_2 - y_s)}{[z - x_s + \alpha(y_2 - y_s)]^2 + [\beta(y_2 - y_s)]^2}, \quad (3.30)$$

where z is the complex variable of integration such that $\text{Re}[z] = x_r$, around a closed contour C consisting of a semi-circle C_R of radius R in the upper half of the complex plane and the x_r axis from negative to positive infinity. The complex integral can be evaluated as:

$$\oint_C S(z) dz = \int_{-\infty}^{\infty} \frac{x - x_r + a(y_1 - y_r)}{[x - x_r + a(y_1 - y_r)]^2 + [b(y_1 - y_r)]^2} \cdot \frac{x_r - x_s + \alpha(y_2 - y_s)}{[x_r - x_s + \alpha(y_2 - y_s)]^2 + [\beta(y_2 - y_s)]^2} dx_r$$

$$+ \oint_C S(z) dz = 2\pi i \sum_k \text{Res}[S(z)]_{z=z_k}, \quad (3.31)$$

where by the residue theorem the right-hand side is $2\pi i$ ($i = \sqrt{-1}$) times the sum of residues of $S(z)$ at the poles *inside* C . It may be proven that the integral over C_R tends to zero as $R \rightarrow \infty$, so that only the real integral along the x_r axis remains. The four first-order poles occupy the complex conjugate locations:

$$z_1, \bar{z}_1 = x + aA_{1r} \pm ibA_{1r}, \quad z_2, \bar{z}_2 = x_s - \alpha A_{2s} \pm i\beta A_{2s}, \quad (3.32)$$

where the new notations

$$\Delta_{1r} = y_1 - y_r, \quad \Delta_{2s} = y_2 - y_s \quad (3.33)$$

have been introduced. The two pole locations within C are those given by Eq. (3.32) with positive imaginary parts, i.e., $x + a\Delta_{1r} + ib\Delta_{1r}$ if $b\Delta_{1r} > 0$ or $x + a\Delta_{1r} - ib\Delta_{1r}$ if $b\Delta_{1r} < 0$, and $x_s - \alpha\Delta_{2s} + i\beta\Delta_{2s}$ if $\beta\Delta_{2s} > 0$ or $x_s - \alpha\Delta_{2s} - i\beta\Delta_{2s}$ if $\beta\Delta_{2s} < 0$. The residues at the poles within C can be easily evaluated:

$$\begin{aligned} \text{Res}[S(z)]_{z=z_1} (\text{if } \text{Im}[z_1] > 0) &= \text{Res}[S(z)]_{z=\bar{z}_1} (\text{if } \text{Im}[\bar{z}_1] > 0) \\ &= \frac{-1}{2} \frac{x - x_s + a\Delta_{1r} + \alpha\Delta_{2s} + i|b\Delta_{1r}|}{\left[x - x_s + a\Delta_{1r} + \alpha\Delta_{2s} + i(|b\Delta_{1r}| - \beta\Delta_{2s}) \right] \cdot \left[x - x_s + a\Delta_{1r} + \alpha\Delta_{2s} + i(|b\Delta_{1r}| + \beta\Delta_{2s}) \right]}, \end{aligned} \quad (3.34)$$

$$\begin{aligned} \text{Res}[S(z)]_{z=z_2} (\text{if } \text{Im}[z_2] > 0) &= \text{Res}[S(z)]_{z=\bar{z}_2} (\text{if } \text{Im}[\bar{z}_2] > 0) \\ &= \frac{1}{2} \frac{x - x_s + a\Delta_{1r} + \alpha\Delta_{2s} - i|\beta\Delta_{2s}|}{\left[x - x_s + a\Delta_{1r} + \alpha\Delta_{2s} - i(|\beta\Delta_{2s}| - b\Delta_{1r}) \right] \cdot \left[x - x_s + a\Delta_{1r} + \alpha\Delta_{2s} - i(|\beta\Delta_{2s}| + b\Delta_{1r}) \right]}, \end{aligned} \quad (3.35)$$

where the modulus sign has been introduced. The residue assumes the same value whether it is z_1 or $\bar{z}_1$ that is inside C (same conclusion for z_2 or $\bar{z}_2$). Evaluation of the sum of the two residues is facilitated by noting that Eqs. (3.34) and (3.35) are respectively of the form of the first and second term on the left-hand side of the following sum:

$$\begin{aligned}
& -\frac{1}{2} \frac{A_1 + i|A_2|}{[A_1 + i(|A_2| - A_3)] \cdot [A_1 + i(|A_2| + A_3)]} + \frac{1}{2} \frac{A_1 - i|A_3|}{[A_1 - i(|A_3| - A_2)] \cdot [A_1 - i(|A_3| + A_2)]} \\
& = \frac{i}{2} \frac{|A_2| + |A_3|}{A_1^2 + (|A_2| + |A_3|)^2},
\end{aligned} \tag{3.36}$$

where $A_1 = x - x_s + a\Delta_{1r} + \alpha\Delta_{2s}$, $A_2 = b\Delta_{1r}$ and $A_3 = \beta\Delta_{2s}$. The identity of Eq. (3.36) can be verified by direct expansion of the terms on the left-hand side. Using this identity, Eq. (3.31) becomes:

$$\begin{aligned}
& \int_{-\infty}^{\infty} \frac{x - x_r + a(y_1 - y_r)}{[x - x_r + a(y_1 - y_r)]^2 + [b(y_1 - y_r)]^2} \cdot \frac{x_r - x_s + \alpha(y_2 - y_s)}{[x_r - x_s + \alpha(y_2 - y_s)]^2 + [\beta(y_2 - y_s)]^2} dx_r \\
& = -\pi \frac{|b(y_1 - y_r)| + |\beta(y_2 - y_s)|}{[x - x_s + a(y_1 - y_r) + \alpha(y_2 - y_s)]^2 + [|b(y_1 - y_r)| + |\beta(y_2 - y_s)|]^2},
\end{aligned} \tag{3.37}$$

and Eq. (3.29) reduces to:

$$\begin{aligned}
& H(a(y_1 - y_r), b(y_1 - y_r)) \cdot H(\alpha(y_2 - y_s), \beta(y_2 - y_s)) [\rho(x)] \\
& = \frac{-1}{\pi} \int_{-\infty}^{\infty} \rho(x_s) \frac{|b(y_1 - y_r)| + |\beta(y_2 - y_s)|}{[x - x_s + a(y_1 - y_r) + \alpha(y_2 - y_s)]^2 + [|b(y_1 - y_r)| + |\beta(y_2 - y_s)|]^2} dx_s \\
& = -I(a(y_1 - y_r) + \alpha(y_2 - y_s), |b(y_1 - y_r)| + |\beta(y_2 - y_s)|) [\rho(x)],
\end{aligned} \tag{3.38}$$

where the last line is obtained via Eqs. (3.2) and (3.10). Equation (3.38) thus establishes Eq. (3.13). The iterative transforms as expressed by Eqs. (3.14)-(3.16) can be similarly proved by using residue calculus.

CHAPTER FOUR

SINGLE DISLOCATION IN ANISOTROPIC TWO-LAYER SYSTEMS

In this chapter, the problems of single dislocation in two-layer systems are presented and solved. Section 4.1 introduces the formulation of the problem. Sections 4.2 and 4.3 develop the solutions for a single edge dislocation and a single screw dislocation, respectively, in a film-substrate system. Section 4.4 outlines the formulation for the mixed dislocation. Section 4.5 presents the numerical results. Conclusions for the chapter are given in Section 4.6.

4.1 Problem formulation by image dislocation method

Figure 4.1(a) shows a film (A) of thickness h bonded to a semi-infinite substrate (B). For analysis, a rectangular frame $x_1 - x_2$ is attached to the interface. According to the right-hand rule, the x_3 - axis points out of the $x_1 - x_2$ plane. The film A and substrate B are elastically anisotropic and dissimilar. The film has the thickness h . The source dislocation, represented by a cross, is situated at (x_1^o, x_2^o) in the system. The type of the source dislocation could be pure edge, pure screw, or mixed. The dislocation could be anywhere in the system, including on the interface. The problem is to determine the stress field in the dissimilar anisotropic film-substrate system.

The solution strategy is to transform the film-substrate problem to a bimaterial problem in which the interface boundary conditions are always exactly satisfied *a priori* and it remains to satisfy only the free surface conditions. Thus, the original problem of fig. 4.1 (a) is transformed into the problem of fig. 4.1 (b), which consists of an *infinite* bimaterial $A-B$ loaded by the source dislocation at (x_1^o, x_2^o) and by the infinitely extended, continuous image dislocation distributions on $x_2 = h$.

Fig. 4.1. (a) The problem of a discrete dislocation at (x_1^o, x_2^o) in an anisotropic film-substrate ($A-B$) system. The film thickness is denoted by h . (b) The equivalent infinite bimaterial problem with image dislocations of densities on $y = h$.

For the general film-substrate systems, the equations for determining the density functions are derived from the traction-free conditions of the film surface, i.e., the stresses $\sigma_{21}, \sigma_{22}, \sigma_{23}$ all vanish on the free surface:

$$\sigma_{21}(x_1, x_2 = h) = 0, \quad \sigma_{22}(x_1, x_2 = h) = 0, \quad \sigma_{23}(x_1, x_2 = h) = 0. \quad (4.1)$$

The stress field in the film-substrate system is given by the field in the corresponding region of the bimaterial containing the image dislocations. In a decoupled problem, the edge and screw components of the source dislocation can be treated separately using edge and screw dislocation images respectively. The most general matrix of elastic constants (where $C_{14} = C_{15} = C_{24} = C_{25} = C_{46} = C_{56} = 0$) allowing a mixed dislocation problem to be solved as a decoupled problem is given in Hirth and Lothe (1982). In Sections 4.2 and 4.3, the solutions for single edge and screw dislocations in decoupled film-substrate problems are studied, respectively. The solution for a mixed dislocation in a coupled problem is briefly illustrated in Section 4.4.

4.2 Solutions for single edge dislocation in decoupled film-substrate problems

A source edge dislocation oriented at the angle of α to the x_1 – axis is situated at (x_1^o, x_2^o) in the system, as shown in fig. 4.2 (a). For convenience, the dislocation is called “glide” dislocation when $\alpha = 0^\circ$, and “climb” dislocation when $\alpha = 90^\circ$. The decoupled problem is considered here, so that no screw dislocation images are needed to satisfy the boundary conditions. The image edge dislocation densities $\rho_1(x_1), \rho_2(x_1)$ are distributed on the position of the free surface, as shown in fig. 4.2 (b).

Fig. 4.2. The transformation of the problem of a film-substrate with an edge dislocation into the problem of an infinite bimaterial. The problem is assumed to be decoupled.

4.2.1 Stress field due to an edge dislocation in infinite bimaterial

In the bimaterial problem, the contributions arise from the source dislocation and the distributed image dislocations. The problem of a single dislocation in a bimaterial must therefore be solved before the governing equations for the film-substrate problem can be formulated.

Consider a single edge dislocation located at (x_1^r, x_2^r) in an infinite bimaterial $(A-B)$. Using the image dislocation method, the problem is decomposed into the two *homogeneous* subproblems A and B as shown in fig. 4.3.

Fig. 4.3. Decomposition of the bimaterial problem into two homogeneous subproblems, A and B .

The image dislocations are collectively denoted by $\rho_{At}(x_1)$ and $\rho_{Bt}(x_1)$, $t=1,2$. They are introduced to satisfy the conditions of continuity of the normal and shear tractions and of the normal and tangential displacement gradients across the interface, i.e.:

$$\sigma_{22}(x_1, 0^+) = \sigma_{22}(x_1, 0^-), \quad \sigma_{12}(x_1, 0^+) = \sigma_{12}(x_1, 0^-), \quad (4.2)$$

$$\frac{\partial u_1}{\partial x_1}(x_1, 0^+) = \frac{\partial u_1}{\partial x_1}(x_1, 0^-), \quad \frac{\partial u_2}{\partial x_1}(x_1, 0^+) = \frac{\partial u_2}{\partial x_1}(x_1, 0^-), \quad (4.3)$$

where u_1, u_2 denote the displacements in the x_1, x_2 – directions, respectively.

The stress and displacement gradient components of a general straight dislocation located at the origin of a rectangular frame $x_1 - x_2$ in a homogeneous anisotropic solid can be written by using Stroh's (1958) formalism, as was done in Wu et al. (2003). These components can be written in a compact form using Eqs. (3.1) and (3.2):

$$\sigma_{ij} = 2 \sum_{\alpha=1}^3 \left[\xi_{\alpha ij}^{iR} P(x_1, p_{\alpha}^R x_2, p_{\alpha}^I x_2) + \xi_{\alpha ij}^{iI} Q(x_1, p_{\alpha}^R x_2, p_{\alpha}^I x_2) \right] b_i, \quad (4.4)$$

$$\frac{\partial u_k}{\partial x_l} = 2 \sum_{\alpha=1}^3 \left[\zeta_{\alpha kl}^{iR} P(x_1, p_{\alpha}^R x_2, p_{\alpha}^I x_2) + \zeta_{\alpha kl}^{iI} Q(x_1, p_{\alpha}^R x_2, p_{\alpha}^I x_2) \right] b_i, \quad (4.5)$$

where $i, j, k, l = 1, 2, 3$, $t' = 1, 2, 3$ denote a general dislocation with Burgers vector components b_1, b_2 and b_3 along the $x_1 -$, $x_2 -$ and $x_3 -$ directions respectively, and $\xi_{\alpha ij}^{iR}$, $\xi_{\alpha ij}^{iI}$ and $\zeta_{\alpha kl}^{iR}, \zeta_{\alpha kl}^{iI}$ are respectively the real and imaginary parts of

$$\xi_{\alpha ij}^i = \frac{C_{ijkl} [m_l + p_{\alpha} n_l] A_{\alpha k} L_{\alpha i'}}{2\pi i}, \quad (4.6)$$

$$\zeta_{\alpha kl}^i = \frac{[m_l + p_{\alpha} n_l] A_{\alpha k} L_{\alpha i'}}{2\pi i}. \quad (4.7)$$

In Eqs. (4.4)-(4.5), the repeated subscript t' implies summation, C_{ijkl} are the components of the elasticity tensor, $m_l = \delta_{l1}$ and $n_l = \delta_{l2}$ are the Kronecker deltas, and $A_{\alpha k}$ and $L_{\alpha t'}$ are the k -th and t' -th components of a certain normalized six-dimensional eigenvector $\{A_{\alpha 1}, A_{\alpha 2}, A_{\alpha 3}, L_{\alpha 1}, L_{\alpha 2}, L_{\alpha 3}\}$ with the associated eigenvalue p_α (real and imaginary parts p_α^R and p_α^I), where $\alpha = 1, 2, \dots, 6$. The eigenvalues p_α and the quantities $\xi_{\alpha ij}^i$ and $\zeta_{\alpha kl}^i$ occur in complex conjugate pairs, so that only three values of α need be considered. In Eqs. (4.4)-(4.5), α ranges from 1 to 3 only and the p_α 's chosen are those with positive imaginary parts, i.e., $\text{sgn}(p_\alpha^I) > 0$. Furthermore, p_α , $\xi_{\alpha ij}^i$ and $\zeta_{\alpha kl}^i$ assume two sets of values corresponding to Materials A and B . The notations $p_{A\alpha}$, $p_{B\alpha}$, etc. will be used where necessary.

Consider now a source edge dislocation with Burgers vector components b_1 and b_2 at (x_1^r, x_2^r) . The stress and displacement gradients, by Eqs. (4.4)-(4.5), on $x_2 = 0$ in either Material A or B are:

$$\sigma_{22}(x_1, 0) = 2 \sum_{\alpha=1}^3 b_s \left[\xi_{\alpha 22}^{sR} P(x_1 - x_1^r, -p_\alpha^R x_2^r, -p_\alpha^I x_2^r) + \xi_{\alpha 22}^{sI} Q(x_1 - x_1^r, -p_\alpha^R x_2^r, -p_\alpha^I x_2^r) \right], \quad (4.8)$$

$$\sigma_{12}(x_1, 0) = 2 \sum_{\alpha=1}^3 b_s \left[\xi_{\alpha 12}^{sR} P(x_1 - x_1^r, -p_\alpha^R x_2^r, -p_\alpha^I x_2^r) + \xi_{\alpha 12}^{sI} Q(x_1 - x_1^r, -p_\alpha^R x_2^r, -p_\alpha^I x_2^r) \right], \quad (4.9)$$

$$\frac{\partial u_1}{\partial x_1}(x_1, 0) = 2 \sum_{\alpha=1}^3 b_s \left[\zeta_{\alpha 11}^{sR} P(x_1 - x_1^r, -p_\alpha^R x_2^r, -p_\alpha^I x_2^r) + \zeta_{\alpha 11}^{sI} Q(x_1 - x_1^r, -p_\alpha^R x_2^r, -p_\alpha^I x_2^r) \right], \quad (4.10)$$

$$\frac{\partial u_2}{\partial x_1}(x_1, 0) = 2 \sum_{\alpha=1}^3 b_s \left[\zeta_{\alpha 21}^{sR} P(x_1 - x_1^r, -p_{\alpha}^R x_2^r, -p_{\alpha}^I x_2^r) + \zeta_{\alpha 21}^{sI} Q(x_1 - x_1^r, -p_{\alpha}^R x_2^r, -p_{\alpha}^I x_2^r) \right], \quad (4.11)$$

where s implies summation ($s = 1, 2$).

The limiting quantities on $y = 0$ can be deduced from Eqs. (4.8)-(4.11):

$$\begin{aligned} \sigma_{22}(x_1, 0) &= \frac{D_{22}^t b_t}{\pi} P(x_1 - x_1'', 0, 0), \\ \sigma_{12}(x_1, 0) &= \frac{D_{12}^t b_t}{\pi} P(x_1 - x_1'', 0, 0), \end{aligned} \quad (4.12)$$

$$\begin{aligned} \frac{\partial u_1}{\partial x_1}(x_1, 0) &= \frac{E_{11}^t b_t}{\pi} P(x_1 - x_1'', 0, 0) - \frac{b_t}{2\pi} Q(x_1 - x_1'', 0, 0) \delta_{1t}, \\ \frac{\partial u_2}{\partial x_1}(x_1, 0) &= \frac{E_{21}^t b_t}{\pi} P(x_1 - x_1'', 0, 0) - \frac{b_t}{2\pi} Q(x_1 - x_1'', 0, 0) \delta_{2t}, \end{aligned} \quad (4.13)$$

where t implies summation ($t = 1, 2$), δ_{1t} and δ_{2t} are Kronecker deltas,

$$D_{22}^t = 2\pi \sum_{\alpha=1}^3 \zeta_{\alpha 22}^{tR}, \quad D_{12}^t = 2\pi \sum_{\alpha=1}^3 \zeta_{\alpha 12}^{tR}, \quad E_{11}^t = 2\pi \sum_{\alpha=1}^3 \zeta_{\alpha 11}^{tR}, \quad E_{21}^t = 2\pi \sum_{\alpha=1}^3 \zeta_{\alpha 21}^{tR}, \quad (4.14)$$

and $Q(x_1 - x_1'', 0, 0) = \pi \operatorname{sgn}(x_2) \delta(x_1 - x_1'')$ by Eq. (3.8). The $\operatorname{sgn}(x_2)$ term will have implications when $x_2 \rightarrow 0^+$ or 0^- according to the interface boundary conditions of Eqs. (4.2) and (4.3). Also, Q does not appear in Eq. (4.12) because the coefficients of Q are

zero in these cases. Where Q does appear, as in $\partial u / \partial x_1(x_1, 0)$ for the glide case and

$\partial v / \partial x_1(x_1, 0)$ for the climb case, the corresponding coefficients equal $-\frac{1}{2}$. In fact,

$$\begin{aligned} 2\pi \sum_{\alpha=1}^3 \xi_{\alpha 22}^{1I} &= 2\pi \sum_{\alpha=1}^3 \xi_{\alpha 12}^{1I} = 2\pi \sum_{\alpha=1}^3 \xi_{\alpha 22}^{2I} = 2\pi \sum_{\alpha=1}^3 \xi_{\alpha 12}^{2I} = 0, \\ 2\pi \sum_{\alpha=1}^3 \xi_{\alpha 11}^{1I} &= -\frac{1}{2}, 2\pi \sum_{\alpha=1}^3 \xi_{\alpha 21}^{1I} = 2\pi \sum_{\alpha=1}^3 \xi_{\alpha 11}^{2I} = 0, 2\pi \sum_{\alpha=1}^3 \xi_{\alpha 21}^{2I} = -\frac{1}{2}. \end{aligned} \quad (4.15)$$

These results arise from the physical requirement that a line integral of the stresses σ_{22} and σ_{12} in Eq. (4.12) along a closed loop around the dislocation in the x_1 – and x_2 – directions must yield a zero force per unit thickness, whereas a similar line integral of the displacement gradients $\frac{\partial u_1}{\partial x_1}$ and $\frac{\partial u_2}{\partial x_1}$ in Eq. (4.13) must yield the Burgers vector magnitudes of b_1 and 0 for the glide case and 0 and b_2 for the climb case (Wu et al., 2003).

After integration, the corresponding stresses and displacement gradients are obtained from Eqs. (4.12) and (4.13):

$$\sigma_{22}(x_1, 0) = \frac{D_{22}^t}{\pi} \int_{-\infty}^{\infty} P(x_1 - x_1'', 0, 0) \rho(x_1'') dx_1'' = D_{22}^t H(0, 0) [\rho(x_1)], \quad (4.16)$$

$$\sigma_{12}(x_1, 0) = \frac{D_{12}^t}{\pi} \int_{-\infty}^{\infty} P(x_1 - x_1'', 0, 0) \rho(x_1'') dx_1'' = D_{12}^t H(0, 0) [\rho(x_1)], \quad (4.17)$$

$$\begin{aligned}
\frac{\partial u_1}{\partial x_1}(x_1, 0) &= \frac{E_{11}^t}{\pi} \int_{-\infty}^{\infty} P(x_1 - x_1'', 0, 0) \rho(x_1'') dx_1'' - \frac{1}{2\pi} \int_{-\infty}^{\infty} Q(x_1 - x_1'', 0, 0) \rho(x_1'') \delta_{1t} dx_1'' \\
&= E_{11}^t H(0, 0) [\rho(x_1)] - \frac{1}{2} \rho(x_1) \operatorname{sgn}(x_2) \delta_{1t},
\end{aligned} \tag{4.18}$$

$$\begin{aligned}
\frac{\partial u_2}{\partial x_1}(x_1, 0) &= \frac{E_{21}^t}{\pi} \int_{-\infty}^{\infty} P(x_1 - x_1'', 0, 0) \rho(x_1'') dx_1'' - \frac{1}{2\pi} \int_{-\infty}^{\infty} Q(x_1 - x_1'', 0, 0) \rho(x_1'') \delta_{2t} dx_1'' \\
&= E_{21}^t H(0, 0) [\rho(x_1)] - \frac{1}{2} \rho(x_1) \operatorname{sgn}(x_2) \delta_{2t}.
\end{aligned} \tag{4.19}$$

The interfacial boundary conditions of Eqs. (4.2) and (4.3) can now be written by using Eqs. (4.8)-(4.11) and Eqs. (4.16)-(4.19). For an edge dislocation with Burgers vector components b_i occupying (x_1^r, x_2^r) , the stresses or displacement gradients on $x_2 = 0^+$ (or $x_2 = 0^-$) in Subproblem A (or B) arise from the discrete source and from the glide and climb dislocation images with densities $\rho_{A1}(x_1)$ and $\rho_{A2}(x_1)$ (or $\rho_{B1}(x_1)$ and $\rho_{B2}(x_1)$). The continuity conditions thus become:

$$D_{A22}^t H(0, 0) [\rho_{At}(x_1)] - D_{B22}^t H(0, 0) [\rho_{Bt}(x_1)] = R_1(x_1), \tag{4.20}$$

$$D_{A12}^t H(0, 0) [\rho_{At}(x_1)] - D_{B12}^t H(0, 0) [\rho_{Bt}(x_1)] = R_2(x_1), \tag{4.21}$$

$$E_{A11}^t H(0, 0) [\rho_{At}(x_1)] - E_{B11}^t H(0, 0) [\rho_{Bt}(x_1)] - \frac{1}{2} \rho_{A1}(x_1) - \frac{1}{2} \rho_{B1}(x_1) = R_3(x_1), \tag{4.22}$$

$$E_{A21}^t H(0,0)[\rho_{At}(x_1)] - E_{B21}^t H(0,0)[\rho_{Bt}(x_1)] - \frac{1}{2}\rho_{A2}(x_1) - \frac{1}{2}\rho_{B2}(x_1) = R_4(x_1), \quad (4.23)$$

where it is emphasized that the repeated t symbols imply summation over $t = 1, 2$, and

$$R_1(x_1) = 2 \sum_{\alpha=1}^3 b_s \left[\begin{aligned} &\zeta_{B\alpha 22}^{sR} P(x_1 - x_1^r, -p_{B\alpha}^R x_2^r, -p_{B\alpha}^I x_2^r) + \zeta_{B\alpha 22}^{sI} Q(x_1 - x_1^r, -p_{B\alpha}^R x_2^r, -p_{B\alpha}^I x_2^r) \\ &- \zeta_{A\alpha 22}^{sR} P(x_1 - x_1^r, -p_{A\alpha}^R x_2^r, -p_{A\alpha}^I x_2^r) - \zeta_{A\alpha 22}^{sI} Q(x_1 - x_1^r, -p_{A\alpha}^R x_2^r, -p_{A\alpha}^I x_2^r) \end{aligned} \right], \quad (4.24)$$

$$R_2(x_1) = 2 \sum_{\alpha=1}^3 b_s \left[\begin{aligned} &\zeta_{B\alpha 12}^{sR} P(x_1 - x_1^r, -p_{B\alpha}^R x_2^r, -p_{B\alpha}^I x_2^r) + \zeta_{B\alpha 12}^{sI} Q(x_1 - x_1^r, -p_{B\alpha}^R x_2^r, -p_{B\alpha}^I x_2^r) \\ &- \zeta_{A\alpha 12}^{sR} P(x_1 - x_1^r, -p_{A\alpha}^R x_2^r, -p_{A\alpha}^I x_2^r) - \zeta_{A\alpha 12}^{sI} Q(x_1 - x_1^r, -p_{A\alpha}^R x_2^r, -p_{A\alpha}^I x_2^r) \end{aligned} \right], \quad (4.25)$$

$$R_3(x_1) = 2 \sum_{\alpha=1}^3 b_s \left[\begin{aligned} &\zeta_{B\alpha 11}^{sR} P(x_1 - x_1^r, -p_{B\alpha}^R x_2^r, -p_{B\alpha}^I x_2^r) + \zeta_{B\alpha 11}^{sI} Q(x_1 - x_1^r, -p_{B\alpha}^R x_2^r, -p_{B\alpha}^I x_2^r) \\ &- \zeta_{A\alpha 11}^{sR} P(x_1 - x_1^r, -p_{A\alpha}^R x_2^r, -p_{A\alpha}^I x_2^r) - \zeta_{A\alpha 11}^{sI} Q(x_1 - x_1^r, -p_{A\alpha}^R x_2^r, -p_{A\alpha}^I x_2^r) \end{aligned} \right], \quad (4.26)$$

$$R_4(x_1) = 2 \sum_{\alpha=1}^3 b_s \left[\begin{aligned} &\zeta_{B\alpha 21}^{sR} P(x_1 - x_1^r, -p_{B\alpha}^R x_2^r, -p_{B\alpha}^I x_2^r) + \zeta_{B\alpha 21}^{sI} Q(x_1 - x_1^r, -p_{B\alpha}^R x_2^r, -p_{B\alpha}^I x_2^r) \\ &- \zeta_{A\alpha 21}^{sR} P(x_1 - x_1^r, -p_{A\alpha}^R x_2^r, -p_{A\alpha}^I x_2^r) - \zeta_{A\alpha 21}^{sI} Q(x_1 - x_1^r, -p_{A\alpha}^R x_2^r, -p_{A\alpha}^I x_2^r) \end{aligned} \right]. \quad (4.27)$$

Exact solutions for Eqs. (4.20)-(4.23) are constructed:

$$\rho_{At}(x_1) = \sum_{i=1}^4 (c_{Ati} R_i(x_1) + c'_{Ati} H(0,0)[R_i(x_1)]), \quad (4.28)$$

$$\rho_{Bt}(x_1) = \sum_{i=1}^4 (c_{Bti} R_i(x_1) + c'_{Bti} H(0,0)[R_i(x_1)]), \quad (4.29)$$

where $t=1,2$ denotes the glide or climb type of image dislocations. A total of 32 coefficients c_{Aii} , c'_{Aii} , c_{Bii} and c'_{Bii} completely specify the image dislocations. Equations (4.28) and (4.29) are substituted back into Eqs. (4.20)-(4.23), and noting the iterative property of the Hilbert transform shown in Eq. (3.25), eight linear algebraic equations can be obtained by collecting the coefficients of the eight functions in each of Eqs. (4.20)-(4.23), leading to a total of 32 linear algebraic equations. There are, however, essentially eight equations as shown below:

$$D_{A22}^1 c_{A1i} + D_{A22}^2 c_{A2i} - D_{B22}^1 c_{B1i} - D_{B22}^2 c_{B2i} = 0, \quad (4.30)$$

$$-D_{A22}^1 c'_{A1i} - D_{A22}^2 c'_{A2i} + D_{B22}^1 c'_{B1i} + D_{B22}^2 c'_{B2i} = \delta_{i1} \eta_{AB}, \quad (4.31)$$

$$D_{A12}^1 c_{A1i} + D_{A12}^2 c_{A2i} - D_{B12}^1 c_{B1i} - D_{B12}^2 c_{B2i} = 0, \quad (4.32)$$

$$-D_{A12}^1 c'_{A1i} - D_{A12}^2 c'_{A2i} + D_{B12}^1 c'_{B1i} + D_{B12}^2 c'_{B2i} = \delta_{i2} \eta_{AB}, \quad (4.33)$$

$$E_{A11}^1 c_{A1i} + E_{A11}^2 c_{A2i} - E_{B11}^1 c_{B1i} - E_{B11}^2 c_{B2i} = \frac{1}{2} (c'_{A1i} + c'_{B1i}), \quad (4.34)$$

$$-E_{A11}^1 c'_{A1i} - E_{A11}^2 c'_{A2i} + E_{B11}^1 c'_{B1i} + E_{B11}^2 c'_{B2i} = \frac{1}{2} (c_{A1i} + c_{B1i}) + \delta_{i3} \eta_{AB}, \quad (4.35)$$

$$E_{A21}^1 c_{A1i} + E_{A21}^2 c_{A2i} - E_{B21}^1 c_{B1i} - E_{B21}^2 c_{B2i} = \frac{1}{2} (c'_{A2i} + c'_{B2i}), \quad (4.36)$$

$$-E_{A21}^1 c'_{A1i} - E_{A21}^2 c'_{A2i} + E_{B21}^1 c'_{B1i} + E_{B21}^2 c'_{B2i} = \frac{1}{2} (c_{A2i} + c_{B2i}) + \delta_{i4} \eta_{AB}, \quad (4.37)$$

where $i = 1, 2, 3, 4$ and $\eta_{AB} = 0$ if $A \equiv B$ and 1 otherwise. If material A is identical to B , it means the material is homogeneous and the continuity conditions are automatically satisfied. Also, the solutions for c_{A1i} , c'_{A1i} , c_{B1i} and c'_{B1i} are independent of whether the source is a mixed edge, pure glide or pure climb dislocation.

The stress components at any position (x_1, x_2) due to the source at (x_1^r, x_2^r) can now be derived exactly from the known image dislocation densities. Suffice to consider stress σ_{22} . In Material A , the contribution from the discrete source is, by Eq. (4.4):

$$\sigma_{22}^{(1)}(x_1, x_2 \geq 0) = 2 \sum_{\alpha=1}^3 b_s \left(\xi_{A\alpha 22}^{sR} P_A + \xi_{A\alpha 22}^{sI} Q_A \right), \quad (4.38)$$

where s implies summation ($s = 1, 2$), and the rational functions are given by:

$$\begin{aligned} P_A &\equiv P(x_1 - x_1^r, p_{A\alpha}^R(x_2 - x_2^r), p_{A\alpha}^I(x_2 - x_2^r)), \\ Q_A &\equiv Q(x_1 - x_1^r, p_{A\alpha}^R(x_2 - x_2^r), p_{A\alpha}^I(x_2 - x_2^r)). \end{aligned} \quad (4.39)$$

The contribution from the image dislocation densities can be obtained by using the density expression of Eq. (4.28), the total contribution of both glide and climb images can be written as:

$$\begin{aligned} & \sigma_{22}^{(2)}(x_1, x_2 \geq 0) \\ &= 2\pi \sum_{\alpha=1}^3 \left\{ \left[\begin{array}{l} \xi_{A\alpha 22}^{tR} H(p_{A\alpha}^R x_2, p_{A\alpha}^I x_2) + \\ \xi_{A\alpha 22}^{tI} I(p_{A\alpha}^R x_2, p_{A\alpha}^I x_2) \end{array} \right] \cdot \left[\sum_{i=1}^4 (c_{A\alpha i} R_i(x_1) + c'_{A\alpha i} H(0,0)[R_i(x_1)]) \right] \right\}, \end{aligned} \quad (4.40)$$

where the repeated symbol t implies summation. Using Eqs. (3.21) and (3.22), Eq. (4.40) becomes:

$$\begin{aligned} & \sigma_{22}^{(2)}(x_1, x_2 \geq 0) \\ &= 2\pi \sum_{\alpha=1}^3 \sum_{i=1}^4 \left[\begin{array}{l} (\xi_{A\alpha 22}^{tR} c_{A\alpha i} + \xi_{A\alpha 22}^{tI} c'_{A\alpha i}) H(p_{A\alpha}^R x_2, |p_{A\alpha}^I x_2|) - \\ (\xi_{A\alpha 22}^{tR} c'_{A\alpha i} - \xi_{A\alpha 22}^{tI} c_{A\alpha i}) I(p_{A\alpha}^R x_2, |p_{A\alpha}^I x_2|) \end{array} \right] [R_i(x_1)]. \end{aligned} \quad (4.41)$$

The sum of $\sigma_{22}^{(1)}$ and $\sigma_{22}^{(2)}$ in Eqs. (4.38) and (4.41) gives an exact expression for stress σ_{22} in Material A of the bimaterial. The other stress components σ_{12} and σ_{11} can be obtained if the subscripts 22 in the two equations are changed into 12 and 11, respectively. For Material B , $x_2 \leq 0$ and it can be similarly shown that:

$$\sigma_{22}^{(1)}(x_1, x_2 \leq 0) = 2 \sum_{\alpha=1}^3 b_s (\xi_{B\alpha 22}^{sR} P_B + \xi_{B\alpha 22}^{sI} Q_B), \quad (4.42)$$

$$\begin{aligned} & \sigma_{22}^{(2)}(x_1, x_2 \leq 0) \\ &= 2\pi \sum_{\alpha=1}^3 \sum_{i=1}^4 \left[\begin{array}{l} (\xi_{B\alpha 22}^{tR} c_{B\alpha i} - \xi_{B\alpha 22}^{tI} c'_{B\alpha i}) H(p_{B\alpha}^R x_2, |p_{B\alpha}^I x_2|) - \\ (\xi_{B\alpha 22}^{tR} c'_{B\alpha i} + \xi_{B\alpha 22}^{tI} c_{B\alpha i}) I(p_{B\alpha}^R x_2, |p_{B\alpha}^I x_2|) \end{array} \right] [R_i(x_1)]. \end{aligned} \quad (4.43)$$

Equations (4.41) and (4.43) require the evaluation of the H and I transforms of

$$R_i(x_1) = 2 \sum_{\beta=1}^3 b_s \left(r_{B\beta i}^{sR} P(x_1 - x_1^r, -p_{B\beta}^R x_2^r, -p_{B\beta}^I x_2^r) + r_{B\beta i}^{sI} Q(x_1 - x_1^r, -p_{B\beta}^R x_2^r, -p_{B\beta}^I x_2^r) \right. \\ \left. - r_{A\beta i}^{sR} P(x_1 - x_1^r, -p_{A\beta}^R x_2^r, -p_{A\beta}^I x_2^r) - r_{A\beta i}^{sI} Q(x_1 - x_1^r, -p_{A\beta}^R x_2^r, -p_{A\beta}^I x_2^r) \right), \quad (4.44)$$

where the new notations

$$r_{A\beta i}^{sR} = \begin{cases} \xi_{A\beta 22}^{sR}, & i = 1 \\ \xi_{A\beta 12}^{sR}, & i = 2 \\ \xi_{A\beta 11}^{sR}, & i = 3 \\ \xi_{A\beta 21}^{sR}, & i = 4 \end{cases}, \quad r_{A\beta i}^{sI} = \begin{cases} \xi_{A\beta 22}^{sI}, & i = 1 \\ \xi_{A\beta 12}^{sI}, & i = 2 \\ \xi_{A\beta 11}^{sI}, & i = 3 \\ \xi_{A\beta 21}^{sI}, & i = 4 \end{cases}, \quad (4.45)$$

and similarly for $r_{B\beta i}^{sR}$ and $r_{B\beta i}^{sI}$ have been introduced into Eqs. (4.24)-(4.27). The H and I transforms of P and Q have been explicitly determined in closed form, see Eqs. (3.17)-(3.20).

Thus:

$$H(p_{A\alpha}^R x_2, |p_{A\alpha}^I x_2|) [R_i(x_1)] = 2 \sum_{\beta=1}^3 b_s \left(-r_{B\beta i}^{sR} Q_{AB} - \text{sgn}(x_2^r) r_{B\beta i}^{sI} P_{AB} + r_{A\beta i}^{sR} Q_{AA} + \text{sgn}(x_2^r) r_{A\beta i}^{sI} P_{AA} \right), \quad (4.46)$$

$$I(p_{A\alpha}^R x_2, |p_{A\alpha}^I x_2|) [R_i(x_1)] = 2 \sum_{\beta=1}^3 b_s \left(r_{B\beta i}^{sR} P_{AB} - \text{sgn}(x_2^r) r_{B\beta i}^{sI} Q_{AB} - r_{A\beta i}^{sR} P_{AA} + \text{sgn}(x_2^r) r_{A\beta i}^{sI} Q_{AA} \right), \quad (4.47)$$

$$H\left(p_{B\alpha}^R x_2, \left|p_{B\alpha}^I x_2\right|\right) [R_i(x_1)] = 2 \sum_{\beta=1}^3 b_s \left(-r_{B\beta i}^{sR} Q_{BB} - \text{sgn}(x_2^r) r_{B\beta i}^{sI} P_{BB} + r_{A\beta i}^{sR} Q_{BA} + \text{sgn}(x_2^r) r_{A\beta i}^{sI} P_{BA} \right), \quad (4.48)$$

$$I\left(p_{B\alpha}^R x_2, \left|p_{B\alpha}^I x_2\right|\right) [R_i(x_1)] = 2 \sum_{\beta=1}^3 b_s \left(r_{B\beta i}^{sR} P_{BB} - \text{sgn}(x_2^r) r_{B\beta i}^{sI} Q_{BB} - r_{A\beta i}^{sR} P_{BA} + \text{sgn}(x_2^r) r_{A\beta i}^{sI} Q_{BA} \right), \quad (4.49)$$

where

$$\begin{aligned} P_{AA} &\equiv P\left(x_1 - x_1^r, p_{A\alpha}^R x_2 - p_{A\beta}^R x_2^r, \left|p_{A\alpha}^I x_2\right| + \left| -p_{A\beta}^I x_2^r \right|\right), \\ P_{AB} &\equiv P\left(x_1 - x_1^r, p_{A\alpha}^R x_2 - p_{B\beta}^R x_2^r, \left|p_{A\alpha}^I x_2\right| + \left| -p_{B\beta}^I x_2^r \right|\right), \\ P_{BA} &\equiv P\left(x_1 - x_1^r, p_{B\alpha}^R x_2 - p_{A\beta}^R x_2^r, \left|p_{B\alpha}^I x_2\right| + \left| -p_{A\beta}^I x_2^r \right|\right), \\ P_{BB} &\equiv P\left(x_1 - x_1^r, p_{B\alpha}^R x_2 - p_{B\beta}^R x_2^r, \left|p_{B\alpha}^I x_2\right| + \left| -p_{B\beta}^I x_2^r \right|\right), \end{aligned} \quad (4.50)$$

and the arguments of Q_{AA} , Q_{AB} , Q_{BA} and Q_{BB} are respectively the same as those of P_{AA} , P_{AB} , P_{BA} , P_{BB} , etc.

Finally, Eqs. (4.38), (4.41), (4.46) and (4.47), and Eqs. (4.42), (4.43), (4.48) and (4.49) can be combined to give exact expressions for stress σ_{22} in Materials A and B , respectively:

$$\begin{aligned} \sigma_{22}(x_1, x_2 \geq 0) &= 2 \sum_{\alpha=1}^3 b_s \left(\xi_{A\alpha 22}^{sR} P_A + \xi_{A\alpha 22}^{sI} Q_A \right) \\ &+ 4\pi \sum_{\alpha=1}^3 \sum_{\beta=1}^3 b_s \left(\Psi_{AA22}^{\alpha\beta s} P_{AA} - \Psi_{AB22}^{\alpha\beta s} P_{AB} + \chi_{AA22}^{\alpha\beta s} Q_{AA} - \chi_{AB22}^{\alpha\beta s} Q_{AB} \right), \end{aligned} \quad (4.51)$$

$$\begin{aligned}\sigma_{22}(x_1, x_2 \leq 0) &= 2 \sum_{\alpha=1}^3 b_s \left(\xi_{B\alpha 22}^{sR} P_B + \xi_{B\alpha 22}^{sI} Q_B \right) \\ &+ 4\pi \sum_{\alpha=1}^3 \sum_{\beta=1}^3 b_s \left(\Psi_{BA22}^{\alpha\beta s} P_{BA} - \Psi_{BB22}^{\alpha\beta s} P_{BB} + \chi_{BA22}^{\alpha\beta s} Q_{BA} - \chi_{BB22}^{\alpha\beta s} Q_{BB} \right),\end{aligned}\quad (4.52)$$

where the constants are given by

$$\Psi_{AA22}^{\alpha\beta s} = \sum_{i=1}^4 \left[\operatorname{sgn}(x_2^r) \left(\xi_{A\alpha 22}^{tR} c_{A\alpha i} + \xi_{A\alpha 22}^{tI} c'_{A\alpha i} \right) r_{A\beta i}^{sI} + \left(\xi_{A\alpha 22}^{tR} c'_{A\alpha i} - \xi_{A\alpha 22}^{tI} c_{A\alpha i} \right) r_{A\beta i}^{sR} \right], \quad (4.53)$$

$$\Psi_{AB22}^{\alpha\beta s} = \sum_{i=1}^4 \left[\operatorname{sgn}(x_2^r) \left(\xi_{A\alpha 22}^{tR} c_{A\alpha i} + \xi_{A\alpha 22}^{tI} c'_{A\alpha i} \right) r_{B\beta i}^{sI} + \left(\xi_{A\alpha 22}^{tR} c'_{A\alpha i} - \xi_{A\alpha 22}^{tI} c_{A\alpha i} \right) r_{B\beta i}^{sR} \right], \quad (4.54)$$

$$\chi_{AA22}^{\alpha\beta s} = \sum_{i=1}^4 \left[\left(\xi_{A\alpha 22}^{tR} c_{A\alpha i} + \xi_{A\alpha 22}^{tI} c'_{A\alpha i} \right) r_{A\beta i}^{sR} - \operatorname{sgn}(x_2^r) \left(\xi_{A\alpha 22}^{tR} c'_{A\alpha i} - \xi_{A\alpha 22}^{tI} c_{A\alpha i} \right) r_{A\beta i}^{sI} \right], \quad (4.55)$$

$$\chi_{AB22}^{\alpha\beta s} = \sum_{i=1}^4 \left[\left(\xi_{A\alpha 22}^{tR} c_{A\alpha i} + \xi_{A\alpha 22}^{tI} c'_{A\alpha i} \right) r_{B\beta i}^{sR} - \operatorname{sgn}(x_2^r) \left(\xi_{A\alpha 22}^{tR} c'_{A\alpha i} - \xi_{A\alpha 22}^{tI} c_{A\alpha i} \right) r_{B\beta i}^{sI} \right], \quad (4.56)$$

$$\Psi_{BA22}^{\alpha\beta s} = \sum_{i=1}^4 \left[\operatorname{sgn}(x_2^r) \left(\xi_{B\alpha 22}^{tR} c_{B\alpha i} - \xi_{B\alpha 22}^{tI} c'_{B\alpha i} \right) r_{A\beta i}^{sI} + \left(\xi_{B\alpha 22}^{tR} c'_{B\alpha i} + \xi_{B\alpha 22}^{tI} c_{B\alpha i} \right) r_{A\beta i}^{sR} \right], \quad (4.57)$$

$$\Psi_{BB22}^{\alpha\beta s} = \sum_{i=1}^4 \left[\operatorname{sgn}(x_2^r) \left(\xi_{B\alpha 22}^{tR} c_{B\alpha i} - \xi_{B\alpha 22}^{tI} c'_{B\alpha i} \right) r_{B\beta i}^{sI} + \left(\xi_{B\alpha 22}^{tR} c'_{B\alpha i} + \xi_{B\alpha 22}^{tI} c_{B\alpha i} \right) r_{B\beta i}^{sR} \right], \quad (4.58)$$

$$\chi_{BA22}^{\alpha\beta s} = \sum_{i=1}^4 \left[\left(\xi_{B\alpha 22}^{tR} c_{Bti} - \xi_{B\alpha 22}^{tI} c'_{Bti} \right) r_{A\beta i}^{sR} - \text{sgn}(x_2^r) \left(\xi_{B\alpha 22}^{tR} c'_{Bti} + \xi_{B\alpha 22}^{tI} c_{Bti} \right) r_{A\beta i}^{sI} \right], \quad (4.59)$$

$$\chi_{BB22}^{\alpha\beta s} = \sum_{i=1}^4 \left[\left(\xi_{B\alpha 22}^{tR} c_{Bti} - \xi_{B\alpha 22}^{tI} c'_{Bti} \right) r_{B\beta i}^{sR} - \text{sgn}(x_2^r) \left(\xi_{B\alpha 22}^{tR} c'_{Bti} + \xi_{B\alpha 22}^{tI} c_{Bti} \right) r_{B\beta i}^{sI} \right]. \quad (4.60)$$

For stresses σ_{12} and σ_{11} , only the subscripts 22 in $\xi_{A\alpha 22}^{sR}$, $\Psi_{AA22}^{\alpha\beta s}$, etc. need be changed to 12 and 11, respectively. The subscripts of the terms in $r_{A\beta i}^{sI}$, etc. in Eq. (4.45) are not changed. The stress components in Material *A* contain six rational forms P_A , Q_A , P_{AA} , P_{AB} , Q_{AA} and Q_{AB} , while those in Material *B* contain the forms P_B , Q_B , P_{BA} , P_{BB} , Q_{BA} and Q_{BB} . These rational functions are defined in Eqs. (3.1) and (3.2). Thus, Eqs. (4.51) and (4.52) express the stress components in terms of rational functions multiplied by appropriate material coefficients. Also, the various summations in the above equations can be explained as follows. The repeated symbol *s* expresses the contribution of the two Burgers vector components b_1 and b_2 of the mixed edge dislocation source. The repeated symbol *t* characterizes the contributions of both glide and climb image dislocations located on $x_2 = 0$. The summation over *i* is related to the satisfaction of the four interfacial boundary conditions using image dislocations. Summations over β and α reflect the effect of anisotropic elasticity on image and source dislocations.

4.2.2 Governing equations for edge dislocation in film-substrate

According to fig. 4.2(b) and the traction-free conditions in Eq. (4.1), it is necessary to write down expressions for σ_{22} and σ_{12} due to the source dislocation located at (x_1^o, x_2^o)

and due to the glide and climb images with densities $\rho^1(x_1)$ and $\rho^2(x_1)$ distributed on the free surface. By setting $x_1^r = x_1^o$ and $x_2^r = x_2^o$ in Eq. (4.51), the stress components at $(x_1, x_2 = h)$ due to the source with Burgers vector components b_s in the film can be written as:

$$\begin{aligned} f_{22}(x_1) = \sigma_{22}(x_1, x_2 = h) = & 2 \sum_{\alpha=1}^3 b_s \left(\xi_{A\alpha 22}^{sR} P_{A1} + \xi_{A\alpha 22}^{sI} Q_{A1} \right) \\ & + 4\pi \sum_{\alpha=1}^3 \sum_{\beta=1}^3 b_s \left(\Psi_{AA22}^{\alpha\beta s} P_{AA1} - \Psi_{AB22}^{\alpha\beta s} P_{AB1} + \chi_{AA22}^{\alpha\beta s} Q_{AA1} - \chi_{AB22}^{\alpha\beta s} Q_{AB1} \right), \end{aligned} \quad (4.61)$$

$$\begin{aligned} f_{12}(x_1) = \sigma_{12}(x_1, x_2 = h) = & 2 \sum_{\alpha=1}^3 b_s \left(\xi_{A\alpha 12}^{sR} P_{A1} + \xi_{A\alpha 12}^{sI} Q_{A1} \right) \\ & + 4\pi \sum_{\alpha=1}^3 \sum_{\beta=1}^3 b_s \left(\Psi_{AA12}^{\alpha\beta s} P_{AA1} - \Psi_{AB12}^{\alpha\beta s} P_{AB1} + \chi_{AA12}^{\alpha\beta s} Q_{AA1} - \chi_{AB12}^{\alpha\beta s} Q_{AB1} \right), \end{aligned} \quad (4.62)$$

where

$$\begin{aligned} P_{A1} &\equiv P(x_1 - x_1^o, p_{A\alpha}^R(h - x_2^o), p_{A\alpha}^I(h - x_2^o)), \\ P_{AA1} &\equiv P(x_1 - x_1^o, p_{A\alpha}^R h - p_{A\beta}^R x_2^o, |p_{A\alpha}^I h| + |-p_{A\beta}^I x_2^o|). \end{aligned} \quad (4.63)$$

Similarly for Q_{A1} , P_{AB1} , Q_{AA1} and Q_{AB1} . Also, $\text{sgn}(x_2^r)$ in $\Psi_{AA22}^{\alpha\beta s}$, etc. becomes $\text{sgn}(x_2^o)$.

Similarly, the stress components on $x_2 = h$ due to the glide and climb images $\rho_u dx_1^u$, $u = 1, 2$ at the location (x_1^u, h) can be obtained using Eqs. (4.51) and (4.52). For the entire distribution, integration with respect to x_1^u yields:

$$\begin{aligned}
 \sigma_{22}(x_1, x_2 = h) = & 2 \sum_{\alpha=1}^3 \int_{-\infty}^{\infty} \left(\xi_{A\alpha 22}^{uR} P(x_1 - x_1', 0, 0) + \xi_{A\alpha 22}^{uI} Q(x_1 - x_1', 0, 0) \right) \rho_u(x_1') dx_1' \\
 & + 4\pi \sum_{\alpha=1}^3 \sum_{\beta=1}^3 \int_{-\infty}^{\infty} \left\{ \Psi_{AA22}^{\alpha\beta u} P(x_1 - x_1', (p_{A\alpha}^R - p_{A\beta}^R)h, |p_{A\alpha}^I h| + |-p_{A\beta}^I h|) \right. \\
 & \quad - \Psi_{AB22}^{\alpha\beta u} P(x_1 - x_1', (p_{A\alpha}^R - p_{B\beta}^R)h, |p_{A\alpha}^I h| + |-p_{B\beta}^I h|) \\
 & \quad + \chi_{AA22}^{\alpha\beta u} Q(x_1 - x_1', (p_{A\alpha}^R - p_{A\beta}^R)h, |p_{A\alpha}^I h| + |-p_{A\beta}^I h|) \\
 & \quad \left. - \chi_{AB22}^{\alpha\beta u} Q(x_1 - x_1', (p_{A\alpha}^R - p_{B\beta}^R)h, |p_{A\alpha}^I h| + |-p_{B\beta}^I h|) \right\} \rho_u(x_1') dx_1', \tag{4.64}
 \end{aligned}$$

and similarly for $\sigma_{12}(x_1, h)$. Note here $\text{sgn}(x_2') = \text{sgn}(h) = 1$ in $\Psi_{AA22}^{\alpha\beta u}$, etc. These expressions can be written as the Hilbert transform and the H and I transforms. By Eq. (4.14), the coefficient of $P(x - x', 0, 0)$ in the above equation is D_{A22}^u / π . By Eq. (4.15) the coefficient of $Q(x - x', 0, 0)$ is zero, and it is immaterial whether the third argument in Q is 0^+ or 0^- . Hence, Eq. (4.64) reduces to:

$$\begin{aligned}
 \sigma_{22}(x_1, x_2 = h) = & D_{A22}^u H(0, 0) [\rho_u(x_1)] \\
 & + 4\pi^2 \sum_{\alpha=1}^3 \sum_{\beta=1}^3 \left\{ \Psi_{AA22}^{\alpha\beta u} H_{AA2} - \Psi_{AB22}^{\alpha\beta u} H_{AB2} + \chi_{AA22}^{\alpha\beta u} I_{AA2} - \chi_{AB22}^{\alpha\beta u} I_{AB2} \right\} [\rho_u(x_1)], \tag{4.65}
 \end{aligned}$$

where $H_{AA2} \equiv H((p_{A\alpha}^R - p_{A\beta}^R)h, (p_{A\alpha}^I + p_{A\beta}^I)h)$, and similar for $H_{AB2}, I_{AA2}, I_{AB2}$.

The governing integral equations corresponding to Eq. (4.1) are obtained by combining Eqs. (4.61) and (4.65) for σ_{22} and similar expressions for σ_{12} , resulting in:

$$D_{A22}^u H(0,0)[\rho_u(x_1)] = -4\pi^2 \sum_{\alpha=1}^3 \sum_{\beta=1}^3 \left\{ \Psi_{AA22}^{\alpha\beta u} H_{AA2} - \Psi_{AB22}^{\alpha\beta u} H_{AB2} + \chi_{AA22}^{\alpha\beta u} I_{AA2} - \chi_{AB22}^{\alpha\beta u} I_{AB2} \right\} [\rho_u(x_1)] - f_{22}(x_1), \quad (4.66)$$

$$D_{A12}^u H(0,0)[\rho_u(x_1)] = -4\pi^2 \sum_{\alpha=1}^3 \sum_{\beta=1}^3 \left\{ \Psi_{AA12}^{\alpha\beta u} H_{AA2} - \Psi_{AB12}^{\alpha\beta u} H_{AB2} + \chi_{AA12}^{\alpha\beta u} I_{AA2} - \chi_{AB12}^{\alpha\beta u} I_{AB2} \right\} [\rho_u(x_1)] - f_{12}(x_1). \quad (4.67)$$

The above are dual "Fredholm-Cauchy" integral equations of the first kind with rational kernels and two unknown density functions $\rho_1(x_1)$ and $\rho_2(x_1)$. Equations (4.66) and (4.67) are first transformed by taking the Hilbert transforms of all terms, resulting in:

$$D_{A22}^u \rho_u(x_1) = T_{1u} [\rho_u(x_1)] + F_{22}(x_1), \quad (4.68)$$

$$D_{A12}^u \rho_u(x_1) = T_{2u} [\rho_u(x_1)] + F_{12}(x_1), \quad (4.69)$$

where the iterative properties of Eqs. (3.21) and (3.22) have been used, and

$$T_{iu} = 4\pi^2 \sum_{\alpha=1}^3 \sum_{\beta=1}^3 \left\{ -\Psi_{AAjk}^{\alpha\beta u} I_{AA2} + \Psi_{ABjk}^{\alpha\beta u} I_{AB2} + \chi_{AAjk}^{\alpha\beta u} H_{AA2} - \chi_{ABjk}^{\alpha\beta u} H_{AB2} \right\}, \quad (4.70)$$

with $j = k = 2$ when $i = 1$ and $j = 1, k = 2$ when $i = 2$. Also,

$$\begin{aligned} F_{22}(x_1) = H(0,0)[f_{22}(x_1)] &= 2 \sum_{\alpha=1}^3 b_s \left(-\xi_{A\alpha 22}^{sR} Q_{A1} + \xi_{A\alpha 22}^{sI} P_{A1} \right) \\ &+ 4\pi \sum_{\alpha=1}^3 \sum_{\beta=1}^3 b_s \left(-\Psi_{AA22}^{\alpha\beta s} Q_{AA1} + \Psi_{AB22}^{\alpha\beta s} Q_{AB1} + \chi_{AA22}^{\alpha\beta s} P_{AA1} - \chi_{AB22}^{\alpha\beta s} P_{AB1} \right), \end{aligned} \quad (4.71)$$

$$\begin{aligned} F_{12}(x_1) = H(0,0)[f_{12}(x_1)] &= 2 \sum_{\alpha=1}^3 b_s \left(-\xi_{A\alpha 12}^{sR} Q_{A1} + \xi_{A\alpha 12}^{sI} P_{A1} \right) \\ &+ 4\pi \sum_{\alpha=1}^3 \sum_{\beta=1}^3 b_s \left(-\Psi_{AA12}^{\alpha\beta s} Q_{AA1} + \Psi_{AB12}^{\alpha\beta s} Q_{AB1} + \chi_{AA12}^{\alpha\beta s} P_{AA1} - \chi_{AB12}^{\alpha\beta s} P_{AB1} \right). \end{aligned} \quad (4.72)$$

Equations (4.68) and (4.69) are dual Fredholm integral equations of the second kind since the unknown $\rho_u(x_1)$ appear directly in the equations. The kernels in I_{AA2} , I_{AB2} , H_{AA2} and H_{AB2} are all rational functions. The equations (4.68) and (4.69) can be solved by Neumann series and Nyström method. In this chapter, Nyström method is used. The Neumann series will be discussed in Section 4.3.

Equation (4.70) and (4.71) can be written into matrix form:

$$\begin{bmatrix} \rho_1(x_1) \\ \rho_2(x_1) \end{bmatrix} = \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} \begin{bmatrix} \rho_1(x_1) \\ \rho_2(x_1) \end{bmatrix} + \begin{bmatrix} G_1(x_1) \\ G_2(x_1) \end{bmatrix}, \quad \text{or } \boldsymbol{\rho}(x_1) = \mathbf{K}\boldsymbol{\rho}(x_1) + \mathbf{G}(x_1), \quad (4.73)$$

where

$$\begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} = \frac{1}{D_{A22}^1 D_{A12}^2 - D_{A22}^2 D_{A12}^1} \begin{bmatrix} D_{A12}^2 & -D_{A22}^2 \\ -D_{A12}^1 & D_{A22}^1 \end{bmatrix} \cdot \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix}, \quad (4.74)$$

$$\begin{bmatrix} G_1(x_1) \\ G_2(x_1) \end{bmatrix} = \frac{1}{D_{A22}^1 D_{A12}^2 - D_{A22}^2 D_{A12}^1} \begin{bmatrix} D_{A12}^2 & -D_{A22}^2 \\ -D_{A12}^1 & D_{A22}^1 \end{bmatrix} \cdot \begin{bmatrix} F_{22}(x_1) \\ F_{12}(x_1) \end{bmatrix}. \quad (4.75)$$

Eq. (4.73) can be rewritten

$$\rho(x_1) = \mathbf{K} \rho(x_1) + \mathbf{G}(x_1) = \int_{-\infty}^{\infty} \mathbf{J}(x_1, x_1') \cdot \rho(x_1') dx_1' + \mathbf{G}(x_1), \quad (4.76)$$

where the matrix kernel function is:

$$\mathbf{J}(x_1, x_1') = \frac{1}{D_{A1}^1 D_{A2}^2 - D_{A1}^2 D_{A2}^1} \begin{bmatrix} D_{A12}^2 & -D_{A22}^2 \\ -D_{A12}^1 & D_{A22}^1 \end{bmatrix} \cdot \begin{bmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{bmatrix}. \quad (4.77)$$

The kernel elements J_{iu} are related to the transforms T_{iu} , i.e.:

$$J_{iu} = 4\pi^2 \sum_{\alpha=1}^3 \sum_{\beta=1}^3 \left\{ -\Psi_{AAjk}^{\alpha\beta u} Q_{AA2} + \Psi_{ABjk}^{\alpha\beta u} Q_{AB2} + \chi_{AAjk}^{\alpha\beta u} P_{AA2} - \chi_{ABjk}^{\alpha\beta u} P_{AB2} \right\}, \quad (4.78)$$

where $P_{AA2} \equiv P(x_1 - x_1', (p_{A\alpha}^R - p_{A\beta}^R)h, (p_{A\alpha}^I + p_{A\beta}^I)h)$, and similarly for $P_{AB2}, Q_{AA2}, Q_{AB2}$. By

the change of variable according to

$$x_1 = \frac{bt}{\sqrt{1-t^2}}, \quad x_1' = \frac{bt'}{\sqrt{1-t'^2}}, \quad (4.79)$$

where b is Burgers vector magnitude, Eq. (4.76) can be transformed into

$$\rho(t) = \int_{-1}^1 \mathbf{J}(t, t') \cdot \rho(t') \frac{b}{(1-t'^2)^{3/2}} dt' + \mathbf{G}(t). \quad (4.80)$$

Replacing the integral by N -point Gaussian-Legendre quadrature, Eq. (4.80) becomes

$$\rho(t) = \sum_{j=1}^N w_j \mathbf{J}(t, t_j') \cdot \rho(t_j') \frac{b}{(1-t_j'^2)^{3/2}} + \mathbf{G}(t), \quad (4.81)$$

where w_j are the weights and t_j' are the quadrature points. Evaluating Eq. (4.81) at the quadrature points t_i yields:

$$\rho(t_i) = \sum_{j=1}^N w_j \mathbf{J}(t_i, t_j') \cdot \rho(t_j') \frac{b}{(1-t_j'^2)^{3/2}} + \mathbf{G}(t_i). \quad (4.82)$$

Defining

$$\tilde{K}_{ij} = w_j \mathbf{J}(t_i, t_j') \frac{b}{(1-t_j'^2)^{3/2}}, \quad (4.83)$$

Eq. (4.82) can be rewritten as:

$$(\mathbf{I} - \tilde{\mathbf{K}}) \cdot \boldsymbol{\rho} = \mathbf{G}, \quad (4.84)$$

where $\mathbf{I}$ is the identity matrix and $\tilde{\mathbf{K}}$ is the matrix of the elements $\tilde{K}_{ij}$. Equation (4.84) is a set of $2N$ linear algebraic equations with $2N$ unknowns $\rho_1(t_i)$ and $\rho_2(t_i)$. After solving for these unknowns, $\boldsymbol{\rho}(t)$ and finally $\boldsymbol{\rho}(x_1)$ can be obtained from Eq. (4.82).

4.3 Solutions for single screw dislocation in decoupled film-substrate problems

The image dislocation method is also applied to solve the decoupled problem of a film-substrate containing a screw dislocation. The film-substrate system is again transformed into an infinite bimaterial system with image screw dislocation distribution on the surface. The physical condition is $\sigma_{23}(x_1, x_2 = h) = 0$. The procedure is similar to that described in Section 4.2. The governing equation reduces to:

$$D_{23}^3 \rho(x_1) = T[\rho(x_1)] + F_{23}(x_1), \quad (4.85)$$

where

$$D_{23}^3 = 2\pi \sum_{\alpha=1}^3 \xi_{\alpha 23}^{3R}, \quad (4.86)$$

$$T = 4\pi^2 \sum_{\alpha=1}^3 \sum_{\beta=1}^3 \left\{ -\Psi_{AA23}^{\alpha\beta 3} I_{AA2} + \Psi_{AB23}^{\alpha\beta 3} I_{AB2} + \chi_{AA23}^{\alpha\beta 3} H_{AA2} - \chi_{AB23}^{\alpha\beta 3} H_{AB2} \right\}, \quad (4.87)$$

$$F_{23}(x_1) = 2 \sum_{\alpha=1}^3 b_3 \left(-\xi_{A\alpha 23}^{3R} Q_{A1} + \xi_{A\alpha 23}^{3I} P_{A1} \right) + 4\pi \sum_{\alpha=1}^3 \sum_{\beta=1}^3 b_3 \left(-\Psi_{AA23}^{\alpha\beta 3} Q_{AA1} + \Psi_{AB23}^{\alpha\beta 3} Q_{AB1} + \chi_{AA23}^{\alpha\beta 3} P_{AA1} - \chi_{AB23}^{\alpha\beta 3} P_{AB1} \right). \quad (4.88)$$

The kernels in I_{AA2} , I_{AB2} , H_{AA2} and H_{AB2} are all rational functions. Equation (4.85) can be solved as Neumann series (Tricomi, 1985).

$$\rho(x_1) = K\rho(x_1) + G(x_1), \quad (4.89)$$

where
$$K = \frac{1}{D_{23}^3} T, \quad G(x_1) = \frac{1}{D_{23}^3} F_{23}(x_1). \quad (4.90)$$

Equation (4.89) has the iterative solution

$$\begin{aligned} \rho_{n+1}(x_1) &= K\rho_n(x_1) + G(x_1) = \\ K \left[K \left[\rho_{n-1}(x_1) + G(x_1) \right] \right] + G(x_1) &= \dots = K_{n+1} \rho_0(x_1) + \sum_{m=0}^n K_m [G(x_1)], \end{aligned} \quad (4.91)$$

where $n = 0, 1, 2, \dots, \infty$, K_0 is the identify matrix with diagonal unity elements and null off-diagonal elements, K_m is the K matrix acting upon itself m times, and ρ_n is the n -th iterative solution of ρ . In particular, one can set the first solution $\rho_0(x_1) = G(x_1)$. Equation (4.88) is the solution of Eq. (4.89) when n tends to infinity.

In the current problem, each time K operates on itself the integral operators have their second arguments increase in absolute value, as stated in Eqs. (3.13)-(3.16). This implies that the rational kernels associated with K_{n+1} tend to zero as $n \rightarrow \infty$. Physically, the transforms in K are associated with the stresses produced on the free surface by the interface images, and surface images are needed to compensate for these additional stresses. These surface images in turn induce interface images, which further produce stresses and images on the free surface and so on. The stresses so induced will progressively become weaker as they must for dislocations, and mathematically this corresponds to K operating on itself repeatedly. Hence, Eq. (4.91) is the exact series solution to the integral Eq. (4.89). A closed-form summation of Eq. (4.89) in the limit $n \rightarrow \infty$ cannot yet be found due to the complexity of the coefficients of the integral transforms.

4.4 Solutions for a mixed dislocation in coupled film-substrate problems

Consider a mixed dislocation with Burgers vector $\mathbf{b} = (b_1, b_2, b_3)$ located in a film-substrate. Assume that the problem is coupled, i.e., both edge and screw images are needed to satisfy the boundary conditions even if the source dislocation is pure edge or pure screw in character. The boundary conditions are $\sigma_{2i} = 0$ on the free surface, as in Eq. (4.1). Three image dislocation densities $\rho_1(x_1), \rho_2(x_1), \rho_3(x_1)$ must be distributed on the free surface as shown in fig. 4.1.

The Green's function for a mixed dislocation in a coupled bimaterial problem is obtained first. The film-substrate system is decomposed into two homogenous systems, where the image dislocation densities $\rho_{At''}(x)$ and $\rho_{Bt''}(x)$, where $t''=1,2,3$ are distributed at the position of the interface in each homogenous system. The continuous conditions across the interface are:

$$\sigma_{12}(x_1, 0^+) = \sigma_{12}(x_1, 0^-), \quad \sigma_{22}(x_1, 0^+) = \sigma_{22}(x_1, 0^-), \quad \sigma_{23}(x_1, 0^+) = \sigma_{23}(x_1, 0^-), \quad (4.92)$$

$$\frac{\partial u_1}{\partial x_1}(x_1, 0^+) = \frac{\partial u_1}{\partial x_1}(x_1, 0^-), \quad \frac{\partial u_2}{\partial x_1}(x_1, 0^+) = \frac{\partial u_2}{\partial x_1}(x_1, 0^-), \quad \frac{\partial u_3}{\partial x_1}(x_1, 0^+) = \frac{\partial u_3}{\partial x_1}(x_1, 0^-). \quad (4.93)$$

The derivation procedure is similar to those used for the pure edge and pure screw dislocations. Also, the solutions for Eqs. (4.92)-(4.93) are constructed as for Eqs. (4.28)-(4.29). After obtaining the solutions for the mixed dislocation in the infinite bimaterial system, the governing equations for the film-substrate system can be obtained by combining contributions from the source dislocation and the image dislocations on the free surface. Numerical solutions can be obtained by using the Neumann series or Nyström method. The final equations are similar to those obtained in the previous subsections, and are omitted here.

4.5 Numerical results

In this section, numerical results for both decoupled and coupled two-layer problems will be presented.

The problem of a single dislocation is studied for three film-substrate systems of indium nitride on silicon carbide (InN/SiC), zinc on zinc (Zn/Zn), and germanium-silicon alloy on silicon ($\text{Ge}_x\text{Si}_{1-x}/\text{Si}$). The study also includes an infinite bimaterial of potassium on potassium (K/K) and a potassium (K) strip. The elastic constants of the cubic and hexagonal materials are listed in Table 4.1.

Hexagonal	InN ¹	SiC ²	Zn ³		Cubic	K ⁴	Si ⁵	$\text{Ge}_x\text{Si}_{1-x}$ ⁶
C'_{11} (GPa)	182	553	61		C'_{11}	4.57	165.7	$128.9x+165.7(1-x)$
C'_{33}	190	501	161		C'_{12}	3.74	63.9	$48.3x+63.9(1-x)$
C'_{12}	121	52	50.1		C'_{44}	2.63	79.6	$67.1x+79.6(1-x)$
C'_{23}	104	111	34.2					
C'_{66}	9.9	163	38.3					

¹Sheleg and Savastenko (1979), ²Kamitani et al. (1997), ^{3,4}Hirth and Lothe (1982), ^{5,6}Jain et al. (1997)

Table 4.1. Elastic constants of hexagonal and cubic crystals with respect to the crystal frame $x'_1 - x'_2 - x'_3$. For the hexagonal crystals, the x'_1 - axis is perpendicular to the basal plane.

4.5.1 Edge dislocation in decoupled film-substrate problems

Figure 4.4 plots, in full lines, the stresses $\sigma_{11}, \sigma_{22}, \sigma_{12}$ at the free surface due to an interfacial edge dislocation in an InN/SiC film-substrate. The Neumann series with $n = 2$ are used as the solutions. The parameters are $h = 500b$, and $(x_1^o, x_2^o) = (0, 0)$. The in-plane c -axis orientations of the InN and SiC crystals are respectively $\theta_A = 15^\circ$ and $\theta_B = 130^\circ$. The column (a)-(c) and the column (d)-(f) show the cases of $\alpha = 0^\circ$ and $\alpha = 90^\circ$,

respectively. For comparison, the stresses on $x_2 = 500b$ due to the same dislocation in an infinite InN/SiC bimaterial ($h = \infty$) are also plotted in dashed lines. It can be seen that the

Fig. 4.4. (a)-(c): Plot of stresses $\sigma_{11}, \sigma_{22}, \sigma_{12}$ at $x_2 = 500b$ versus the normalized distance x_1/b due to an edge dislocation with Burgers vector magnitude b and orientation $\alpha = 0^\circ$ at the origin in InN/SiC. The full and dashed lines show the results for a film of thickness $h = 500b$ and $h = \infty$, respectively. (d)-(f): Plot of the stresses for the case of $\alpha = 90^\circ$.

stresses σ_{21}, σ_{22} at the free surface are essentially zero, while they are of significant values at the corresponding location in the infinite bimaterial. This verifies that the solved image densities satisfy the governing integral equations rather well. For $\alpha = 0^\circ$, stress σ_{11} at the free surface reduces in magnitude compared to the infinite bimaterial case. For $\alpha = 90^\circ$, the reverse is true.

To compare the solutions obtained from the Neumann series and Nyström methods, Figure 4.5 plots stress σ_{22} on the free surface for the material system of fig. 4.4 for $\alpha = 0^\circ$ and $\alpha = 90^\circ$. The c -axis orientations of InN and SiC are respectively $\theta_A = 15^\circ$

Fig. 4.5. Comparison of σ_{22} at $x_2 = 500b$ versus the normalized distance x_1/b as calculated by the Neumann series method (a, c) and the Nyström method (b, d). The stress is due to an edge dislocation with Burgers vector magnitude b and orientation $\alpha = 0^\circ$ or 90° at the origin in InN/SiC. The solutions converge to zero as n or N increases.

and $\theta_B = 130^\circ$. The series indices are $n = 0, 1, 2$ and $N = 10, 100, 500$. It can be observed that as n or N increases, σ_{22} tends to the correct value of zero. In the case of $\alpha = 0^\circ$, $n = 2$ appears to yield a better accuracy compared to $N = 500$, but the opposite is true when $\alpha = 90^\circ$.

The image forces in the x_2 – direction on a dislocation with Burgers vector $\mathbf{b} = b(1, 0, 0)$ in $\text{Ge}_\alpha\text{Si}_{1-\alpha}/\text{Si}$ (010) and InN/SiC (0001) are next calculated as a function of position x_2^o/h . For the epitaxial $\text{Ge}_\alpha\text{Si}_{1-\alpha}/\text{Si}$ ($\alpha = 0.1$) film on the (010) plane of the silicon substrate, the x_1 – , x_2 – and x_3 – axes coincide with the crystallographic directions $[10\bar{1}]$, $[010]$ and $[101]$, respectively. For InN/SiC , the axes coincide with $[\bar{1}2\bar{1}0]$, $[0001]$ and $[10\bar{1}0]$, respectively. Figure 4.6 (a) plots F_2 / F_{free} against x_2^o/h for the range $0 < x_2^o/h < 0.8$, where $F_2 = -\sigma_{11}b_1 - \sigma_{12}b_2 - \sigma_{13}b_3$, and F_{free} is the image force F_2 on the dislocation at the distance h from the free surface in a half-space of the *substrate* material. For $\text{Ge}_\alpha\text{Si}_{1-\alpha}/\text{Si}$, the minimum image force occurs when the dislocation is close to the substrate, i.e., $x_2^o/h \sim 0.06$. For InN/SiC , the curve tilts the other way, and the minimum image force occurs when the dislocation is at $x_2^o/h \sim 0.5$. Moreover, F_2 / F_{free} is less than 1 over a wide range of x_2^o/h values for InN/SiC , whereas it is above 1 for $\text{Ge}_\alpha\text{Si}_{1-\alpha}/\text{Si}$. This reveals the complex interaction between the free surface and the interface, which may not be easily rationalized. Strong repulsion of the dislocation from the substrate is also predicted for InN/SiC due to the large dissimilarity between the elastic constants of the two materials. A weaker repulsion occurs for the dislocation in $\text{Ge}_{0.1}\text{Si}_{0.9}$, whose elastic constants are not very different from those of Si. Although not

shown here, the image force F_2 experiences a jump as the dislocation positions change from just above to just below the interface, since σ_{11} experiences a jump across the interface. Furthermore, Figure 4.6 (b) shows the results for a mixed dislocation with Burgers vector $\mathbf{b} = b(1/2, -1/\sqrt{2}, 1/2)$ in $\text{Ge}_\alpha\text{Si}_{1-\alpha}/\text{Si}$ ($\alpha = 0.1$).

Fig. 4.6. (a) Plot of the normalized image force F_2/F_{free} versus normalized dislocation position y_0/h . The Burgers vector $\mathbf{b} = b(1, 0, 0)$. (b) Comparison of present results with the previous for $\text{Ge}_\alpha\text{Si}_{1-\alpha}/\text{Si}$ ($\alpha = 0.1$) and $\mathbf{b} = b(1/2, -1/\sqrt{2}, 1/2)$.

Even though the dislocation is mixed type, the system is still decoupled. It can be seen that the present results agree well with those of Choi and Earmme (2002). The results of fig. 4.6 emphasize the importance of elastic anisotropy and material inhomogeneity in determining the image forces.

Figure 4.7 plots the interfacial stresses due to a glide edge dislocation (b , $\alpha = 0^\circ$) at $(x_1^o, x_2^o) = (0, 0.5h)$ in a Zn/Zn film-substrate, where $h = 500b$ and $\theta_A = 15^\circ$, $\theta_B = 130^\circ$. The components $\sigma_{22}(x_1, 0)$ and $\sigma_{12}(x_1, 0)$ are continuous across the interface, as required in the formulation. In contrast, $\sigma_{11}(x_1, 0^+)$ differs considerably from $\sigma_{11}(x_1, 0^-)$ due to the strong elastic anisotropy of the Zn crystal, for which $C'_{33}/C'_{11} = 2.64$ (see Table 4.1). The stress range between -0.01 and 0.03 GPa in fig. 4.7 will likely be amplified in the presence of multiple dislocations. Indeed, large interfacial stresses due to dislocations in the film may cause further nucleation of defects (dislocations, cracks).

Fig. 4.7. Variation of interfacial stresses with normalized distance x_1/b due to a glide edge dislocation at $(0, 0.5h)$ in Zn/Zn. The film thickness is $h = 500b$, and the c -axis orientations are $\theta_A = 15^\circ$ and $\theta_B = 130^\circ$. Note the jump in σ_{11} across the interface.

Figure 4.8 plots the whole field for the shear stress σ_{12} due to an interfacial dislocation ($b, \alpha = 0^\circ$) located at the origin in InN/SiC. The film thickness is $h = 500b$, and the c -axis orientations of InN and SiC are respectively $\theta_A = 15^\circ$ and $\theta_B = 130^\circ$. The results are shown in the region of $-500 < x_1/b < 500$, $-500 < x_2/b < 500$. The contours are continuous, albeit with kinks, across the interface. The zero stress contours merge at the film surface, in agreement with the free surface condition, and they compartmentalize the region into six sub-regions with shear stresses of alternately opposite signs. These contours are similar to those for the infinite bimaterial case (see Wu et al. 2003), where however the six zero contours extend radially to infinity and the contour loops are of different sizes.

Fig. 4.8. Contour plot of σ_{12} due to an interfacial glide edge dislocation in the InN/SiC film-substrate. The c -axis orientations are $\theta_A = 15^\circ$, $\theta_B = 130^\circ$, and the thickness of the InN film is $h = 500b$. The line $x_2/b = 500$ is the zero stress line corresponding to the film surface. The contours are continuous with kinks across the interface.

4.5.2 Screw dislocation in decoupled film-substrate problems

Consider first an interfacial screw dislocation with the Burgers vector magnitude b at the origin in an InN/SiC film-substrate of thickness $h = 500b$. The in-plane c -axis orientations of the InN and SiC crystals with respect to the x_1 -axis are respectively $\theta_A = 15^\circ$ and $\theta_B = 130^\circ$. To show the convergence of the results to the correct values, the component σ_{23} on the free surface $x_2 = 500b$ is plotted for different values of the iterative index $n = 0, 1, 2$ in fig. 4.9. For comparison, σ_{23} on $x_2 = 500b$ in an infinite InN/SiC bimaterial is also plotted. It can be seen that the solutions converge as n increases, and they converge to the value of zero, which is correct since σ_{23} must vanish on the free surface. The curve $\sigma_{23}(h = \infty)$ shows that the stress in the infinite bimaterial at the position corresponding to the free surface in the film-substrate is rather large, of the order of 0.01 GPa.

Fig. 4.9. Plots of the stress σ_{23} on the free surface $x_2 = 500b$ due to an interfacial screw dislocation with Burgers vector magnitude b in an InN/SiC film-substrate (solid lines) and at the corresponding position due to the same dislocation in an infinite bimaterial (dashed line). The three solid lines indicate the iterative index n used for the dislocation image density $\rho_n(x_1)$.

In fig. 4.10, the stress component σ_{13} for $n = 0, 1, 2$ in the film-substrate and σ_{13} in the infinite bimaterial on the line $x_2 = 500b$ are also plotted. The adjustment of the σ_{13} curve is evident as n increases from 0 to 2. Moreover, the marked difference between the $n = 2$ and the $h = \infty$ solutions illustrate the significant influence of the free surface on the elastic field.

Fig. 4.10. Plots of the stress σ_{13} on the free surface $x_2 = 500b$ due to an interfacial screw dislocation with Burgers vector magnitude b in an InN/SiC film-substrate (solid lines) and at the corresponding position due to the same dislocation in an infinite bimaterial (dashed line). The three solid lines indicate the iterative index n used for the dislocation image density $\rho_n(x_1)$. The influence of the free surface is evident from the marked difference between the $n = 2$ and $h = \infty$ curves.

The results in figs. 4.9 and 4.10 show that the stress components converge with the inclusion of more, albeit progressively weaker, image components $n = 0, 1, 2$, etc., and that the governing integral equation is satisfied quite well by the image solution for $n = 2$. The latter check is important since although the convergence of solutions has been studied

in previous works, how well the converged solution satisfies the governing equation has rarely been reported.

We consider the $\text{Ge}_\alpha\text{Si}_{1-\alpha}/\text{Si}$ and $\text{Si}/\text{Ge}_\alpha\text{Si}_{1-\alpha}$ systems, where $\alpha = 0.5$. Specifically, the image force in the x_2 – direction on a screw dislocation with Burgers vector $\mathbf{b} = b(0, 0, 1)$ in the film is calculated as a function of position x_2^o/h . For the $\{1\ 0\ 0\}$ plane epitaxy, the x_1 – , x_2 – and x_3 – axes coincide with the crystallographic directions $[10\bar{1}]$, $[010]$, $[101]$, respectively. Figure 4.11 plots F_2/F_{free} against x_2^o/h for the range of $0 < x_2^o/h < 0.8$. In the present case, the ratio of F_{free} for a dislocation in silicon and germanium silicon half spaces is 1.1.

Fig. 4.11. Plot of the normalized image force F_2/F_{free} versus normalized dislocation position x_2^o/h in $\text{Ge}_\alpha\text{Si}_{1-\alpha}/\text{Si}$ and $\text{Si}/\text{Ge}_\alpha\text{Si}_{1-\alpha}$ ($\alpha = 0.5$) systems. The Burgers vector $\mathbf{b} = b(0, 0, 1)$.

The results show that the screw dislocation is attracted towards the free surface. If the substrate is harder than the film as in $\text{Ge}_\alpha\text{Si}_{1-\alpha}/\text{Si}$, the dislocation is repelled by the interface. Conversely, if the substrate is softer as in $\text{Si}/\text{Ge}_\alpha\text{Si}_{1-\alpha}$, the dislocation is attracted towards the interface. This example demonstrates the importance of the details of material inhomogeneity on the image force.

We next investigate how the normalized image force F_2 / F_{free} on a screw dislocation varies with the normalized film thickness h/b , where $60 < h/b < 500$, and F_{free} is the image force on a screw dislocation at a depth of $500b$ in a half space of the substrate material. The dislocation has the Burgers vector $\mathbf{b} = b(0, 0, 1)$ and is located at the fixed position $(0, 5b)$. Thus, the dislocation is always closer to the interface than to the free surface in this simulation. Again, the x_1 -, x_2 - and x_3 - axes coincide with the crystallographic directions $[10\bar{1}]$, $[010]$, $[101]$, respectively. Figure 4.12 plots the variation for the $\text{Ge}_\alpha\text{Si}_{1-\alpha}/\text{Si}$ and $\text{Si}/\text{Ge}_\alpha\text{Si}_{1-\alpha}$ ($\alpha = 0.5$) systems. The results show that in the case of $\text{Ge}_\alpha\text{Si}_{1-\alpha}/\text{Si}$ the dislocation is always repelled by the interface. For $\text{Si}/\text{Ge}_\alpha\text{Si}_{1-\alpha}$, the dislocation is attracted towards the interface for thick films $h/b > 120$ but repelled by it for thin films $h/b < 120$. This shows the influence of the free surface overriding that of the soft substrate as the film becomes thin.

Fig. 4.12. Plot of the normalized image force F_2 / F_{free} versus normalized film thickness h/b in $\text{Ge}_\alpha\text{Si}_{1-\alpha}/\text{Si}$ and $\text{Si}/\text{Ge}_\alpha\text{Si}_{1-\alpha}$ ($\alpha = 0.5$) systems.

To verify the continuity of σ_{23} across the interface $x_2 = 0$, Figure 4.13 plots the interfacial stresses due to a screw dislocation with Burgers vector magnitude b at $(x_1^o, x_2^o) = (0, 0.5h)$ in a Zn/Zn and a SiC/SiC film-substrate, respectively. The film thickness is $h = 500b$ and the c -axis orientations are $\theta_A = 15^\circ$, $\theta_B = 130^\circ$. It can be seen that $\sigma_{23}(x_1, 0)$ is indeed continuous across the Zn/Zn or the SiC/SiC interface, as the interface continuity conditions are exactly satisfied in the formulation. In contrast, $\sigma_{11}(x_1, 0^+)$ differs considerably from $\sigma_{11}(x_1, 0^-)$ in the Zn/Zn bicrystal due to the strong elastic anisotropy of the Zn crystal. The difference is somewhat less for the SiC/SiC due to the weaker anisotropy of the SiC crystal.

Fig. 4.13. Variation of interfacial stresses with normalized distance x_1/b due to a screw dislocation at $(0, 0.5h)$ in (a) Zn/Zn and (b) SiC/SiC bicrystal with a free surface. The film thickness is $h = 500b$, and the c -axis orientations are $\theta_A = 15^\circ$ and $\theta_B = 130^\circ$.

Finally, Figure 4.14 plots the whole field for σ_{23} due to an interfacial screw dislocation located at the origin in InN/SiC. Again, the c -axis orientations of the InN and

SiC crystals are taken to be $\theta_A = 15^\circ$ and $\theta_B = 130^\circ$, respectively. Part (a) of the figure refers to an infinite bimaterial. Part (b) refers to a film-substrate with the film thickness $h = 500b$. The results are shown in the region $-500 < x_1/b < 500$, $-500 < x_2/b < 500$. The contours are continuous, albeit with kinks, across the interface. The zero stress contours merge at the film surface, in agreement with the free surface condition. The contour loops in the film-substrate reduce in size compare to the loops in the infinite bimaterial, showing the influence of the free surface.

Fig. 4.14. Contour plots of σ_{23} due to an interfacial screw dislocation in the InN/SiC (a) infinite bicrystal and (b) film-substrate. The c -axis orientations are $\theta_A = 15^\circ$, $\theta_B = 130^\circ$, and the thickness of the InN film is $h = 500b$. The contours are continuous with kinks across the interface.

4.5.3 Dislocation in coupled two-layer problems

For the coupled problem, the stresses and displacement gradients caused by edge and screw components all need to be considered, even though the source dislocation is pure edge or pure screw dislocation.

In fig. 4.15, the stresses of $\sigma_{12}, \sigma_{22}, \sigma_{23}$ across interface are shown in the infinite bimaterial system potassium on potassium (K/K). The source is pure glide dislocation located at $(0, 100b)$. The crystal orientation is such that in the upper potassium, the direction $[14\bar{5}]$ is along the out-of-plane x_3 -axis, and the Burgers vector is along the $[111]$ direction in the x_1-x_2 plane. While, in the lower potassium, coordinate system x_1-, x_2-, x_3- coincide with crystal system x'_1-, x'_2-, x'_3- , respectively. Thus, this is a coupled problem. From the figure below, it can be seen that stress σ_{23} is not zero across interface, and stresses $\sigma_{12}, \sigma_{22}, \sigma_{23}$ are continuous across interface, which satisfy the physical conditions.

Fig. 4.15. Interfacial stresses across bimaterial K/K system. The source glide dislocation with Burgers vector magnitude b is at $(0, 100b)$.

Now consider an edge dislocation, with Burgers vector magnitude b , at the position $(0, x_2^0)$ in a potassium strip of thickness h . The present results for the strip, obtained by using vanishingly small elastic constants for the substrate material. The crystal orientation is such that the direction $[14\bar{5}]$ is along the out-of-plane x_3 - axis, and the Burgers vector is along the $[111]$ direction in the $x_1 - x_2$ plane, making an angle of α with respect to the x_1 - direction.

Fig. 4.16. Comparison of the dependence of the normalized image force on dislocation position in a potassium strip as calculated by the current (dislocation image) method, the alternating technique (Choi and Earmme (2002)) and the Fourier transform technique (Wu and Chiu (1995)).

The Nyström method is used to obtain the numerical solutions, with $N = 250$. It can be shown that the image force pushes the dislocation towards the free surfaces. For the climb edge dislocation ($\alpha = 90^\circ$), the present results agree very well with those of Wu and Chiu (1995), who used the Fourier transform technique, and those of Choi and Earmme (2002), who used the alternating method. For the glide edge dislocation ($\alpha = 0^\circ$), the agreement between the present results and those by Wu and Chiu is also good. However, the alternating method results by Choi and Earmme differ appreciably from these results. Choi and Earmme remarked that up to fifteen terms were used in their functions for the case of $\alpha = 0^\circ$.

We investigate the discrepancy further by plotting the three stress components on the free surfaces versus x/b , see fig. 4.17. Here, the strip has a thickness of $h = 500b$, $\alpha = 0^\circ$, and $x_2^o/h = 0.3$, the position where the results show significant discrepancy.

Fig. 4.17. Variation of stresses on the two free surfaces of a potassium strip with normalized distance x_1/b . The strip thickness $h = 500b$, and the edge dislocation (Burgers vector magnitude b and orientation $\alpha = 0^\circ$) is located at $x_1^o = 0, x_2^o = 0.3h$. The σ_{22} , σ_{12} and σ_{23} on the two free surfaces are approximately zero.

Figure 4.17 shows that stresses σ_{22} , σ_{12} and σ_{23} on both free surfaces are very close to zero, verifying that the integral equations are satisfied quite well. Moreover, σ_{11} above the dislocation at the top surface is tensile, while below the dislocation at the lower surface it is compressive. In an infinite body, σ_{11} would be compressive and tensile above and below the dislocation. The change of sign shows the significant influence of the free surfaces on the dislocation stress field. In passing, note also that the stresses when plotted against x_1/b are independent of b .

4.6 Conclusions

In this chapter, the image method is used to derive the Green's function for an edge and a screw dislocation in an anisotropic film-substrate composite. The semi-infinite film-substrate problem is transformed to an infinite bimaterial problem in which the interface boundary conditions are satisfied exactly *a priori*. The image formulation leads to Fredholm integral equations of the second kind with singular terms, which can be removed by using the properties of the H and I transforms. Exact solutions in the form of Neumann series of rational functions of linear to quadratic polynomials and approximate solutions by the Nyström method are obtained. The accuracy of the present solutions is verified by convergence study, by the satisfaction of free boundary conditions on the film surface, and by comparison with past results. The numerical results demonstrate the importance of elastic anisotropy, film-substrate inhomogeneity and the free surface in determining the various stress components and the image forces. These solutions can

serve as Green's functions for problems of cracks and dislocation pileups, and the image method can be readily extended for the analysis of multilayer solids.

CHAPTER FIVE

A MIXED DISLOCATION IN GENERAL MULTILAYER SYSTEMS

The organization of this chapter is as follows. Section 5.1 introduces the problem of a mixed dislocation in a general multilayer system. Section 5.2 develops the general image decomposition method. Section 5.3 presents the governing equations for the three-layer and N -layer problems, and Section 5.4 illustrates the technique used to transform the governing singular integral equations into non-singular integral equations. Section 5.5 presents the numerical results. Section 5.6 summarizes the major findings of the chapter.

5.1 Problem description

Figure 5.1(a) shows the problem of a single dislocation in a multilayer system. This source dislocation can be pure edge, pure screw or mixed, and is represented by a cross. It can be located anywhere in the multilayer system, which consists of elastically dissimilar anisotropic layers. Two free surfaces at the top and bottom of the multilayer system are also assumed. The problem is in general coupled. The thickness of each layer is denoted by $h_1, h_2, \dots, h_n$. Note that Layers 1 and n may be semi-infinite, in which case $h_1 \rightarrow \infty$ and/or $h_n \rightarrow \infty$ and correspondingly there will be no free surfaces at all or only one free

surface. The aim is to determine the stress field caused by source dislocation, and hence the image force on the source dislocation in the multilayer system.

Fig. 5.1. A mixed dislocation in a dissimilar anisotropic multilayer system with free surfaces. The thickness of each layer is donated by $h_1, h_2, \dots, h_n$.

5.2 Generalized image decomposition technique

To solve the stated problem, an image decomposition technique is developed. The technique is explained with reference to the problem of a mixed dislocation in a simple three-layer system before generalization to an N -layer system.

5.2.1 Formulation for three-layer system

As shown in fig. 5.2, the Layers 1, 2 and 3 from top to bottom are elastically dissimilar and have the thicknesses h_1, h_2 and h_3 respectively. Layers 1 and 3 may be

semi-infinite, in which case $h_1 \rightarrow \infty$ and/or $h_3 \rightarrow \infty$. The mixed dislocation, marked by the cross symbol, may be located anywhere within the multilayer system, say (x_{1s}, x_{2s}) with respect to a coordinate frame $x_1 - x_2$ located on the top surface. The problem is to find the elastic solutions such as the stress field and hence the image force on the mixed dislocation.

Fig. 5.2. A mixed dislocation located at (x_{1s}, x_{2s}) in a finite anisotropic three-layer system. The thicknesses h_1 and h_3 may be infinite so that the solid becomes semi-infinite or infinite.

Assuming that the uppermost and lowermost faces (Face 1 and Face 4) of the three-layer solid are free surfaces and that the interfaces (Face 2 and Face 3) are perfectly

bonded, the physical boundary conditions are that the tractions σ_{2i} vanish on the free surfaces and that the stresses σ_{2i} and the displacement gradients $\partial u_i / \partial x_1$ (equivalently the displacements u_i), where $i = 1, 2, 3$ are continuous across the interfaces:

$$\sigma_{2i}(x_1, x_2 = 0) = 0, \quad (5.1)$$

$$\sigma_{2i}(x_1, x_2 = -h_1^+) = \sigma_{2i}(x_1, x_2 = -h_1^-), \quad (5.2)$$

$$\frac{\partial u_i}{\partial x_1}(x_1, x_2 = -h_1^+) = \frac{\partial u_i}{\partial x_1}(x_1, x_2 = -h_1^-), \quad (5.3)$$

$$\sigma_{2i}(x_1, x_2 = -(h_1 + h_2)^+) = \sigma_{2i}(x_1, x_2 = -(h_1 + h_2)^-), \quad (5.4)$$

$$\frac{\partial u_i}{\partial x_1}(x_1, x_2 = -(h_1 + h_2)^+) = \frac{\partial u_i}{\partial x_1}(x_1, x_2 = -(h_1 + h_2)^-), \quad (5.5)$$

$$\sigma_{2i}(x_1, x_2 = -(h_1 + h_2 + h_3)) = 0. \quad (5.6)$$

Equations (5.1) and (5.6) are the traction-free conditions on Face 1 and Face 4, respectively, and Eqs. (5.2)-(5.3) and Eqs. (5.4)-(5.5) are the continuity conditions across Face 2 and Face 3, respectively.

The above problem is solved by the method of continuously distributed image dislocations (also called virtual dislocations). The original problem is decomposed into

three subproblems. The first, second and third subproblem is a problem of an infinite homogeneous body of the material 1, 2 and 3, respectively. Each also contains the mixed dislocation at (x_{1s}, x_{2s}) . This is shown in fig. 5.3. The shaded region in each subproblem in the figure corresponds to the real region in the original problem, and image dislocations are distributed on the upper and lower faces of these shaded regions to satisfy the boundary conditions Eqs. (5.1)-(5.6). For instance, if the boundary condition Eq. (5.2) is to be satisfied, the stress components $\sigma_{2i}(x_1, x_2 = -h_1^+)$ and $\sigma_{2i}(x_1, x_2 = -h_1^-)$ are calculated from all sources, i.e., the source dislocation and image dislocations, in Subproblems 1 and 2, respectively, and then set equal to each other. In this approach, all field quantities in Layers 1, 2 and 3 of the original problem must be calculated respectively from Subproblems 1, 2 and 3 and not by the superposition of the subproblems.

Fig. 5.3. Decomposition of a three-layer problem (left) into three infinite homogeneous subproblems denoted by $k = 1, 2$ and 3 . The elastic fields in Layers 1, 2 and 3 of the original problem are determined from summing the contributions of the source (marked by the cross symbol) and all dislocation images in Subproblems 1, 2 and 3, respectively. The partial image density solutions ρ_{1U}^t , ρ_{1L}^t , etc. are determined by the consistency condition when the three-layer problem degenerates into one- and two-layer problems.

The densities of the image dislocations are denoted by ρ^t , where $t = 1, 2, 3$ denotes the $x_1 -$, $x_2 -$ and $x_3 -$ components (the first two are the edge components, the last is the screw component). Thus, image dislocations $(\rho_{1U}^t, \rho_{1L}^t)$, $(\rho_{2U}^t, \rho_{2L}^t)$ and $(\rho_{3U}^t, \rho_{3L}^t)$ are distributed to the upper and lower faces of the shaded regions in Subproblems 1, 2 and 3 of fig. 5.3, respectively. These six densities (not counting the edge and screw components) are to be determined via the satisfaction of the boundary conditions. However, they are insufficient for the solution of the problem because they do not satisfy the consistency condition that when two contiguous layers are identical in material the corresponding subproblems must likewise be identical. Consequently, if Layers 1 and 2 are identical in material (thickness may or may not be the same), then images with the density ρ_{2L}^t must also be distributed on “Face” 3 in Subproblem 1, and similarly images with the density ρ_{1U}^t must be located on “Face” 1 in Subproblem 2. Boundary conditions will then ensure that on Face 2 $\rho_{1L}^t = \rho_{2U}^t$, (which must be zero since Face 2 is not an interface when Layers 1 and 2 are identical). Using the same reasoning, if Layers 2 and 3 are identical, then images with the densities ρ_{1U}^t and ρ_{2U}^t on “Face” 1 and “Face” 2 in Subproblem 2 must also be distributed at the corresponding locations in Subproblem 3, and images with the density ρ_{3L}^t in Subproblem 3 must be correspondingly located in Subproblem 2 and hence also in Subproblem 1. Consistency is also achieved if all three layers are identical. However, if the identical layers are not contiguous, e.g., if Layers 1 and 3 only are identical, Subproblems 1 and 3 will not be the same. Also, the consistency condition requires that the mixed dislocation source in the original problem be present in each subproblem as already assumed above. Thus, partial solutions have been found in the

three subproblems via the consistency condition, which must hold when the original three-layer problem is degenerated into two- and one-layer problems. They are partial in the sense that the forms or numerical values of these density functions are yet to be determined from the boundary conditions. This concept was not developed in the earlier works (Wu and Wang, 2005; Wang and Wu, 2005), where the two-layer film-substrate problem was not decomposed into homogeneous subproblems. Rather, infinite bi-layers were used as the basic elements in the previous works.

5.2.2 Formulation for general N -layer system

The generalization to an N -layer system can be achieved without difficulty. The problem is similarly divided into N infinite homogeneous subproblems, each with the dislocation source at (x_{1s}, x_{2s}) . Using the consistency requirement, the partial solutions ρ_{JK}^t in Layer J of Subproblem K are determined to be:

$$\rho_{JK}^t = \begin{cases} \rho_{JU}^t, J = 1, K \\ \rho_{(J-1)L}^t, J = K + 1, N + 1 \end{cases} \quad (5.7)$$

Applying Eq. (5.7) to a four-layer system, the partial solutions in the four subproblems are:

$$\begin{aligned} \rho_{J1}^t &= \{\rho_{1U}^t, \rho_{1L}^t, \rho_{2L}^t, \rho_{3L}^t, \rho_{4L}^t\}, \\ \rho_{J2}^t &= \{\rho_{1U}^t, \rho_{2U}^t, \rho_{2L}^t, \rho_{3L}^t, \rho_{4L}^t\}, \\ \rho_{J3}^t &= \{\rho_{1U}^t, \rho_{2U}^t, \rho_{3U}^t, \rho_{3L}^t, \rho_{4L}^t\}, \\ \rho_{J4}^t &= \{\rho_{1U}^t, \rho_{2U}^t, \rho_{3U}^t, \rho_{4U}^t, \rho_{4L}^t\}. \end{aligned} \quad (5.8)$$

These image densities are also shown in fig. 5.4 and can be verified to be correct using the consistency condition. Furthermore, if the topmost layer is semi-infinite with $h_1 \rightarrow \infty$, then the image densities ρ'_{1K} , $K=1, \dots, N$ on Face 1 of all the subproblems are zero. Likewise, if the lowermost layer is semi-infinite, $\rho'_{(N+1)K} = 0$ on Face $N+1$ of all the subproblems. This is because the boundaries infinitely far from the source are not affected by it and no images are necessary to satisfy the free boundary conditions. Hence, the image solutions of Eq. (5.7) are the (partial) solutions for the problem of a dislocation in a finite, semi-infinite or infinite anisotropic multilayer system. It should be noted that in a finite N -layer problem, the actual number of unknown densities is $2N$ (or $6N$ if the edge and screw components are counted separately). In a semi-infinite N -layer problem, the number of unknowns is $2N-1$ or alternatively $3(2N-1)$.

Fig. 5.4. Decomposition of a four-layer problem (left) into four infinite homogeneous subproblems by image decomposition method.

5.3 Governing integral equations

Based on Stroh's (1958) formalism, the stress and displacement gradient fields due to a mixed dislocation with Burgers vector components b_t ($t=1,2,3$) located at (x_{1s}, x_{2s}) in a homogeneous anisotropic solid under plane strain can be expanded in terms of P and Q (see Chapter 4). For the current multilayer system problem, assuming that Subproblem K ($K=1,2,\dots,N$) is considered. Then, the stresses and displacement gradients at a general position (x_1, x_2) in terms of $\Delta x_1 = x_1 - x_{1s}$ and $\Delta x_2 = x_2 - x_{2s}$ can be written as:

$$\begin{aligned} \sigma_{ij}(K, b_t, \Delta x_1, \Delta x_2) \\ = 2 \sum_{\alpha=1}^3 \left(\zeta_{K\alpha ij}^{tR} P(\Delta x_1, p_{K\alpha}^R \Delta x_2, p_{K\alpha}^I \Delta x_2) + \zeta_{K\alpha ij}^{tI} Q(\Delta x_1, p_{K\alpha}^R \Delta x_2, p_{K\alpha}^I \Delta x_2) \right) b_t, \end{aligned} \quad (5.9)$$

$$\begin{aligned} \frac{\partial u_i}{\partial x_j}(K, b_t, \Delta x_1, \Delta x_2) \\ = 2 \sum_{\alpha=1}^3 \left(\zeta_{K\alpha ij}^{tR} P(\Delta x_1, p_{K\alpha}^R \Delta x_2, p_{K\alpha}^I \Delta x_2) + \zeta_{K\alpha ij}^{tI} Q(\Delta x_1, p_{K\alpha}^R \Delta x_2, p_{K\alpha}^I \Delta x_2) \right) b_t, \end{aligned} \quad (5.10)$$

where $p_{K\alpha}^R$ and $p_{K\alpha}^I$ are the real (indicated by superscript R) and imaginary (superscript I) parts of the three pairs of complex conjugate eigenvalues in Stroh's sextic formulation for Subproblem K (no sum over K), and $\zeta_{K\alpha ij}^{tR}$, $\zeta_{K\alpha ij}^{tI}$, $\zeta_{K\alpha ij}^{tR}$, $\zeta_{K\alpha ij}^{tI}$ have the same meanings as in previous chapters. It can also be seen that the expressions for the stress and displacement components differ only in the constants $\zeta_{K\alpha ij}^{tR}$, $\zeta_{K\alpha ij}^{tI}$, $\zeta_{K\alpha ij}^{tR}$, $\zeta_{K\alpha ij}^{tI}$. The four arguments of σ_{ij} and $\partial u_i / \partial x_j$ in Eqs. (5.9)-(5.10) emphasize their dependence on the

subproblem, the Burgers vector of the source dislocation, and the position of the point of interest relative to the source position. It should be noted that if the anisotropic materials degenerate into isotropic ones, Eqs. (5.9)-(5.10) take a form different from P and Q . However, numerically isotropic materials can be approximated very closely by weakly anisotropic materials.

According to the decomposition scheme, the stresses and displacement gradients on Face F due to the image dislocations ρ_{JK}^t of Eq. (5.7) distributed on Face J in Subproblem K must also be evaluated. Let the position of interest be (x_1, x_{2F}) , where x_{2F} is the x_2 coordinate of Face F , and the image dislocation density is at (x_1', x_{2J}) , where x_{2J} is the x_2 coordinate of Face J . Replacing b_t in Eq. (5.9) by $\rho_{JK}^t(x_1')$ and integrating from $x_1' = -\infty$ to $x_1' = +\infty$ yields the stresses :

$$\begin{aligned}
 & \sigma_{ij}(K, \rho_{JK}^t, x_1, \Delta x_2) \\
 &= \int_{-\infty}^{\infty} 2 \sum_{\alpha=1}^3 \left(\xi_{K\alpha ij}^{tR} P(\Delta x_1, p_{K\alpha}^R \Delta x_2, p_{K\alpha}^I \Delta x_2) + \xi_{K\alpha ij}^{tI} Q(\Delta x_1, p_{K\alpha}^R \Delta x_2, p_{K\alpha}^I \Delta x_2) \right) \rho_{JK}^t(x_1') dx_1' \\
 &= 2\pi \sum_{\alpha=1}^3 \left(\xi_{K\alpha ij}^{tR} H(p_{K\alpha}^R \Delta x_2, p_{K\alpha}^I \Delta x_2) + \xi_{K\alpha ij}^{tI} I(p_{K\alpha}^R \Delta x_2, p_{K\alpha}^I \Delta x_2) \right) [\rho_{JK}^t(x_1)],
 \end{aligned} \tag{5.11}$$

where $\Delta x_1 = x_1 - x_1'$ and $\Delta x_2 = x_{2F} - x_{2J}$. Similarly, the displacement gradients due to the image distribution are obtained when $(\xi_{K\alpha ij}^{tR}, \xi_{K\alpha ij}^{tI})$ are replaced by $(\zeta_{K\alpha ij}^{tR}, \zeta_{K\alpha ij}^{tI})$:

$$\begin{aligned}
& \frac{\partial u_i}{\partial x_j}(K, \rho_{JK}^t, x_1, \Delta x_2) \\
& = 2\pi \sum_{\alpha=1}^3 \left(\zeta_{K\alpha ij}^{tR} H(p_{K\alpha}^R \Delta x_2, p_{K\alpha}^I \Delta x_2) + \zeta_{K\alpha ij}^{tI} I(p_{K\alpha}^R \Delta x_2, p_{K\alpha}^I \Delta x_2) \right) [\rho_{JK}^t(x_1)].
\end{aligned} \tag{5.12}$$

In summary, the stresses and displacement gradients due to a discrete mixed dislocation have been expressed as the sum of P and Q functions as given by Eqs. (5.9)-(5.10), while those due to distributed images as the sum of H and I transforms of the density function as given by Eqs. (5.11)-(5.12).

The governing equations of the finite three-layer problem with top and bottom free surfaces can now be derived. Consider the top free surface ($F=1$) as shown in fig. 5.2. The boundary condition to be satisfied is $\sigma_{2i}(x_1, x_2=0)=0$ (Eq. (5.1)) and according to the decomposition scheme of fig. 5.3, $\sigma_{2i}(x_1, x_2=0)$ is the sum of the stress due to the dislocation source at (x_{1s}, x_{2s}) and those due to the images ρ_{JK}^t at (x_1', x_{2J}) on Face J (for $J=1, 2, 3, 4$) in Subproblem $K=1$. Using Eqs. (5.9) and (5.11), this can be written as:

$$\sigma_{2i}(x_1, x_{21}) = \sigma_{2i}(1, b_i, x_1 - x_{1s}, x_{21} - x_{2s}) + \sum_{J=1}^{J=4} \sigma_{2i}(1, \rho_{J1}^t, x_1, x_{21} - x_{2J}) = 0, \tag{5.13}$$

where $i=1, 2, 3$ and $x_{21}=0$ is the x_2 coordinate of Face 1. Similarly, the traction free condition on the bottom free surface ($F=4$) given by Eq. (5.6) can be written as:

$$\sigma_{2i}(x_1, x_{24}) = \sigma_{2i}(3, b_i, x_1 - x_{1s}, x_{24} - x_{2s}) + \sum_{J=1}^{J=4} \sigma_{2i}(3, \rho_{J3}^t, x_1, x_{24} - x_{2J}) = 0, \tag{5.14}$$

where $x_{24} = -h_1 - h_2 - h_3$ is the x_2 coordinate of Face 4. The stress continuity condition across Face 2 is similarly written using Subproblem 1 (just above Face 2) and Subproblem 2 (just below Face 2):

$$\begin{aligned} & \sigma_{2i}(1, b_t, x_1 - x_{1s}, x_{22} - x_{2s}) + \sum_{J=1}^{J=4} \sigma_{2i}(1, \rho_{J1}^t, x_1, x_{22} - x_{2J}) \\ &= \sigma_{2i}(2, b_t, x_1 - x_{1s}, x_{22} - x_{2s}) + \sum_{J=1}^{J=4} \sigma_{2i}(2, \rho_{J2}^t, x_1, x_{22} - x_{2J}), \end{aligned} \quad (5.15)$$

where $x_{22} = -h_1$ is the x_2 coordinate of Face 2. Likewise, the stress continuity across Face 3 is expressed by:

$$\begin{aligned} & \sigma_{2i}(2, b_t, x_1 - x_{1s}, x_{23} - x_{2s}) + \sum_{J=1}^{J=4} \sigma_{2i}(2, \rho_{J2}^t, x_1, x_{23} - x_{2J}) \\ &= \sigma_{2i}(3, b_t, x_1 - x_{1s}, x_{23} - x_{2s}) + \sum_{J=1}^{J=4} \sigma_{2i}(3, \rho_{J3}^t, x_1, x_{23} - x_{2J}), \end{aligned} \quad (5.16)$$

where $x_{23} = -h_1 - h_2$ is the x_2 coordinate of Face 3. For the continuity of the displacement gradient across Face 2 and Face 3, the equations are analogous to Eqs. (5.15)-(5.16):

$$\begin{aligned} & \frac{\partial u_i}{\partial x_1}(1, b_t, x_1 - x_{1s}, x_{22} - x_{2s}) + \sum_{J=1}^{J=4} \frac{\partial u_i}{\partial x_1}(1, \rho_{J1}^t, x_1, x_{22} - x_{2J}) \\ &= \frac{\partial u_i}{\partial x_1}(2, b_t, x_1 - x_{1s}, x_{22} - x_{2s}) + \sum_{J=1}^{J=4} \frac{\partial u_i}{\partial x_1}(2, \rho_{J2}^t, x_1, x_{22} - x_{2J}), \end{aligned} \quad (5.17)$$

$$\begin{aligned}
& \frac{\partial u_i}{\partial x_1}(2, b_t, x_1 - x_{1s}, x_{23} - x_{2s}) + \sum_{j=1}^{J=4} \frac{\partial u_i}{\partial x_1}(2, \rho_{j2}^t, x_1, x_{23} - x_{2j}) \\
& = \frac{\partial u_i}{\partial x_1}(3, b_t, x_1 - x_{1s}, x_{23} - x_{2s}) + \sum_{j=1}^{J=4} \frac{\partial u_i}{\partial x_1}(3, \rho_{j3}^t, x_1, x_{23} - x_{2j}).
\end{aligned} \tag{5.18}$$

Equations (5.13)-(5.18) are thus the governing equations for the finite three-layer problem. The number of unknowns ρ_{jK}^t for $j=1,2,3,4$ and $K=1,2,3$ for each value of t is actually six as given by the partial solutions of Eq. (5.7), which are indicated in fig. 5.3. By induction, these equations can be generalized for the finite N -layer problem with $N+1$ faces (2 free surfaces and $N-1$ interfaces). For the free surface condition on Face F ($F=1$ and $F=N+1$), the governing equations are:

$$\sigma_{2i}(K, b_t, x_1 - x_{1s}, x_{2F} - x_{2s}) + \sum_{j=1}^{J=N+1} \sigma_{2i}(K, \rho_{jK}^t, x_1, x_{2F} - x_{2j}) = 0, \tag{5.19}$$

where x_{2F} is the x_2 -coordinate of Face F . For $F=1$, $K=F$, while for $F=N+1$, $K=F-1$, indicating the subproblem to be used in evaluating Eq. (5.19). For stress and displacement gradient continuity across the interfaces $F=2,3,\dots,N$, the governing equations are respectively:

$$\begin{aligned}
& \sigma_{2i}(K, b_t, x_1 - x_{1s}, x_{2F} - x_{2s}) + \sum_{j=1}^{J=N+1} \sigma_{2i}(K, \rho_{jK}^t, x_1, x_{2F} - x_{2j}) \\
& = \sigma_{2i}(K+1, b_t, x_1 - x_{1s}, x_{2F} - x_{2s}) + \sum_{j=1}^{J=N+1} \sigma_{2i}(K+1, \rho_{j(K+1)}^t, x_1, x_{2F} - x_{2j}),
\end{aligned} \tag{5.20}$$

$$\begin{aligned}
& \frac{\partial u_i}{\partial x_1}(K, b_t, x_1 - x_{1s}, x_{2F} - x_{2s}) + \sum_{J=1}^{J=N+1} \frac{\partial u_i}{\partial x_1}(K, \rho_{JK}^t, x_1, x_{2F} - x_{2J}) \\
& = \frac{\partial u_i}{\partial x_1}(K+1, b_t, x_1 - x_{1s}, x_{2F} - x_{2s}) + \sum_{J=1}^{J=N+1} \frac{\partial u_i}{\partial x_1}(K+1, \rho_{J(K+1)}^t, x_1, x_{2F} - x_{2J}),
\end{aligned} \tag{5.21}$$

where $K = F - 1$, which implies that for Interface F the left and right sides of Eqs. (5.20)-(5.21) are to be calculated from Subproblems $F - 1$ and F , respectively. If either Layer 1 or Layer N or both are infinite, the corresponding free surface condition expressed by Eq. (5.19) is dropped accordingly, and Eqs. (5.20)-(5.21) still hold with $\rho_{JK}^t = 0$ for $J = 1$ and/or $N + 1$ (equivalently the summation over J ranges from 2 to $N + 1$ or 1 to N or 2 to N , instead of from 1 to $N + 1$). Thus, Eqs. (5.19)-(5.21) are the governing equations for the general N -layer finite, semi-infinite or infinite problems.

The derived governing equations are of two basic types. The terms containing b_t as an argument are associated with the source dislocation and are composed of the rational functions P and Q , while those containing ρ_{JK}^t are associated with the distributed images and are composed of the H and I transforms of ρ_{JK}^t . When $x_{2F} - x_{2J} \rightarrow 0^\pm$, the terms $\sigma_{2i}(K, \rho_{JK}^t, x_1, x_{2F} - x_{2J})$ (and similarly $\sigma_{2i}(K+1, \rho_{J(K+1)}^t, x_1, x_{2F} - x_{2J})$) in Eqs. (5.19)-(5.20) reduce to the following according to Eq. (5.11) :

$$\begin{aligned}
& \sigma_{2i}(K, \rho_{JK}^t, x_1, 0) \\
&= 2\pi \sum_{\alpha=1}^3 \left(\xi_{K\alpha 2i}^{tR} H(0, 0) + \xi_{K\alpha 2i}^{tI} I(0, 0^\pm) \right) [\rho_{JK}^t(x_1)] \\
&= 2\pi \sum_{\alpha=1}^3 \xi_{K\alpha 2i}^{tR} H(0, 0) [\rho_{JK}^t(x_1)] + 2\pi \operatorname{sgn}(0^\pm) \sum_{\alpha=1}^3 \xi_{K\alpha 2i}^{tI} \rho_{JK}^t(x_1) \\
&= 2\pi \sum_{\alpha=1}^3 \xi_{K\alpha 2i}^{tR} H(0, 0) [\rho_{JK}^t(x_1)],
\end{aligned} \tag{5.22}$$

Eq. (5.22) consists of only the Hilbert transform, which gives rise to the singular term in the governing equations. Physically, it represents the stresses on a face due to image dislocations distributed on the face itself. Thus, the governing equations, Eqs. (5.19)-(5.20), consist of both the singular terms $H(0,0)[\rho_{JK}^t(x_1)]$ and the non-singular terms $H(a,b)[\rho_{JK}^t(x_1)]$, $a \neq 0, b \neq 0$. They are Cauchy integral equations of the first type, since the unknown densities $\rho_{JK}^t(x_1)$ do not appear independently, i.e., they appear only as integrands. In contrast, the terms $\frac{\partial u_i}{\partial x_1}(K, \rho_{JK}^t, x_1, x_{2F} - x_{2J})$ in Eq. (5.22) reduce to:

$$\begin{aligned}
& \frac{\partial u_i}{\partial x_1}(K, \rho_{JK}^t, x_1, 0) \\
&= 2\pi \sum_{\alpha=1}^3 \left(\xi_{K\alpha i1}^{tR} H(0, 0) + \xi_{K\alpha i1}^{tI} I(0, 0^\pm) \right) [\rho_{JK}^t(x_1)] \\
&= 2\pi \sum_{\alpha=1}^3 \xi_{K\alpha i1}^{tR} H(0, 0) [\rho_{JK}^t(x_1)] + 2\pi \operatorname{sgn}(0^\pm) \sum_{\alpha=1}^3 \xi_{K\alpha i1}^{tI} \rho_{JK}^t(x_1),
\end{aligned} \tag{5.23}$$

where $2\pi \sum_{\alpha=1}^3 \zeta_{K\alpha i}^{II}$ equals zero if $i \neq t$ and equals $-1/2$ if $i = t$. This is because integrating $\partial u_i / \partial x_1$ along the infinitely long rectangular path enclosing a dislocation with Burgers vector purely in the x_t direction must yield a non-zero displacement jump in that direction but no jump in the other two directions. Thus, when $i = t$ the second term in Eq. (5.23) will not vanish and its sign depends on the signum function of $x_{2F} - x_{2J}$. It will make equal but opposite contributions to $\partial u_i / \partial x_1$ evaluated just above and just below Face F . Consequently, Eq. (5.22) contains the singular term $H(0,0)[\rho'_{JK}(x_1)]$, non-singular terms $H(a,b)[\rho'_{JK}(x_1)]$, $a \neq 0, b \neq 0$ and the density $\rho'_{JK}(x_1)$ itself, and it is thus a Cauchy integral equation of the second type.

If the governing equations are exclusively Cauchy integral equations of the first type, which are derived from the stress boundary conditions, then the singular terms $H(0,0)[\rho'_{JK}(x_1)]$ can be eliminated by taking the Hilbert transform of each term in the integral equations, resulting in non-singular integral equations. This can be explained using Eq. (5.19) as an example. Taking the Hilbert transform of the first term of this equation will yield $H(0,0)[P(x_1)]$ and $H(0,0)[Q(x_1)]$. Taking the Hilbert transform of the second term will yield terms involving $H(0,0)H(a,b)$ and $H(0,0)I(a,b)$ (here $a \neq 0, b \neq 0$), all of which correspond to non-singular integrals. However, if some of the governing equations are of the second kind (displacement gradient boundary conditions), then the singular terms cannot be eliminated simply by taking the Hilbert transform. This is because the unknown densities appear by themselves in these equations and taking the

Hilbert transform of them will yield singular terms. In next section, a method is devised to eliminate all singular terms from the governing equations.

5.4 Development of non-singular integral equations

5.4.1. Elimination of singular terms from Cauchy integral equations

The proposed method of removing singularities from the integral equations is explained by considering two Cauchy integral equations with the unknown densities $\rho_1(x_1)$ and $\rho_2(x_1)$. Generalization of the method to n integral equations is straightforward. First, write the integral equations in matrix form as:

$$\mathbf{C}\boldsymbol{\rho} + \mathbf{C}_0\mathbf{H}_0\boldsymbol{\rho} + \mathbf{C}_H\mathbf{H}\boldsymbol{\rho} + \mathbf{C}_I\mathbf{I}\boldsymbol{\rho} = \mathbf{C}_R\mathbf{R}, \quad (5.24)$$

where

$$\begin{aligned} \boldsymbol{\rho} &= \begin{Bmatrix} \rho_1(x_1) \\ \rho_2(x_1) \end{Bmatrix}, \mathbf{H}_0 = \begin{bmatrix} H(0,0) & 0 \\ 0 & H(0,0) \end{bmatrix}, \mathbf{H} = \begin{bmatrix} H(a,b) & 0 \\ 0 & H(c,d) \end{bmatrix}, \\ \mathbf{I} &= \begin{bmatrix} I(a',b') & 0 \\ 0 & I(c',d') \end{bmatrix}, \mathbf{R} = \begin{Bmatrix} P(x_1, \alpha, \beta) \\ Q(x_1, \alpha', \beta') \end{Bmatrix}, \end{aligned} \quad (5.25)$$

denote the densities, Hilbert transforms, H transforms, I transforms and the rational functions, respectively. For the H transform, a and b , and similarly c and d , cannot both be zero. The same restriction applies to a' and b' , and c' and d' , in the I transform. The arguments $\alpha, \beta, \alpha', \beta'$ in P and Q are arbitrary constants. Only the $H(0,0)$ terms are

singular and are to be eliminated. Also, $\mathbf{C}$, $\mathbf{C}_0$, $\mathbf{C}_H$, $\mathbf{C}_I$ and $\mathbf{C}_R$ are the coefficient matrices premultiplying the five matrices in Eq. (5.25), and $\mathbf{C}_0 \neq \mathbf{0}$ since otherwise Eq. (5.24) would have already been non-singular. The singular terms $\mathbf{H}_0 \boldsymbol{\rho}$ can be eliminated according to the following three cases depending on $\mathbf{C}$ and $\mathbf{C}_0$.

Case 1: $\mathbf{C}=\mathbf{0}$. Equation (5.24) is a Cauchy integral equation of the first kind corresponding to the stress boundary conditions Eqs. (5.19)-(5.20). Taking the Hilbert transforms of all terms in Eq. (5.24) yields:

$$-\mathbf{C}_0 \boldsymbol{\rho} + \mathbf{C}_H \mathbf{H}_0 \mathbf{H} \boldsymbol{\rho} + \mathbf{C}_I \mathbf{H}_0 \mathbf{I} \boldsymbol{\rho} = \mathbf{C}_R \mathbf{H}_0 \mathbf{R}, \quad (5.26)$$

Note in particular that:

$$\mathbf{H}_0 \mathbf{H} = \begin{bmatrix} H(0,0)H(a,b) & 0 \\ 0 & H(0,0)H(c,d) \end{bmatrix} = \begin{bmatrix} -I(a,|b|) & 0 \\ 0 & -I(c,|d|) \end{bmatrix}, \quad (5.27)$$

$$\mathbf{H}_0 \mathbf{I} = \begin{bmatrix} H(0,0)I(a',b') & 0 \\ 0 & H(0,0)I(c',d') \end{bmatrix} = \begin{bmatrix} \text{sgn}(b')H(a',|b'|) & 0 \\ 0 & \text{sgn}(d')H(c',|d'|) \end{bmatrix}, \quad (5.28)$$

so that $\mathbf{H}_0 \mathbf{H}$ and $\mathbf{H}_0 \mathbf{I}$ contain the I and H transforms respectively. Equation (5.26) is thus non-singular. It is in fact a Fredholm integral equation of the second kind since the unknown $\boldsymbol{\rho}$ is not integrated in the first term of the equation.

Case 2: $\mathbf{C} \neq \mathbf{0}$. Equation (5.24) is a Cauchy integral equation of the second kind corresponding to the displacement gradient boundary conditions Eq. (5.21). Two sub-cases can be considered as follows.

Case 2(a): $\det \mathbf{C} \neq 0$ and $\det \mathbf{C}_0 = 0$. First, solve for $\mathbf{p}$ in terms of $\mathbf{H}_0\mathbf{p}$, $\mathbf{H}\mathbf{p}$, $\mathbf{I}\mathbf{p}$ and $\mathbf{R}$:

$$\mathbf{p} = -\mathbf{C}^{-1} (\mathbf{C}_0\mathbf{H}_0\mathbf{p} + \mathbf{C}_H\mathbf{H}\mathbf{p} + \mathbf{C}_I\mathbf{I}\mathbf{p} - \mathbf{C}_R\mathbf{R}). \quad (5.29)$$

Substitute Eq. (5.29) back into the singular term (i.e., the second term) of Eq. (5.24) yields after rearrangement:

$$(\mathbf{C} + \mathbf{C}_0\mathbf{C}^{-1}\mathbf{C}_0)\mathbf{p} + (\mathbf{C}_H\mathbf{H} + \mathbf{C}_I\mathbf{I} - \mathbf{C}_0\mathbf{C}^{-1}\mathbf{C}_H\mathbf{H}_0\mathbf{H} - \mathbf{C}_0\mathbf{C}^{-1}\mathbf{C}_I\mathbf{H}_0\mathbf{I})\mathbf{p} = (\mathbf{C}_R - \mathbf{C}_0\mathbf{C}^{-1}\mathbf{C}_R\mathbf{H}_0)\mathbf{R}. \quad (5.30)$$

Equation (5.30) is non-singular, since $\mathbf{H}$, $\mathbf{I}$, $\mathbf{H}_0\mathbf{H}$ and $\mathbf{H}_0\mathbf{I}$ operating on $\mathbf{p}$ all give rise to non-singular integrals.

Case 2(b): $\det \mathbf{C} = 0$ and $\det \mathbf{C}_0 \neq 0$. Unlike Case 2(a), one cannot first solve for $\mathbf{p}$ since $\det \mathbf{C} = 0$. Instead, the Hilbert transform is taken of all terms in Eq. (5.24), yielding:

$$\mathbf{C}\mathbf{H}_0\mathbf{p} - \mathbf{C}_0\mathbf{p} + \mathbf{C}_H\mathbf{H}_0\mathbf{H}\mathbf{p} + \mathbf{C}_I\mathbf{H}_0\mathbf{I}\mathbf{p} = \mathbf{C}_R\mathbf{H}_0\mathbf{R}, \quad (5.31)$$

where $\mathbf{p}$ can now be solved for since the determinant of its coefficient matrix is non-zero.

Thus, we might then proceed as in Case 2(a).

Case 3: Cauchy integral equations of both the first and second kinds. Consider for instance the two equations:

$$\begin{aligned}
 & \begin{bmatrix} 0 & 0 \\ c_{21} & c_{22} \end{bmatrix} \begin{Bmatrix} \rho_1(x_1) \\ \rho_2(x_1) \end{Bmatrix} + \begin{bmatrix} c_{011} & c_{012} \\ c_{021} & c_{022} \end{bmatrix} \begin{bmatrix} H(0, 0) & 0 \\ 0 & H(0, 0) \end{bmatrix} \begin{Bmatrix} \rho_1(x_1) \\ \rho_2(x_1) \end{Bmatrix} \\
 & + \begin{bmatrix} c_{H11} & c_{H12} \\ c_{H21} & c_{H22} \end{bmatrix} \begin{bmatrix} H(a, b) & 0 \\ 0 & H(c, d) \end{bmatrix} \begin{Bmatrix} \rho_1(x_1) \\ \rho_2(x_1) \end{Bmatrix} + \begin{bmatrix} c_{I11} & c_{I12} \\ c_{I21} & c_{I22} \end{bmatrix} \begin{bmatrix} I(a', b') & 0 \\ 0 & I(c', d') \end{bmatrix} \begin{Bmatrix} \rho_1(x_1) \\ \rho_2(x_1) \end{Bmatrix} \\
 & = \begin{bmatrix} c_{R11} & c_{R12} \\ c_{R21} & c_{R22} \end{bmatrix} \begin{Bmatrix} P(x_1, \alpha, \beta) \\ Q(x_1, \alpha', \beta') \end{Bmatrix},
 \end{aligned} \tag{5.32}$$

where the first and second equations are of the first and second kind, respectively, since $c_{11} = c_{12} = 0$ in the matrix $\mathbf{C}$. It can be seen that $\det \mathbf{C} = 0$ necessarily. We consider also two sub-cases. In Case 3(a), $\det \mathbf{C}_0 \neq 0$ then one may proceed as in Case 2(b). In Case 3(b), $\det \mathbf{C}_0 = C_{011}C_{022} - C_{012}C_{021}$ may be zero or very close to zero. In such a case, Hilbert transform is taken of all the terms in either the first (or second) equation and the resulting equation is then solved in conjunction with the second (or first) equation. For instance, taking the Hilbert transform of the first equation only yields:

$$\begin{aligned}
 & \begin{bmatrix} -c_{011} & -c_{012} \\ c_{21} & c_{22} \end{bmatrix} \begin{Bmatrix} \rho_1(x_1) \\ \rho_2(x_1) \end{Bmatrix} + \begin{bmatrix} 0 & 0 \\ c_{021} & c_{022} \end{bmatrix} \begin{bmatrix} H(0, 0) & 0 \\ 0 & H(0, 0) \end{bmatrix} \begin{Bmatrix} \rho_1(x_1) \\ \rho_2(x_1) \end{Bmatrix} \\
 & + \begin{bmatrix} c_{H11}H(0, 0) & c_{H12}H(0, 0) \\ c_{H21} & c_{H22} \end{bmatrix} \begin{bmatrix} H(a, b) & 0 \\ 0 & H(c, d) \end{bmatrix} \begin{Bmatrix} \rho_1(x_1) \\ \rho_2(x_1) \end{Bmatrix} \\
 & + \begin{bmatrix} c_{I11}H(0, 0) & c_{I12}H(0, 0) \\ c_{I21} & c_{I22} \end{bmatrix} \begin{bmatrix} I(a', b') & 0 \\ 0 & I(c', d') \end{bmatrix} \begin{Bmatrix} \rho_1(x_1) \\ \rho_2(x_1) \end{Bmatrix} \\
 & = \begin{bmatrix} c_{R11}H(0, 0) & c_{R12}H(0, 0) \\ c_{R21} & c_{R22} \end{bmatrix} \begin{Bmatrix} P(x_1, \alpha, \beta) \\ Q(x_1, \alpha', \beta') \end{Bmatrix}.
 \end{aligned} \tag{5.33}$$

If the determinant of the coefficient matrix premultiplying $\mathbf{p}$ is not zero, i.e., $-C_{011}C_{22} + C_{012}C_{21} \neq 0$, $\mathbf{p}$ may now be expressed as a function of the other terms and substituted back into the second term of Eq. (5.32) to remove all singularities. Alternatively, if Hilbert transform is taken of the second equation, express $\mathbf{H}_0\mathbf{p}$ as a function of all the other terms and substitute the resulting expression into the second term of Eq. (5.32). Here it is assumed that the determinant of the coefficient matrix premultiplying $\mathbf{H}_0\mathbf{p}$ is $C_{011}C_{22} - C_{012}C_{21} \neq 0$. The new equation will no longer have terms involving $\mathbf{H}_0\mathbf{p}$ and is therefore non-singular. Furthermore, it is unlikely that the determinant $C_{011}C_{022} - C_{012}C_{021}$ in Case 3(a) and the determinant $\pm(-C_{011}C_{22} + C_{012}C_{21})$ in case 3(b) will both be zero, since C_{022} and C_{021} are constants associated with stresses and will unlikely be equal to C_{22} and C_{21} which are associated with displacements.

In the three cases above, the Cauchy integral equations reduce to Fredholm integral equations of the second kind, which can be solved using standard techniques such as the the Neumann series or Nyström method. A very simple and effective algorithm for the Nyström method contained in the book “Numerical Recipes in C” (Press et al., 1992) was used in this work. Essentially, the integrals in the governing equations are approximated by Gaussian quadratures using Gaussian points and weights, and the resulting approximate equations are to be satisfied at the same set of Gaussian points, yielding a system of linear algebraic equations with the image densities at the Gaussian points as unknown. Analytical forms for the densities can be obtained by substituting the solved densities at the Gaussian points back into the approximate equations. The analytical image densities can then be used to evaluate the stresses using Eq. (5.11).

The singular terms in governing equations in bi-layer problems can be eliminated by using the method in Case 2 (a). Exactly the same results can be obtained, comparing with the results by the method of solution construction in Chapter 4.

5.4.2 Current problem

Among the governing equations, Eq. (5.19) is the traction free condition and consists of three Cauchy integral equations of the first type ($i = 1, 2, 3$). Figure 5.3 shows that the singular terms in Eq. (5.19) are associated with the density ρ_{1U}^t in Subproblem 1 (top surface) or ρ_{NL}^t in Subproblem N (bottom surface) since these images are directly on the faces where the traction free condition is to be satisfied. Thus, three Hilbert transform terms $H(0, 0)[\rho_{1U}^t]$ or $H(0, 0)[\rho_{NL}^t]$ ($t = 1, 2$ and 3) are to be eliminated from Eq. (5.19) for each traction free surface. The elimination of these singular terms can be done as for Case 1. In contrast, Eq. (5.20) or Eq. (5.21) involves six singular terms for each interface considered, since three densities from two neighboring subproblems must be considered for continuity across the interface of two materials. However, Eq. (5.20) or Eq. (5.21) consists of only three equations for each interface. Thus, they are combined to form six equations of the first and second types with six Hilbert transform terms. The elimination of the singular terms is carried out as for Case 3, which leads to a matrix equation similar to Eq. (5.33). In particular, the equation corresponding to Eq. (5.33) for the interface F is:

$$\begin{bmatrix} D_{K12}^1 & D_{K12}^2 & D_{K12}^3 & -D_{(K+1)12}^1 & -D_{(K+1)12}^2 & -D_{(K+1)12}^3 \\ D_{K22}^1 & D_{K22}^2 & D_{K22}^3 & -D_{(K+1)22}^1 & -D_{(K+1)22}^2 & -D_{(K+1)22}^3 \\ D_{K23}^1 & D_{K23}^2 & D_{K23}^3 & -D_{(K+1)23}^1 & -D_{(K+1)23}^2 & -D_{(K+1)23}^3 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{bmatrix} \begin{Bmatrix} \rho_K^1(x_1) \\ \rho_K^2(x_1) \\ \rho_K^3(x_1) \\ \rho_{(K+1)}^1(x_1) \\ \rho_{(K+1)}^2(x_1) \\ \rho_{(K+1)}^3(x_1) \end{Bmatrix} = \text{RHS}, \quad (5.34)$$

where the constants $D_{Kij}^t = 2\pi \sum_{\alpha=1}^3 \xi_{K\alpha ij}^{tR}$ and $K = F - 1$, i.e., for Interface F the subproblems considered are $F - 1$ and F . Also, RHS denotes the right-hand side terms, including the $H(0, 0)$, H , I transforms and the rational functions. Evaluation of the determinant of the coefficient matrix leads to a non-zero value and consequently the densities in Eq. (5.34) can be expressed as a function of the RHS terms and substituted back into the governing equations to yield six Fredholm equations of the second kind. For brevity, the transformed equations are not listed.

In the section on numerical results, a three-layer semi-infinite solid in which two thin films are bonded to a semi-infinite substrate is considered. The three-layer problem consists of one free surface (three equations) and two interfaces (six equations for each interface), resulting in a total of fifteen integral equations with the same number of unknown densities.

5.4.3 Discussion

There are several advantages associated with the proposed method of transforming the integral equations. The key advantage is the elimination of all singular terms, which saves

considerable computational effort and completely removes inaccuracies associated with singularities. Second, degenerate problems (in which adjacent layers are identical) can be treated without difficulty. This means $D_{Kij}^t = D_{(K+1)ij}^t$ in Eq. (5.34) and the determinant of the coefficient matrix remains non-zero. Third, decoupled and coupled problems can be handled directly with no additional manipulation. In a decoupled problem, the edge and screw components of the source dislocation can be treated separately using edge and screw dislocation images respectively. Fourth, the coefficient matrix in Eq. (5.34) for any given interface F remains the same for any number of layers in the multilayer solid. This is because the elements in this coefficient matrix are associated with the stresses and displacement gradients caused by image dislocations on themselves, and will not be affected by the addition or reduction of *other* faces. Varying the number of faces only requires changes to the RHS of Eq. (5.34).

5.5 Numerical results

In this section, numerical results for the image forces on dislocations in multilayer systems composed of various materials are presented, specifically the cubic materials nickel (Ni), copper (Cu), silicon (Si), and germanium-silicon alloy ($\text{Ge}_\alpha\text{Si}_{1-\alpha}$), where α is the fraction of lattice sites occupied by germanium atoms, as well as the hexagonal materials zinc (Zn), indium nitride (InN), silicon carbide (SiC). The crystal elastic constants of these materials are shown in Tables 4.1 and Table 5.1. Furthermore, isotropic multilayer systems are considered. Both coupled and decoupled problems are also investigated. The results are grouped into two subsections: this section shows two

examples of comparison with previous results and a verification that the boundary conditions are indeed satisfied, while next section contains new results for rather complex multilayer systems.

Cubic	Ni ¹	Cu ¹
C'_{11} (GPa)	246.5	168.4
C'_{12}	147.3	121.4
C'_{44}	124.7	75.4

¹Hirth and Lothe (1982)

Table 5.1. Elastic constants of cubic crystals Ni and Cu with respect to the crystal frame $x'_1 - x'_2 - x'_3$.

5.5.1 Verification of results

Kamat and Hirth (1987) calculated the image force F_2 in the $x_2 -$ direction on a screw dislocation with the Burgers vector $\mathbf{b} = b(0, 0, 1)$ in an infinite isotropic three-layer composite 1-2-1, where Layer 2 is finite with thickness h and Layers 1 are semi-infinite. The dislocation is located in Layer 2 at the distance of d from the upper interface. They employed discrete screw images to numerically obtain the answers in the form of series. The normalized image forces F_2/F_{free} at several values of the normalized position $a = d/h$ are shown as crosses in fig. 5.5 for two values of the material inhomogeneity parameter $\gamma = (\mu_1 - \mu_2)/(\mu_1 + \mu_2)$, where μ is the shear modulus. Here F_{free} is the reference image force in the $x_2 -$ direction on the screw dislocation located at the depth of h below the free surface of a half-space of Material 2. This problem was also solved by our decomposition technique using only four Gaussian points when approximating the integrals in the Nyström method. The image force is calculated by the Peach-Koehler

formula: $F_2 = -\sigma_{11}b_1 - \sigma_{12}b_2 - \sigma_{13}b_3 = -\sigma_{13}b$, where the stress components are those due to all the continuously distributed images in Subproblem 2 (the dislocation is in Layer 2). The results are shown as squares and superimposed on the results of Kamat and Hirth (1987). It can be seen that they agree very well. The antisymmetric dependence of the image force on a is expected for a screw dislocation in the infinite three-layer system. The significant increase in image force magnitude is also apparent as the material inhomogeneity γ increases.

Fig. 5.5. Comparison of the results of Kamat and Hirth (1987) and the current results for a screw dislocation in an infinite 1-2-1 multilayer system for two values of the inhomogeneity parameter γ .

Next, we consider a $\text{Ge}_a\text{Si}_{1-a}$ film of thickness h on a semi-infinite silicon substrate. For the $\{1\ 0\ 0\}$ plane epitaxy, the x_1 -, x_2 -, x_3 -axis coincides with the crystallographic

directions $[1\ 0\ \bar{1}]$, $[0\ 1\ 0]$ and $[1\ 0\ 1]$, respectively. The dislocation with the Burgers vector $\mathbf{b} = b(1/2, -1/\sqrt{2}, 1/2)$ is located at $(0, x_2)$ in the film, where $-h < x_2 < 0$. This is a decoupled problem even though the dislocation is mixed. Figure 5.6 plots the normalized image force F_2/F_{free} on the dislocation, where F_{free} is the image force in the x_2 – direction on the dislocation located at the depth of h from the free surface of a silicon half-space. Two cases $\alpha = 0.1$ and $\alpha = 0.5$ are considered. The present results, again calculated using four Gaussian points in the Nyström method, are shown as full lines. They compare very well with the earlier results of Choi and Earmme (2002a) marked in symbols.

Fig. 5.6. Comparison of current results with the results of Choi and Earmme (2002a) for a mixed dislocation in a $\text{Ge}_\alpha\text{Si}_{1-\alpha}/\text{Si}$ two-layer solid with $\{1\ 0\ 0\}$ plane epitaxy.

The satisfaction of boundary conditions is also verified. Consider a semi-infinite three-layer composite Zn-InN-Zn. Both the first (Zn) and second (InN) layers have the same thickness of $500b$ (b is a Burgers vector magnitude), and the Zn substrate is semi-infinite. A screw dislocation with the Burgers vector $\mathbf{b} = b(0, 0, 1)$ is located in the middle $(0, -750b)$ of the InN layer. For all three layers, the x_1 -axis coincides with the crystallographic direction $[0001]$. This is a decoupled problem solved by using 15 Gaussian points. The boundary conditions require that σ_{23} on the free surface $x_2 = 0$ to vanish, and that σ_{23} to be continuous across the upper and lower interfaces $x_2 = -500b$ and $-1000b$. Figure 5.7(a) shows that σ_{23} on the free surface is indeed very close to zero, compared to the value that it would otherwise assume if the top layer is semi-infinite. Figure 5.7(b) shows that σ_{23} is indeed continuous across the upper interface, as the dashed line representing the stress $\sigma_{23}(x_1, x_2 = -h_1^+)$ on its upper side is almost indistinguishable from the full line representing the stress $\sigma_{23}(x_1, x_2 = -h_1^-)$ on its lower side. The same agreement is found for the lower interface, as shown in fig 5.7(c).

Fig. 5.7. Verification of boundary conditions for a screw dislocation located in the middle of the InN layer in a Zn-InN-Zn multilayer system. (a) The stress σ_{23} on the free surface is almost zero (full line) while it would acquire finite magnitude (dashed line) if the top Zn layer is semi-infinite. (b) Across the upper interface at $x_2 = -500b$, the stress $\sigma_{23}(x_1, x_2 = -h_1^+)$ represented by the dashed line overlaps the stress $\sigma_{23}(x_1, x_2 = -h_1^-)$ represented by the solid line. (c) Similar agreement is found for the lower interface at $x_2 = -1000b$.

5.5.2 Numerical results for semi-infinite three-layer systems

Next, the dependence of the image force on the dislocation position, relative layer thicknesses, dislocation mixity and elastic anisotropy is investigated. All calculations are performed using fifteen Gaussian points.

Figure 5.8 plots the variation of the normalized image force F_2/F_{free} as an edge dislocation with the Burgers vector $\mathbf{b} = b(1, 0, 0)$ changes its position from near the free surface to within the substrate in two semi-infinite multilayer systems: InN-Zn-InN and Zn-InN-Zn. For both multilayer systems, the thickness of the first and second layers is $h_1 = h_2 = h$, and the normalizing constant F_{free} is the image force F_2 on the dislocation at the depth of h in a Zn half-space. Note that F_{free} is positive since it is the force that pushes the dislocation to the top free surface of the Zn half-space. Also, F_2/F_{free} plotted against $-x_2/h$ is independent of h . For simplicity, the x_1 -axis coincides with the crystallographic direction $[0001]$ in all layers, resulting in a decoupled problem. Based on the results for isotropic bimetals, a dislocation approaching the interface of a bimaterial will be repelled from the interface if it is within the softer material but attracted towards it if it is within the stiffer material. Table 4.1 shows that all the elastic constants of Zn, except C'_{66} , are smaller than those of InN. Also, the shear constant $C'_{44} = 1/2(C'_{33} - C'_{23})$ of Zn is larger than that of InN. Hence, for a Zn-InN interface it is not immediately clear if a dislocation in Zn will be repelled by or attracted towards InN. Figure 5.8(a) shows that for the InN-Zn-InN multilayer system, the image force F_2/F_{free} changes sign if the dislocation is in the middle Zn layer, i.e., it tends to push the dislocation in the middle Zn layer into the InN layers on the upper and lower sides of it. Similarly, Figure 5.8 (b) shows that for the Zn-InN-Zn multilayer system, the dislocation in the middle InN layer will be repelled

Fig. 5.8. The variation of the normalized image force F_2/F_{free} with the normalized position $-x_2/h$ of an edge dislocation in (a) InN-Zn-InN, and (b) Zn-InN-Zn. The dislocation in the Zn layer is always attracted towards the InN layer.

from its interfaces with Zn. Hence, the shear elastic constant C'_{66} or C'_{44} is relevant if the general idea of repulsion from the stiffer material and attraction towards the less stiff

material is to be retained. Such results reveal the complex dependence of the image force on the inhomogeneity of the bonded anisotropic materials, which may not be easily assessed by intuition. Based on the shear stiffness, the sign of the image force when the dislocation is in the top layer or in the substrate can be similarly assessed. The results in figs. 5.8(a) and (b) are in agreement with this assessment.

In fig. 5.9, the variation of F_2 / F_{free} with the film thickness for an edge dislocation $\mathbf{b} = b(1,0,0)$ in the InN-SiC-InN and SiC-InN-SiC multilayer systems is simulated. The multilayer systems are semi-infinite with the top two layers having the thicknesses of h_1 and h_2 . The thickness h_1 (or h_2) is varied while keeping h_2 (or h_1) fixed at h . The dislocation is *always* located at $10b$ above the upper interface in Layer 1. The x_1 -axis coincides with the crystallographic direction $[0001]$ in all layers, and this is a decoupled problem. For *both* multilayer systems, F_{free} is the force F_2 on the dislocation at the depth of h in a SiC half-space. The dependence of the image force on thickness can be rationalized in terms of the superposition of image forces arising from various faces (free surface and interfaces). Note that SiC has a higher normal and shear stiffness compared to InN, as Table 4.1 shows. This implies that a dislocation in InN will likely be repelled from the InN-SiC interface. In fig. 5.9(a), it can be seen that the dislocation is attracted by F_2 to the free surface, and this force decreases as the thickness h_1 of Layer 1 increases. This may be attributed to a decrease in the attracting force exerted by the free surface as it moves away from the dislocation. In fig. 5.9(b), the repulsive force exerted on the dislocation in the top InN layer by the middle SiC layer becomes stronger as h_2 increases, i.e., as the lower SiC-InN interface recedes from the dislocation. This result can be understood since layer 3 is elastically less stiff compared to layer 2 and it will mitigate

the repulsive force due to layer 2 on the dislocation in layer 1. However, as the lower interface recedes, this mitigating influence weakens and there is an overall increase in the repulsive force. In figs. 5.9(c) and (d), the dislocation is within the top SiC layer of the SiC-InN-SiC multilayer system, and the variation of the image force with h_1 and h_2 can be similarly rationalized. Finally, fig. 5.9 also shows that when a dislocation is close to the interface, the influence of the thickness ratio of the thin to thick layers on the image force is most significant when that ratio is less than 0.5.

Fig. 5.9. Plot of the normalized image force F_2/F_{free} versus the normalized film layer thickness. Variation with (a) h_1 and (b) h_2 in InN-SiC-InN, and variation with (c) h_1 and (d) h_2 in SiC-InN-SiC. The edge dislocation is located at $10b$ above the upper interface in the top layer.

Attention is turned next to the dependence of F_2 / F_{free} on the relative strength of the screw and edge components of the Burgers vector. For simplicity, infinite Cu-Ni-Cu and Ni-Cu-Ni multilayer systems are considered. The middle layer has the thickness h and layers 1 and 3 are semi-infinite. In each layer, the x_1 -, x_2 -, and x_3 -axis coincides with the crystallographic directions $[110]$, $[\bar{1}11]$ and $[1\bar{1}2]$, respectively. This is a coupled problem. The dislocation is located in the middle layer at the distance of $0.2h$ below the upper interface. It has the Burgers vector magnitude $b = |\mathbf{b}| = \sqrt{b_1^2 + b_2^2 + b_3^2}$. The special case is considered whereby $b_2/b = 0$ and b_3/b is varied from zero (pure edge) to one (pure screw). Furthermore, we choose F_{free} to be the image force F_2 acting on a reference edge dislocation with the Burgers vector $b(1, 0, 0)$ located at the depth of h in a nickel half-space. Figure 5.10 summarizes the results for the two multilayer systems.

Fig. 5.10. Plot of the normalized image force F_2 / F_{free} versus normalized dislocation component $b_3 / |\mathbf{b}|$ in infinite (a) Cu-Ni-Cu and (b) Ni-Cu-Ni multilayer systems.

It can be seen that F_2 / F_{free} decreases in magnitude as b_3 / b increases, i.e., a larger image force acts on the dislocation with a larger edge component. The variation is also quite significant, amounting to -25% to -30% change as b_3 / b increases from zero to one.

Similarly, the effect of dislocation mixity on F_2 / F_{free} in hexagonal materials can be investigated. Consider the following two cases of a mixed dislocation in an infinite three-layer InN-SiC-InN solid with the middle layer thickness h . In the first case, the c -axis $[0001]$ direction in each layer coincides with the x_1 -axis direction ($[001]$ in the reference x_1 - x_2 - x_3 coordinate frame). In the second case, the c -axis direction in each layer coincides with the $[101]$ direction. As in the previous figure, the dislocation has the Burgers vector $(b_1, 0, b_3)$ with magnitude b and is located at the distance of $0.2h$ below the upper interface. In both cases, F_{free} is the image force F_2 on a dislocation with the Burgers vector $\mathbf{b} = b(1, 0, 0)$ located at the depth of h in a SiC half-space where the c -axis and the x_1 -axis directions coincide. The first case is a decoupled problem because of the special orientation of the c -axis. The second case is a coupled problem. As in fig. 5.10, fig. 5.11 shows that for the first case F_2 decreases in magnitude with increase in b_3 . However, for the second case F_2 increases with b_3 until $b_3 \approx 0.8|\mathbf{b}|$, after which it decreases. These examples show the complex dependence of the image force on dislocation mixity, material anisotropy and inhomogeneity. Finally, it is interesting that although in both figs. 5.10 and 5.11 F_{free} is defined with respect to a pure edge dislocation at a depth of h in a half-space, F_2 is smaller than F_{free} for the cubic materials but larger than F_{free} for the hexagonal materials.

Fig. 5.11. Plot of the normalized image force F_2 / F_{free} versus the normalized dislocation component $b_3 / |\mathbf{b}|$ in an infinite InN-SiC-InN multilayer system.

In the last numerical example, the variation of the image force with the c -axis orientation for a screw dislocation $\mathbf{b} = b(0\ 0\ 1)$ and an edge dislocation $\mathbf{b} = b(1\ 0\ 0)$ in a semi-infinite SiC-InN-Zn multilayer system is investigated. The SiC and InN layers have the thickness h and the Zn layer is semi-infinite. The c -axis of the hexagonal materials in all three layers lies in the x_1 - x_3 plane and makes an angle of θ with respect to the x_1 -axis. The dislocation is located at the distance of $h/5$ below the SiC-InN interface. This is generally a coupled problem. Defining F_{free} as the image force F_2 on the *edge* dislocation at the depth of h in an InN half-space with $\theta = 0^\circ$, F_2 / F_{free} is plotted against θ in fig. 5.12, which shows a very strong dependence on θ . For the screw dislocation, the image

force magnitude has a minimum at $\theta = 90^\circ$ and a maximum around $\theta = 35^\circ$, while for the edge dislocation, it has a maximum at $\theta = 90^\circ$ and a minimum around $\theta = 30^\circ$. The variation of the image force with θ essentially shows the significant influence of elastic anisotropy of the hexagonal materials, and the differences between the screw and edge dislocation curves highlight the dependence on dislocation mixity.

Fig. 5.12. Plot of the normalized image force F_2 / F_{free} versus the angle θ between the c -axis and the x_1 -axis for a screw dislocation and an edge dislocation in a SiC-InN-Zn multilayer system.

5.6 Conclusions

In this chapter, the image decomposition method is developed for solving the problem of a mixed dislocation in a multilayer system consisting of an arbitrary number of layers

of various materials and thicknesses. The development of the method has the following four significant points. First, partial solutions which automatically satisfy the consistency requirement when the original N -layer problem degenerates into an M -layer problem ($M < N$) can be determined through the method of decomposition. Without the inclusion of these partial solutions, the formulation of the governing equations would be improper and accurate numerical solutions may not be attained. Second, all singular integrals in the governing Cauchy integral equations of the first and second kind can be eliminated through the H and I transforms, resulting in non-singular Fredholm integral equations and thus removing at the outset inaccuracies associated with singularities. Third, we believe that solutions for a mixed dislocation in a general multilayer system (as opposed to a pure edge or pure screw dislocation in a bimaterial or periodic multilayer system) based on the image method are reported for the first time. Finally, since Cauchy integral equations arise not only in dislocation problems but also in other engineering problems, e.g., contact mechanics (Fan and Keer, 1994; Fan et al., 1996), the current method of solving Cauchy integral equations may be applicable to these other problems.

The method was used to calculate image forces acting on mixed dislocations in three-layer composites of cubic or hexagonal materials. In particular, the investigation of the dependence of the image forces (acting in the direction perpendicular to the faces) on dislocation position, layer thicknesses, dislocation mixity and material anisotropy was carried out. It was revealed that (a) whether the dislocation in a layer near an interface will be repelled by or attracted towards the other layer depends (at least) on the elastic constants of the two layers in a complex manner, (b) for a dislocation near an interface, the dependence of the image force on the thicknesses of the neighboring layers is very significant when the thickness ratio of the thin to thick layers is less than ~ 0.5 , (c) the

image force magnitude in general depends non-monotonically on the dislocation mixity, and (d) the influence of elastic anisotropy of the materials is significant and is generally also non-monotonic. Consequently, elastic anisotropy, layer inhomogeneity, layer thicknesses, dislocation mixity and dislocation position all influence the image forces in a complex manner and the actual values of the forces can be determined only through a computational model capable of simultaneously handling all these factors.

CHAPTER SIX

MULTILAYER SYSTEM YIELDING PREDICTED BY DISCRETE DISLOCATION PILEUP MODEL

In this chapter, Sections 6.1, 6.2 and 6.3 present the model for analyzing a discrete dislocation pileup in a multilayer system, the numerical predictions of multilayer system yield strength and the comparison of theoretical results with experimental data, and the conclusions, respectively.

6.1 Discrete dislocation pileup in multilayer system

A discrete dislocation pileup in a finite anisotropic N -layer system is shown in fig. 6.1. The dislocation lines are all infinitely long, straight, and parallel to each other. The thicknesses of the layers are denoted by $h_1, h_2, \dots, h_n$, respectively. Layers 1 and n may be semi-infinite. The dislocation pileup is located within layer i , which is softer than the neighboring layers $i-1$ and $i+1$. The angle between the dislocation glide direction and the interface is denoted by θ . The cross symbol represents a mixed dislocation in general. The applied shear stress is denoted by τ .

Fig. 6.1. Illustration of a dislocation pileup in a finite anisotropic N -layer system. The film thickness of each layer is represented by h_i , $i = 1, 2, \dots, n$. The dislocation pileup is subjected to the applied shear stress τ . The angle between the glide direction and the interface is denoted by θ .

Consider the equilibrium of the discrete dislocations in the pileup. Any dislocation experiences a force due to the applied shear loading, forces from all the other dislocations, and image forces from the boundaries. The physical condition is that any dislocation in the pileup is in its equilibrium position, and the sum of forces acting on it in the pileup direction must be zero:

$$\tau \cdot b_i + \sum_{j=1}^{i-1} F_i^j + \sum_{j=i+1}^N F_i^j + \bar{F}_i = 0, \quad (6.1)$$

where b_i denotes the Burgers vector magnitude of i^{th} dislocation, F_i^j the image force on the i^{th} dislocation contributed by the j^{th} dislocation, and $\bar{F}_i$ the image force on the i^{th} dislocation from all the boundaries.

Computationally, it is necessary to reduce the complexity of the multilayer while still capturing its essential elements. Clearly, a one layer model, either in the form of an infinite medium, a half space or a strip, is unsatisfactory. A two-layer model, such as a film-substrate 1-2 with a free surface is also unsatisfactory because the effect of the thickness of Layer 2 cannot be captured by such a simplified model. A three-layer model 1-2-3 with a free surface for Layer 1, seems to be the simplest acceptable model, since the thicknesses and elasticity of the layers sharing the interface against which the pileup occurs can both be incorporated in the analysis. The material and geometry of these two neighboring layers will be most relevant to the analysis. Thus, a dislocation pileup in a three-layer anisotropic system with a free surface is considered in the present work.

The coordinate system $x_1 - x_2$ is constructed on the free surface as shown in fig. 6.2. Assume that Materials 1 and 3 are both elastically harder than Material 2 so that the dislocations pile up in Material 2. It can be observed from fig. 6.2 that this system consists of a top free surface and two interfaces. Furthermore, it is assumed that the dislocation source, represented by an open circle, is located at the lower interface. Under the applied shear stress τ , dislocations pile up against the upper interface in Layer 2. To simplify the analysis, it is also assumed that the glide plane is perpendicular to the interfaces ($\theta = 90^\circ$) and τ is along the $x_2 -$ direction, all the dislocations have the same Burgers vector, and only a single pileup occurs. These simplifications do not fundamentally alter the physics of the problem and are consistent with the approximate nature of the model.

Furthermore, it should be mentioned that each layer can be monocrystalline or polycrystalline. In the present work, all layers are taken to be single crystals since the multilayer thickness varies from a few to a few hundred nanometers only and each layer does not contain sufficiently many crystals to result in a homogeneous polycrystal. Thus, the present work focuses on a single crystal nanolaminate.

Fig. 6.2. Discrete single-ended dislocation pileup in a semi-infinite anisotropic three-layer system. The thicknesses of Layers 1 and 2 are denoted by h_1 and h_2 , respectively. The dislocations are emitted by the source, represented by the open circle, and pile up against the upper interface in the presence of an applied shear stress τ . The pileup plane is vertical to the interfaces.

The pileup occurs according to the following hypothesis. When the applied shear stress τ exceeds the threshold stress τ^0 necessary for the source to generate a dislocation, the first or leading dislocation is emitted. The back stress on the dislocation source produced by the first dislocation temporarily stops the emission of a second dislocation. However, the second dislocation will be generated when τ is larger than the sum of the threshold stress and the back stress on the dislocation source. Thus, more dislocations can be generated by increasing the applied shear stress. The equilibrium positions of the dislocations will be reached under their mutual interaction, the applied shear, as well as the image forces. Eventually, the leading dislocation may penetrate the barrier and propagate to the next layer, resulting in yielding of the multilayer. Koehler's criterion (Koehler, 1970) is used in the present work to determine when this yielding occurs. Essentially, this criterion states that the leading dislocation moves closer to the

barrier as more dislocations are generated and the barrier is overcome when the leading dislocation moves to within a small distance, say $1b$, of the barrier.

In order to obtain the governing equations for the dislocation pileup, the Green's function of a single dislocation is first obtained. The three-layer system is decomposed into three homogeneous problems, as shown in fig. 6.3. The decomposition process is discussed in detail in Chapter 5, and all the symbols used in this chapter have the same meaning as those in Chapter 5.

Fig. 6.3. Image decomposition for a semi-infinite three-layer system. The mixed dislocation, represented by a cross, can be located anywhere in the system. The symbols $\rho'_{1U}, \rho'_{1L}, \rho'_{2U}, \rho'_{2L}, \rho'_{3U}$ denote image dislocation densities in the positions indicated by dashed lines.

As fig. 6.3 shows, there are 5 unknown image dislocation densities $\rho'_{1U}, \rho'_{1L}, \rho'_{2U}, \rho'_{2L}, \rho'_{3U}$. The boundary conditions are that the tractions vanish on the free surface and the stresses and displacement gradients are continuous across the upper and lower interfaces:

$$\sigma_{2i}(x_1, x_2 = 0) = 0, \quad (6.2)$$

$$\sigma_{2i}(x_1, x_2 = -h_1^+) = \sigma_{2i}(x_1, x_2 = -h_1^-), \quad (6.3)$$

$$\frac{\partial u_i}{\partial x}(x_1, x_2 = -h_1^+) = \frac{\partial u_i}{\partial x}(x_1, x_2 = -h_1^-), \quad (6.4)$$

$$\sigma_{2i}(x_1, x_2 = -(h_1 + h_2)^+) = \sigma_{2i}(x_1, x_2 = -(h_1 + h_2)^-), \quad (6.5)$$

$$\frac{\partial u_i}{\partial x}(x_1, x_2 = -(h_1 + h_2)^+) = \frac{\partial u_i}{\partial x}(x_1, x_2 = -(h_1 + h_2)^-), \quad (6.6)$$

where $i = 1, 2, 3$. The above five governing equations, which describe the problem of a single dislocation, are singular Cauchy integral equations. They can be transformed into non-singular Fredholm integral equations of the second kind by the method in Chapter 5. The Fredholm integral equations are then solved for the image densities via the Nyström method. The image densities are used to construct the stress field. For the problem of a number of discrete dislocations as in a pileup, the combined stress field is simply the sum of the fields of all the dislocations. These fields will be dependent on the position coordinates of the dislocations. The governing equations (6.1) can thus be set up in terms of these position coordinates. They are nonlinear algebraic equations and are solved via Powell's hybrid method (<http://www.netlib.org/minpack/>).

6.2 Numerical results and comparison with experimental data

Convergence tests have been performed on the image decomposition model, as reported in the previous chapters. In this section, another test of convergence is made on a semi-infinite three-layer system Ni-Cu-Ni, in order to determine the number of Gaussian points appropriate for the numerical solution. After this, the model is used to predict the shear strength of multilayers, assuming that the pileup is single-ended. The predictions are compared to previous theoretical and experimental results.

6.2.1 Convergence test for a semi-infinite three-layer system Ni-Cu-Ni

Consider a screw dislocation with a Burgers vector magnitude of b in the copper layer of a three-layer Ni-Cu-Ni composite, where the thickness is given by $h_1 = h_2 = 100b$. Copper and nickel are face-centered-cubic (FCC), with the major operative slip system of $\{111\}\langle 110\rangle$. In all layers, the crystallographic directions $[\bar{1}11]$, $[110]$ and $[\bar{1}1\bar{2}]$ are parallel to the global coordinate axes x_1 , x_2 and x_3 , respectively. For Cu with relatively large grain size, the threshold stress is $\tau^0 = 0.015$ GPa (Varin et al., 1987), and the three-layer system is subjected to an applied shear stress equal in magnitude. Numerical results of the position of the dislocation and the back stress on the source, obtained by using different Gaussian points, are listed in Table 6.1.

Number of Gaussian points	Position of the dislocation (b)	Back stress on (GPa)
4	$x_2 = -118.2363$	0.06013
10	$x_2 = -118.4527$	0.06039
15	$x_2 = -118.5860$	0.06047
50	$x_2 = -118.9931$	0.06074

Table 6.1. Convergence tests for a screw dislocation in a Ni-Cu-Ni system

The elastic constants of copper and nickel in GPa are respectively $C_{11} = 168.4$, $C_{12} = 121.4$, $C_{44} = 75.4$ and $C_{11} = 246.5$, $C_{12} = 147.3$, $C_{44} = 124.7$, respectively (Hirth and Lothe, 1982). These differences are not negligible. Thus, the numerical results in Table 6.1 show that a small number of Gaussian points are sufficient for solving the problem even though the elastic inhomogeneity is quite significant. Considering the need to balance efficiency against accuracy, four Gaussian points are used for calculation throughout this chapter.

6.2.2. Development of a discrete dislocation pileup model

A discrete dislocation pileup model is developed to predict the number of dislocations in a pileup and the yield strength of multilayers. For the purpose of illustration, consider a single-ended screw dislocation pileup in the soft (Cu) layer of the semi-infinite Ni-Cu-Ni system shown in fig. 6.2. The source is located at the lower interface and the dislocations pile up against the upper interface. The crystallographic directions $[\bar{1}11]$, $[110]$ and $[\bar{1}1\bar{2}]$ in each layer are parallel to the global coordinate x_1 -, x_2 - and x_3 - axes, respectively, as before.

Define τ^* to be the shear strength (by yielding) of the three-layer system, τ_n^* the shear stress necessary to cause yielding in the presence of n dislocations, and τ_n the shear stress required to generate n dislocations. Note that τ_n^* is not necessarily τ^* because a larger number of dislocations may cause yield failure at an applied stress smaller than τ_n^* . If indeed $\tau^* = \tau_n^*$ then the number of dislocations has remained unchanged as the applied shear is increased from τ_n to τ_n^* . The dislocation pileup may be regarded as stable as it can support a stress larger than τ_n . On the other hand, τ_n is the nucleation stress for the

n -th dislocation and is in general not the shear strength unless Koehler's criterion is also satisfied. If indeed $\tau^* = \tau_n$, the dislocation pileup is unstable since the generation of the n -th dislocation immediately causes the system to yield.

Actual numerical examples are next provided. First, consider the layer thickness to be $h_1 = h_2 = 15b$, where b is the Burgers vector magnitude. When the applied shear stress $\tau > \tau_1 = \tau^0 = 0.015$ GPa, where $\tau^0 = 0.015$ GPa is the experimental value for the emission of the first dislocation. Using the image decomposition model, the equilibrium position of the first dislocation is determined to be $x_2(1) = -18.6611b$. The distance d from this first dislocation to the upper interface is then $d = (18.6611 - 15)b > 1b$ and the system does not yield according to Koehler's criterion. It is then necessary to increase the applied stress to τ_1^* (the stress required for yielding in the presence of one dislocation) or τ_2 (the stress required for generating two dislocations). Calculations show that $\tau_1^* = 0.7683$ GPa and $\tau_2 = \tau_1 + \tau_{back} = 0.4480$ GPa, where $\tau_{back} = 0.4330$ GPa is the back stress exerted by the first dislocation on the source. Since $\tau_2 < \tau_1^*$, two dislocations will be generated at τ_2 before the applied stress can reach τ_1^* . Under the interaction between the dislocations, the boundaries and the applied shear $\tau = \tau_2$, the positions of the two dislocations will be reorganized. Calculations show that $x_2(1) = -15.6540b$, $x_2(2) = -24.9996b$, where $x_2(1)$ and $x_2(2)$ denote the positions of the first and second dislocations, respectively. The distance between the leading dislocation and the upper interface is now $d = (15.6540 - 15)b < 1b$, and so the system yields. Thus, the generation of the second dislocation at τ_2 causes the system to yield and the dislocation pileup is immediately unstable, resulting in the shear strength $\tau^* = \tau_2$. The corresponding number of dislocations is $n = 2$.

Consider next thicker layers, i.e., $h_1 = h_2 = 25b$. Under the threshold stress $\tau_1 = \tau^0 = 0.015$ GPa, the first dislocation emerges and its equilibrium position is $x_2(1) = -30.8354b$. Since $d = (30.8354 - 25)b > 1b$, the system does not yield. Calculations then show that $\tau_1^* = 0.8725$ GPa and $\tau_2 = 0.2718$ GPa, and since $\tau_2 < \tau_1^*$ the system will have two dislocations. The positions of the two dislocations are given by $x_2(1) = -26.0872b$, $x_2(2) = -41.6407b$, and since $d = (26.0872 - 25)b > 1b$ the system does not yield. Consequently, further calculations are performed, giving $\tau_2^* = 0.33$ GPa and $\tau_3 = 0.8319$ GPa. This implies that when τ reaches τ_2^* the system yields before the third dislocation can be generated. Thus, the dislocation pileup with two dislocations is stable upon generation at τ_2 and only becomes unstable when the applied shear stress reaches τ_2^* . In this case, $\tau^* = \tau_2^*$ and $n = 2$. The general procedure for determining the shear strength and the corresponding number of dislocations is shown in the flow chart of fig. 6.4.

Fig. 6.4. Flow chart for calculating the shear strength τ^* and the corresponding number of dislocations n in the pileup.

The procedure developed above is used to predict τ^* and the corresponding n as the layer thickness $h = h_1 = h_2$ increases from $15b$ to $750b$. The final results are listed in Table 6.2. The arrow symbol “ $\rightarrow$ ” between numbers in the third column of the table is

used to represent the “unstable pileup” case, while numbers without the arrow symbol represent the “stable pileup” case .

Layer thickness ($h = h_1 = h_2$) Units of b	Shear Strength τ^* (GPa)	Final number of dislocations in the system, n
15	0.4480	$1 \rightarrow 2$
25	0.3300	2
50	0.4164	$2 \rightarrow 3$
100	0.2814	$3 \rightarrow 4$
150	0.2786	$4 \rightarrow 5$
200	0.2520	$5 \rightarrow 6$
300	0.2115	$6 \rightarrow 7$
400	0.1710	8
500	0.1802	$8 \rightarrow 9$
750	0.1454	$10 \rightarrow 11$

Table 6.2. Results of shear strength and final number of screw dislocations in Ni-Cu-Ni system.

Assuming $b \sim 2 \times 10^{-10}$ m and after normalizing τ^* by $\tau^0 = 0.015$ GPa, the predicted results are compared with the theoretical results of Anderson and Li (1995) and the experimental results of Bunshah et al. (1980). The experimental data are normalized by the shear yield strength of Cu at large layer thickness. Anderson and Li’s results were obtained from a double-ended discrete screw dislocation pileup in an infinite three-layer Ni-Cu-Ni solid, where each layer is assumed to be isotropic. They also used the $d = 1b$ distance criterion but employed an additional parameter of interfacial resistance to fit the experimental data. From fig. 6.5, it can be seen that the current model predictions (diamonds) based on discrete single-ended screw dislocation pileup agree very well with the previous theoretical and experimental results when $h^{-1/2} < 0.08 \text{ nm}^{-1/2}$ or when $h >$

156 nm. The current results actually predict a Hall-Petch relation (highlighted by the straight line) down to $h \sim 40$ nm. For $h > 40$ nm, i.e., $h > 200b$, the number of dislocations in the pileup is larger than six (see Table 6.2). Thus the current results also agree with the statement that for single-ended dislocation pile-ups $\sigma \propto h^{-1/2}$ is only applicable when the number of dislocations in the pileup is larger than six (Misra et al., 2005).

Fig. 6.5. Comparison of current theoretical results with those of Anderson and Li (1995), and with the experimental data of Bunshah et al. (1980) for Ni-Cu multilayers. The straight line is the linear fit of the experimental data.

The current predictions in fig. 6.5 not only show deviations from the Hall-Petch relation at $h \sim 40$ nm but also an inverse relation at $h \sim 10$ nm. Also, the “erratic” behavior at small h is due to the discreteness of the model and whether the yield occurs by the failure of a “stable” or “unstable” pileup, which consists of only one or two dislocations. To explore the reason why the current model predicts a deviation from the Hall-Petch

relation, the normalized force F_2/b acting on the leading dislocation, as contributed from the free surface image, upper interface image, lower interface image, dislocation interaction, and the applied stress, are listed in Table 6.3 for the two cases of $h = 5$ nm and 80 nm. A positive force pushes or draws the leading dislocation towards the upper interface, while a negative force repels it from the upper interface. In the case of the larger thickness, the contribution of the free surface and lower interface images is about 8.5% of the dislocation interaction contribution, while in the case of the smaller thickness it is 66.2% of the dislocation interaction contribution. This suggests that as the thickness reduces, the free surface and the lower interface images get closer to the leading dislocation and assist in pushing it towards the upper interface. This in turn reduces the applied shear necessary to cause yielding (a weakening effect). This is the origin of the deviation from the Hall-Petch relation in the current model. If the weakening is severe, an inverse relation, i.e., a decrease in shear strength as thickness decreases, may even be predicted, as in the case of $h = 5$ nm.

The negative force due to the upper interface image always resists the approaching leading dislocation. This contribution is relatively independent of the layer thickness since the leading dislocation is approximately at the distance of $1b$ from the interface at failure. In fact, the upper interface image contribution reflects the Koehler image force strengthening effect (Koehler, 1970): the applied stress must overcome this image force to cause yielding. Koehler calculated this image force for an infinite isotropic bimaterial, which therefore cannot take into account image effects associated with layer thickness. The current model shows for the first time that the image effects are of two kinds: a Koehler strengthening effect relatively insensitive to layer thickness, and a weakening effect due to layer thickness reduction, and it is the latter image effect that can account for the deviation from the Hall-Petch relation.

Furthermore, it is noted that the force acting on the leading dislocation due to interaction with other dislocations decreases by $\sim 50\%$ as the thickness decreases from 80 to 5 nm. This is expected as there are eight and two dislocations in the 80 nm ($400b$) and 5 nm ($25b$) thickness cases, respectively, as can be seen Table 6.2. Also, the sum of all the forces in each of the two columns in Table 6.3 must be zero since the pileup is in equilibrium just before yield.

Normalized Force F_2/b (GPa) on Leading Dislocation as Contributed From:	Layer Thickness $h = 5$ nm	Layer Thickness $h = 80$ nm
Free Surface Image	0.2062	0.05752
Upper Interface Image	-1.1366	-1.2396
Lower Interface Image	0.1151	0.02638
Dislocation Interaction	0.4853	0.9847
Applied Shear	0.3300	0.1710

Table 6.3. Force acting on the leading dislocation as contributed from various sources. The image sources on the free surface and the lower interface become important as compared to the dislocation sources, when h reduces from 80 to 5 nm.

In summary, the current investigation establishes the importance of image effects on the strength of multilayers, and identifies a strengthening image effect due to the interface barrier and a weakening image effect due to layer thickness reduction. It should be mentioned that various mechanisms have been proposed to explain the deviation from Hall-Petch relation. For instance, the inverse relation has been explained in terms of (1) absence of misfit dislocations as the layer thickness reduces, thus lowering the resistance to dislocation penetration across the interface barrier, (2) the loss of chemical sharpness of the interface when the layer thickness decreases, thus lowering the barrier resistance, (3) the dislocation core becoming comparable in size to the layer thickness, and (4) the

reduction of the Koehler strengthening effect with layer thickness reduction. The current results, which are based on actual calculations, offer the image mechanism as a possible explanation of the departure from the Hall-Petch relation in addition to the other proposed mechanisms.

6.2.3. Comparison with experimental data

Eighteen sets of experimental data on the relation between the shear strength and the layer thickness of various multilayer systems are collected and shown in fig. 6.6. The original data of hardness are divided by 3 to obtain the tensile yield strength (Johnson, 1970), which are further divided by 3.1 to obtain the shear strength (Misra et al. 2005). The divisors used to convert the data are approximate, but do not affect the basic nature of the dependence of the shear strength on layer thickness.

The bottommost data for the Cu-Ni multilayer system, represented by the smaller solid box symbols, were obtained by Ebrahimi and Kong (1999). The uppermost data for the Au-Ni multilayer system, as represented by the larger open box symbols, were obtained by Schweitz et al. (2001). These data represent the upper and lower bounds of the shear strength, respectively, i.e., ~ 0.9 GPa and ~ 0.1 GPa. The layer thickness for most of the data lies between 1 nm and 500 nm, and the multilayers can be considered as microlaminates and nanolaminates. Significant deviations from the Hall-Petch relation are observed, and the inverse relation is also evident for most data sets. Typically, peaks in the curves can be seen for layer thickness in the range of 1 to 10 nm.

Shear Strength, τ^* (GPa)

Fig. 6.6. Data showing the relationship between shear strength and layer thickness in multilayer systems. In the legend, Symbol 1 denotes data by Misra et al. (2005); 2~5 by Misra and Kung (2001); 6~7 by Schweitz et al. (2001); 8~12 by Hoagland et al. (2004); 13 by Zhang et al. (2003); 14 by Ebrahimi and Kong (1999); 15~16 by Verdier et al. (2001); 17 by Lehoczky (1978); and 18 by Zhang et al. (2004).

To verify the developed discrete dislocation pileup model, numerical predictions are made for Ni-Cu multilayers and compared to the experimental data in fig. 6.7. The predicted results are obtained by assuming pileups of both pure screw and pure edge dislocations. The pure edge dislocations have the Burgers vector in the x_2 - direction. All geometrical, material and loading parameters are the same as those in the previous subsection. It can be observed that the experimental data, except for one data set, are essentially bounded from the top and from the bottom by the predicted results for the edge and screw dislocations, respectively.

Shear Strength, τ^* (GPa)

Fig. 6.7. Comparison of predicted shear strength with experimental data for Cu-Ni multilayers. Legend symbols a, b denote the data of Misra and Kung (2001); c Hoagland et al. (2004); d Zhang et al. (2003); e Ebrahimi and Kong (1999); f Verdier et al. (2001); and g Zhang et al. (2004). The cross and pentagon symbols denote the model predictions for screw and edge dislocation pileups, respectively.

The developed pileup model is further verified against the experimental results for Au-Ni multilayers. It is assumed that the dislocation pileup occurs in the softer layer, i.e., Au. The set of data by Schweitz et al. (2001) is available for this purpose. Zimmerman et al. (2001) remarked that the threshold stress necessary for dislocation nucleation in Au is in the range of 1.5 to 2 GPa. In this work, the threshold stress for Au is taken to be $\tau^0 = 0.7$ GPa, since the data of Schweitz et al. (2001) show shear strengths between 0.7 and 1 GPa. From fig. 6.8, it can be seen that the results predicted by the screw dislocation pileup model agree quite well with the experimental data. The model predictions also show an inverse Hall-Petch relation, although this relation is not apparent in the data. Nevertheless,

the agreement may be considered reasonably good, since no fitting parameters are used in the model predictions and the model is quite simple, i.e., it accounts for only image effects and does not incorporate other possible mechanisms.

Fig. 6.8. Comparison of model predictions of the shear strength of Au-Ni multilayers with experimental data. The open star symbol denotes the data of Schweitz et al. (2001); the solid diamond and open box symbols denote the model predictions for pure screw and pure edge dislocation pileups, respectively.

6.3 Conclusions

Based on the solutions for a mixed dislocation in a general N -layer system obtained by the image decomposition method, the problem of a discrete dislocation pileup is solved. In the pileup model, it is assumed that a dislocation is generated when the threshold stress and the back stress from previously generated dislocations are overcome by the applied shear stress. Koehler's criterion of $1b$ between the leading dislocation and the interface barrier is adopted as the yield criterion.

To simplify calculations, semi-infinite three-layer systems are used to model the multilayers. The number of dislocations, their positions and the shear strength are predicted. The Hall-Petch relation is predicted for large layer thickness, and deviation from the relation and an inverse relation are predicted for small layer thickness. It is shown for the first time that image effects can account for the deviation and the inverse relation. These image effects add to the pileup effect, thus weakening the multilayer strength. The predicted shear strengths agree well with the experimental data for Cu-Ni and Au-Ni multilayers.

CHAPTER SEVEN

CONCLUSIONS AND RECOMMENDATIONS

In this chapter, the major contributions are listed in Section 7.1. Based on the results obtained, some recommendations are made for future research in Section 7.2.

7.1 Major contributions

The research focuses on the mechanics of anisotropic multilayer materials embedded with mixed dislocations under the plane strain condition. It is believed that the following advances have been made:

- 1) Development and application of the general H and I transforms and their operation properties, which result in the complete elimination of singular kernels from the governing integral equations and hence improvement in solution accuracy and efficiency. This work is reported in Chapter 3.
- 2) Development of the solutions for the problems of pure edge, pure screw and mixed dislocations located anywhere in anisotropic two-layer systems, including infinite bi-layers and semi-infinite film-substrates, and demonstration of the influence of elastic anisotropy, film-substrate inhomogeneity and the free surface on the various stress components and image forces. This work is reported in Chapter 4.

- 3) Generalization of the image decomposition technique for solving N -layer systems embedded with mixed dislocations. The development of partial solutions and the elimination of singular integrals greatly improve the solution accuracy and efficiency. Numerical investigations show that elastic anisotropy, layer inhomogeneity, layer thicknesses, dislocation mixity and dislocation position all influence the image forces in a complex manner. This work is reported in Chapter 5.
- 4) Development of a discrete dislocation pileup model and prediction of the shear strength of multilayer systems. Koehler's criterion is adopted as the yield criterion. The Hall-Petch relation is successfully simulated for layer thickness greater than 40 nm, while deviation of the relation and an inverse relation are also predicted for layer thickness less than 40 nm. The agreement with experimental data is reasonably good, given the simplicity of the physical model. A key finding is that the deviation from the classical relation and the inverse relation can be accounted for by the image effects of the approaching boundaries. The work is reported in Chapter 6.

7.2 Recommendations for future work

Based on the research reported in this thesis, further work can be carried out. Some topics are suggested as follows.

- 1) Investigation of dislocations in complex multilayer systems with possibly different types of constitutive equations for the layers. Such study is important for the

understanding of the behavior of multilayer devices such as smart actuators where the layers can be piezoelectric, dielectric and conducting.

- 2) Development of the mechanics of cracks in multilayer systems. Cracks degrade the material integrity and their study is thus of great importance for the evaluation of device performance.
- 3) Study of the influence of defect evolution and interaction on the long-term performance of miniaturized multilayer devices, e.g., crack growth along interfaces.
- 4) Optimization of the multilayer geometry and material to minimize the degradation effects caused by defects.

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