Mechanics of disclinated interfaces and cracks in polycrystalline an nanocrystalline materials

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**Mechanics of Disclinated Interfaces and
Cracks in Polycrystalline and
Nanocrystalline Materials**

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Abstract

Grain boundaries (GBs) and crystal lattices in nanocrystalline materials contain defects, which may grow and induce failure of the materials. A critical issue for developing nanocrystalline materials is thus the modeling of material microstructures and constituent defects as well as the simulation of their behavior under load. In particular, the disclination defect, commonly found in nanocrystalline materials, is investigated in this research. The research focuses on the description of material interfaces by a disclination dipole wall and on the investigation of cracks initiating from disclinations.

First, the mechanics model of an interfacial wedge disclination dipole wall in a hexagonal bicrystal is established by the method of image dislocations. The exact closed-form solutions for the elastic stress and strain energy density are shown to be of the form of the logarithm of hyperbolic and trigonometric functions of complex parameters. The results show that the stress, strain energy density and strain energy all depend significantly on the orientational and material inhomogeneities.

Second, the disclination-structural unit model in conjunction with the mechanics model of the dipole wall is developed for the physical description of GBs in hexagonal bicrystals. For $[1\bar{1}00]$ symmetrical tilt GBs in cobalt and titanium, it is shown that the GB stress field and energy depend strongly on the misorientation. In particular, the GB stress field is more localized in high-angle boundaries than in small-angle boundaries and severe distortion of the stress field results from even a small inhomogeneity. The energy-misorientation curve is characterized by cusps associated with favored

boundaries, local energy maxima between the cusps, and regions of high and low average energies demarcated by the $(11\bar{2}2)$ favored boundary. The maximum energy occurs near the misorientation of 23° corresponding to the $(1\ 1\ \bar{2}\ 16)$ plane.

Third, the stability of a cylindrical bicrystalline nanowire containing a negative wedge disclination is studied via continuum mechanics and atomistic simulations. The continuum theory considers stable and unstable double-ended equilibrium cracks initiating from the disclination in an isotropic cylinder, and takes into account the redistribution of stress due to crack disturbance. For the atomistic simulations, molecular statics relaxations are performed starting from structures both without and with an initial interfacial crack. The continuum and atomistic calculations show very close agreement in the critical disclination strength (11.6° and 11.1° for a nanowire of 25 nm radius), and general agreement in the stable crack length, the crack opening profile, and the stress field of the disclinated crack in the nanowire.

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List of Symbols

Symbol	Definition
a	Crystal lattice constant
a_d	Half arm length of a disclination dipole
$\bar{a}_d$	Value of a_d normalized by the disclination dipole wall period h
a'_{ij}	Compliance components of a crystal in the local coordinate system $x' - y' - z'$
A_α	Normalized vectors arising from Stroh's sextic formulation
$\mathbf{b}$	Burgers vector of a discrete dislocation
b	Magnitude of the Burgers vector of a discrete dislocation
b_x	x -component of the Burgers vector of a discrete dislocation
b_y	y -component of the Burgers vector of a discrete dislocation
c	Crystal lattice constant
c_θ	$c_\theta = \cos \theta$
C_{ij}	Elastic constant components of a crystal in the global coordinate system $x - y - z$
C'_{ij}	Elastic constant components of a crystal in the local coordinate system $x' - y' - z'$
e	Volume expansion of a grain boundary
G	Shear Modulus
h	Half period vector of a grain boundary

h	Period of a disclination dipole wall
H	Period vector of a grain boundary
K_I	Stress intensity factor of a mode I crack
K_{IC}	Critical stress intensity factor of a mode I crack
l	Half length of a crack
L_α	Normalized vectors arising from Stroh's sextic formulation
p_α	Eigenvalues arising from Stroh's sextic formulation
r_c	Cut-off distance of an atomistic potential
R	Cylinder radius
s_θ	$s_\theta = \sin \theta$
u_x	Displacement in the x -direction
u_y	Displacement in the y -direction
v_1, v_2	Roots of the characteristic equation of the elastic constant components C'_{ij}
W	Strain energy density
γ_t	Cleavage energy of a grain boundary
γ_{gb}	Energy of a grain boundary
γ_s	Surface energy
γ_ϵ	Strain energy
θ	Orientation of the c -axis of a hexagonal crystal with respect to x -direction in the global coordinate system $x - y - z$

ρ^c	Density of climb dislocations
ρ^g	Density of glide dislocations
ρ_x	Density of dislocations with Burgers vector in the x -direction
ρ_y	Density of dislocations with Burgers vector in the y -direction
σ	Stress field with components σ_x , σ_y , and σ_{xy}
σ_x	Normal stress in the x -direction
σ_y	Normal stress in the y -direction
σ_{xy}	Shear stress in the x - y plane
σ_{ij}	Stress tensor components in the global coordinate system $x - y - z$
σ'_i	Stress tensor components in the local coordinate system $x' - y' - z'$
σ_r	Radial stress in the polar coordinate system $r - \phi - z$
$\sigma_{r\phi}$	Shear stress in the polar coordinate system $r - \phi - z$
Σ	Reciprocal coincidence site density of a grain boundary
ν	Poisson's ratio
θ	Grain boundary misorientation
ω	Frank vector of a disclination
ω	Strength of a disclination
ω_c	Critical disclination strength

Chapter 1

Introduction

The present research aims to study disclinated interfaces and cracks in polycrystalline and nanocrystalline materials. In this chapter, the research background is introduced in Section 1.1, followed by an explanation of the research motivation in Section 1.2. Thereafter, the objectives of this research thesis are stated in Section 1.3, and the thesis work is outlined in Section 1.4.

1.1. Background

Nanocrystalline materials are polycrystalline materials with grain sizes smaller than 100 nanometers. Over the past two decades, nanocrystalline materials have gained much interest of material scientists because they demonstrate a number of improved physical and mechanical properties, namely good electrical conductivity, high magnetic permeability, superplasticity, and high strength, ductility and wear resistance, as compared with their coarse-grained counterparts (e.g., Gleiter (1989), Gryaznov and Trusov (1993), Valiev et al. (2000) and Romanov (2003)). These improved properties are mainly determined by two factors: (i) grain size effects and (ii) the presence of high-density interfaces or grain boundaries (GBs) in the material interior. However, the GBs and crystal lattices in nanocrystalline materials are also prone to the growth of defects, which may induce failure of the materials.

Disclinations, which are rotational line defects (Romanov and Vladimirov, 1992), can exist in polycrystalline and nanocrystalline materials. They may appear as disclination dipoles, each of which consists of a positive and a negative disclination. For example, the atomic structure of disclination dipoles was observed directly in mechanically milled, nanocrystalline iron by high-resolution transmission electron microscopy (TEM) (Murayama et al., 2002). Due to the fact that disclinations, similar to dislocations, possess long-range elastic fields, they play an essential role in the plasticity and strength of crystals (Romanov, 2003).

Disclinations are commonly generated in plastic deformation of polycrystals. The studies of substructure evolution during large plastic deformation showed that disclinations are accumulated in triple junctions of grains due to their strain incompatibilities (Rybin, 1986; Rybin et al., 1993; Zisman and Rybin, 1996). These junction disclinations can have strengths up to 3° (Rybin, 1986; Motylenko et al., 2004) and have been observed by TEM (Motylenko et al., 2004). Therefore, triple junction disclinations can constitute an essential element of the structure of nanocrystalline materials produced by severe plastic deformation and as such significantly influence their structural stability as well as mechanical and physical properties (Valiev et al., 2000; Nazarov and Mulyukov, 2003). Furthermore, disclinations formation can be caused by the termination of GBs during the growth of crystal thin films on substrates, as has been observed by Jiang and Jia (1996).

Due to the singular internal stress fields induced by disclinations, they serve as preferential sites for crack formation. Cracks due to disclinations may be termed *disclinated cracks*. Rybin and Zhukovskii (1978) first proposed a model of crack

formation at a triple junction disclination. This model specified the position, shape and dimensions of nucleating microcracks during the late stage of plastic deformation and predicted that for the fragment size of $0.5\ \mu\text{m}$ a wedge disclination with a strength of 1.7° had an equilibrium crack length of about $0.07\ \mu\text{m}$. Essentially, the same estimate was obtained by Gutkin and Ovid'ko (1994) for unsplit wedge disclinations. They also predicted that the splitting of disclinations into ones with smaller strengths resulted in an increase of the equilibrium crack length. Accurate estimates of crack length due to disclinations in micron-size homogeneous isotropic cylinders were made by Wu and Zhou (1996) based on the modeling of the nucleated crack by initially unknown continuous distributions of infinitesimal edge dislocations. Their theory assumed the crack to be Zener-type, growing from the disclination in one direction, and predicted the existence of two equilibrium crack lengths at any value of the disclination strength. Recently, Wu (2001, 2002a) also investigated the characteristics of a mode I Zener crack with and without cohesive end zones and wedge opened by a disclination dipole.

Furthermore, the disclination approach is very helpful in the description of the structures and properties of microstructures where rotational symmetry is violated (Shenderova and Brenner, 2002). In particular, the disclination approach has been successfully used to study GBs since Li (1972) proposed that a GB can be modeled by a disclination dipole wall. For example, Gertsman et al. (1989) developed the disclination-structural unit model (DSUM) to model GBs by combining Li's disclination model and the structural unit model (Sutton and Vitek, 1983a, b, c). In this model, the GB energy is composed of three parts: a weighted sum of the energy of the individual structural units, the elastic energy of the disclination dipole wall, and the

energy of the disclination cores. The GBs modeled in this manner may be termed *disclinated boundaries* or *disclinated interfaces*. The DSUM has been applied to obtain the GB energy versus misorientation curves for $[001]$ and $[1\bar{1}0]$ symmetrical tilt GBs in aluminum (Gertsman et al., 1989; Valiev et al., 1990). The results agreed well with the experimental data obtained by Hasson and Goux (1971). Furthermore, using the DSUM combined with first-principles quantum mechanics simulations, the GB energies have been obtained for the entire misorientation range for $[001]$ and $[011]$ symmetrical tilt GBs in diamond (Shenderova et al., 1998; Nazarov et al., 2000a, b). Recently, the martensite structure in palladium-iron alloy was shown by TEM to possess disclination dipole walls, which induce a locally fluctuating residual stress field (Mori et al., 2004).

1.2. Motivation

A critical issue for developing nanocrystalline materials is the ability to understand, model and simulate the behavior of material microstructures and constituent defects and to make the connection between structures, properties and functions.

1.2.1. Grain Boundaries

Interfaces are ubiquitous in materials and structures. A polycrystalline or nanocrystalline material contains numerous interfaces or GBs between the crystals or grains. GBs are essentially planar microstructural defects, and are the direct cause of the immense differences between properties of single crystals and polycrystalline materials. Indeed, the modeling of GB structures is the key to success in the control and engineering of modern high-performance polycrystalline or nanocrystalline materials.

Detailed knowledge of the stress fields and energies of GBs is of great significance. The GB stress field governs interaction with defects and impurities, and the GB energy is a driving force for processes such as intergranular fracture. Furthermore, the GB misorientation angle is a key parameter. It has been demonstrated that the GB property and behavior depend strongly on the misorientation angle, e.g., the GB energy (Nazarov et al., 2000a, b), the fracture stress (Tsuekawa et al., 1994; Watanabe and Tsuekawa, 1999), the cleavage energy (Shenderova et al., 2000) and the critical current density (Heinig et al., 1999) in bicrystals.

Thus far, much work has focused on the modeling of GBs in face-centered cubic (FCC) materials, and research has yet to be done for materials with other crystal structures. In particular, the hexagonal close-packed (HCP) structures are of great importance since many metals such as titanium and zinc have HCP structures.

In a global coordinate frame, two identical crystals of different crystallographic orientations have different elastic constants referring to that frame and therefore are inhomogeneous across the GB if they are treated as anisotropic, while they have the same elastic constants with respect to that frame and therefore are homogenous if treated as isotropic. In most of the previous studies, the crystals sharing the GB are treated as isotropic and the inhomogeneity resulting from the elastic anisotropy of the crystals is not taken into account. However, the material anisotropy and inhomogeneity may have strong influence on the stress distribution (Wu, 2000b) and the GB stress field and energy. Consequently, it is meaningful to incorporate bicrystal anisotropy and inhomogeneity in the investigation of GBs.

Furthermore, it was discussed in Section 1.1 that the disclination approach provides a good means to study GBs. This approach, however, needs further development for the application to different crystal structures like the HCP.

1.2.2. Cracks

Cracks, being planar microstructural defects with stress singularities or significant stress concentrations, can have detrimental effect on the properties and behaviors of nanocrystalline and polycrystalline materials. Therefore, the investigation of mechanisms or conditions of crack formation and the study of the crack characteristics, e.g., the crack length, the crack opening profile and the stress field of the crack, are of fundamental importance for reliability prediction and failure prevention of nanocrystalline materials.

However, the knowledge of disclinated cracks in nanocrystalline materials remains poorly understood. The nucleation condition and characteristics of a disclinated crack within grains or along GBs become obscure as the grain-size screening effect on the long-range stress field of a disclination becomes strong in nano-sized grains. Nanowires, which have wide applications in nano-devices, can reach a few nanometers in diameter and tens of microns in length (Xu et al., 2003). To understand the fundamental mechanism of cracking in nanocrystalline materials, the disclinated crack in a nanowire, which is a comparatively “simple” type of nanocrystalline material, is studied in this research.

In fracture study, the continuum-mechanics and atomistic simulation approaches each have their own strengths and weaknesses, realm of applicability and limitations. Thus, a multi-approach trying to utilize the merits of both is taken in this investigation.

1.3. Objectives

The proposed research aims to conduct an in-depth investigation into the mechanics of disclinated interfaces and cracks and their physical modeling thus facilitating the prediction of the internal mechanical states of polycrystalline and nanocrystalline materials. The wedge disclination, which is one of two types of disclinations (see Chapter 2.1.1) will be considered only. The specific objectives are to:

- 1) Construct the mechanics model of a wedge disclination dipole wall for GBs in HCP bicrystals. This model takes into account the bicrystal anisotropy and inhomogeneity.
- 2) Develop the physical model of a DSUM for GBs in HCP bicrystals. The DSUM is used in conjunction with the mechanics model of a wedge disclination dipole wall to investigate the GB properties.
- 3) Establish a continuum model and an atomistic model for a disclinated crack in a bicrystalline nanowire. The DSUM approach is incorporated in the construction of the atomistic model.

1.4. Outline of the Thesis

Following this introduction, the other chapters of the thesis are organized as follows.

In Chapter 2, the concept and the formation mechanism of disclinations and their presence in nanostructured materials are described in detail. Previous studies on disclinated GBs and cracks are reviewed.

In Chapter 3, the stress field and strain energy of a disclination dipole wall at the interface of a hexagonal bicrystal are derived, and the influence of the anisotropy and inhomogeneity of the bicrystal on the elastic field is investigated.

In Chapter 4, the DSUM is developed for application in hexagonal bicrystals. For the purpose of comparison, the mechanics model of a disclination dipole wall in homogeneous isotropic crystals is also presented. The stress field of the disclination dipole wall and the dependence of GB energy on misorientation are investigated using the DSUM in conjunction with the inhomogeneous anisotropic model obtained in Chapter 3 and the homogeneous isotropic mechanics model.

In Chapter 5, a continuum model is used to describe a double-ended wedge crack due to a negative disclination in a bicrystalline nanowire, and an atomistic model incorporating the DSUM approach presented in Chapter 4 is then developed to simulate the same crack. The results obtained via the two models are presented and discussed.

In Chapter 6, conclusions are drawn and some suggestions for further research in this field are made.

Chapter 2

Literature Review

This chapter begins with an introduction of the concept of disclinations in Section 2.1, with emphasis on the geometrical properties, the elastic fields, and the relations between disclinations and dislocations. The formation mechanism of disclinations in solids and their presence in nanostructured materials are then described in Sections 2.2 and 2.3, respectively. Thereafter, studies of two types of planar defects, GBs and cracks, associated with disclinations are reviewed. Previous works on the application of disclinations in modeling GBs are briefly described in Section 2.4, while studies of cracks initiated by disclinations are reviewed in Section 2.5. On the basis of the review, the scope of the thesis work is also outlined in Sections 2.4 and 2.5.

2.1 Introduction of Disclinations

2.1.1. Geometry of Disclinations in a Uniform Continuum

A good way to understand disclinations is to start with a geometrical approach. In continuum theory, Volterra has introduced six types of dislocations in a hollow cylinder made of isotropic material (Romanov and Vladimirov, 1992). The cylinder is cut along a plane Γ as shown in Fig. 2.1(a). By translating and turning the faces of the radial cut Γ and subsequently sticking them together, six types of Volterra distortions can be

Fig 2.1. Volterra dislocations. (a) Initial hollow cylinder with a radial cut Γ . (b), (c) Edge dislocations of Burgers vector b . (d) A screw dislocation. (e), (f) Twist disclinations of Frank vector ω . (g) A wedge disclination.

obtained, as illustrated in Figs. 2.1(b)-(g). In this process, material is either inserted into the arising cavities or taken away from the areas of overlap. Shrinking of the inside passage results in a linear singularity in the cylinder, which represents the line of a defect. The first three types of Volterra distortions related to the translation of the cut faces by a Burgers vector $\mathbf{b}$ are said to be dislocations, while the other three types of distortions related to the rotation of the non-deformed cut faces by a Frank vector $\boldsymbol{\omega}$ are said to be disclinations. The Frank vector $\boldsymbol{\omega}$ characterizes the strength of a disclination as the Burgers vector $\mathbf{b}$ characterizes the strength of a dislocation. Disclinations having the Frank vector perpendicular to the defect line are called twist disclinations (Figs. 2.1(e) and (f)). In contrast, straight linear disclinations having the Frank vector parallel to the defect line are called wedge disclinations (Fig. 2.1(g)). A wedge disclination is said to be positive if it is created by taking out a wedge of matter, while it is negative if created by inserting some amount of new matter into the region between the cut faces. This literature review is mainly concerned with the studies of wedge disclinations.

2.1.2. Geometry of Disclinations in Crystals

In the continuum theory the rigid translations and rotations in Volterra's operations may be chosen arbitrarily in magnitudes and signs for isotropic materials. However, crystalline materials, which are not isotropic, are associated with discrete translations and rotations.

Anthony (2002) gave a comprehensive description of disclinations in crystal lattices. Figures 2.2 and 2.3 show how a positive and a negative wedge disclination are created

Fig 2.2. Wedge disclination in the hexagonal triangle lattice. (a) A lattice with a 60° wedge taken out of it. (b) A formed positive 60° wedge disclination in the lattice.

Fig 2.3. Wedge disclination in the hexagonal triangle lattice. (a) A lattice with a 60° wedge inserted into it. (b) A formed negative 60° wedge disclination in the lattice.

Fig 2.4. A partial negative 30° wedge disclination, delineating a lattice plane and a GB, in the hexagonal triangle lattice.

in the hexagonal triangle lattice, respectively. In each of the two figures, the two-dimensional lattice, on which circles represent atoms, is the projection of a three-dimensional hexagonal lattice onto its basal plane along the c -axis. One removes from or inserts into the crystal an appropriate 60° wedge of crystalline material. After rewelding the structure one arrives at two opposite wedge disclinations as shown in Figs. 2.2(b) and 2.3(b). This procedure is consistent with that of Volterra in Fig. 2.1(g). The positive disclination in Fig. 2.2(b) gives rise to a 5-fold rotational symmetry of its crystal structure about the disclination line located at the structure center. The negative disclination in Fig. 2.3(b) gives rise to a 7-fold rotational symmetry. Due to the symmetry, the two disclinations are termed perfect disclinations in contrast to partial disclinations which are commonly discussed in plasticity theory (Romanov and Vladimirov, 1992). Figure 2.4 shows an example of a partial disclination in the hexagonal triangle lattice. Formally, it is produced by the same procedure in Fig. 2.2(a), however, with a 30° wedge angle, which is not a symmetry angle of the lattice. This

procedure results in a GB ending in the partial 30° disclination, which thus delineates a lattice plane and a GB.

2.1.3. Relations with Dislocations

There exists a close interrelation between disclinations and dislocations. Any disclination can be represented in the form of a superposition of dislocations (Romanov and Vladimirov, 1992). Simultaneously, any dislocation defect admits an equivalent representation through a set of disclinations (Romanov, 2003).

Figure 2.5(a) shows that the wedge, which is inserted to create a negative wedge disclination, can be modeled by means of a succession of edge dislocations with infinitesimal Burgers vectors db which are introduced into the matter. Thus, an individual disclination is identical to a semi-infinite wall of edge dislocations having linear density:

$$\rho = \frac{1}{dl} = \frac{2 \tan(\omega/2)}{db}, \quad \text{or} \quad \rho = \frac{\omega}{db} \quad \text{if} \quad \omega \ll 1. \quad (2.1)$$

Disclinations may appear as dipoles (a pair of positive and negative disclinations) and quadrupoles (a pair of dipoles) (Romanov and Vladimirov, 1992). Figure 2.5(b) shows that a double-axis disclination dipole, in which the line of each disclination coincides with its own rotation axis, can be modeled by a wall of edge dislocations cut off from two sides. In a single-axis disclination dipole the wedge disclinations have a single common axis of rotation intersecting the middle of the link between the defect ones as illustrated in Fig. 2.5(c). This dipole can be represented by a portion of a dislocation wall terminated at its ends by two edge dislocations of Burgers vector

Fig 2.5. Dislocation models for wedge disclinations and their dipoles. (a) A single disclination. (b) A double-axis dipole. (c) A single-axis dipole.

magnitude $b = 2a_d \tan(\omega/2)$, where $2a_d$ is the dipole arm length. This method is also appropriate for building dislocation models for disclination quadrupoles.

2.1.4. Elastic Fields of Disclinations

Detailed knowledge of the elastic fields of disclinations is of great significance in investigating the behavior and properties of disclinated solids, e.g., deformation, fracture/damage, interaction with other defects, and excess energy. In this subsection, previous works on the elastic fields of wedge disclinations in homogeneous and inhomogeneous solids are reviewed categorically, and the characteristic of the long-range stress field of a wedge disclination is noted.

2.1.4.1. Disclinations in Homogeneous Solids

As early as 1907, Volterra presented the displacement and stress fields of a hollow-core wedge disclination running along the axis of a long isotropic cylinder (de Wit,

1972). An elegant derivation of the stress field using complex variables was obtained by Muskhelishvili (1953). Friedel (1964) gave the stress field and energy solutions for the case of a large outer radius of the cylinder. The above expressions contain terms that depend on the inner and outer radii of the cylinder and which serve primarily to satisfy the boundary conditions. If they are ignored, the leading terms which are characteristic of the wedge disclination will be left. de Wit (1972) summarized the elastic solutions of a zero-core wedge disclination running along the axis of an infinite isotropic cylinder of radius R . To illustrate, the expressions for the circumferential stress $\sigma_{\phi\phi}$ in polar coordinates (r, ϕ) and strain energy γ_ϵ (per unit length along the z -axis) are given below:

$$\sigma_{\phi\phi} = \frac{G\omega}{2\pi(1-\nu)} \left(\ln \frac{r}{R} + 1 \right), \quad \gamma_\epsilon = \frac{G\omega^2 R^2}{16\pi(1-\nu)}, \quad (2.2)$$

where G and ν denote the shear modulus and Poisson's ratio of the cylinder material, respectively. Equation (2.2) shows that a wedge disclination has logarithmically divergent long-range stresses and its energy quickly grows with the body dimension R . In contrast, stresses of a dislocation in a cylinder approach zero at large distances and its energy grows only very slowly with R , as can be seen in the stress and energy expressions for an edge dislocation in a cylinder with inner radius $r_0 \rightarrow 0$ (Hirth and Lothe, 1982), i.e.,

$$\sigma_{\phi\phi} = \frac{Gb}{2\pi(1-\nu)} \sin \phi \left(-\frac{1}{r} - \frac{r_0^2}{r^3} + \frac{3r}{R^2} \right), \quad \gamma_\epsilon = \frac{Gb^2}{4\pi(1-\nu)} \ln \frac{R}{r_0}, \quad (2.3)$$

where the Burgers vector of the edge dislocation is along the direction of $\phi = 0$. Furthermore, Eq. (2.2) shows that a weak logarithmic singularity exists at the

disclination line: $\sigma_{\phi\phi} \sim \ln r$ as $r \rightarrow 0$ and the contribution of stresses from the region around the disclination line to the energy γ_e is negligible. This is again in contrast to that of a dislocation, where stresses at the dislocation line have a strong singularity of the type $1/r$ and the energy would diverge (refer to the limiting behavior of $\sigma_{\phi\phi}$ and γ_e at $r \rightarrow 0$ and $r_0 \rightarrow 0$ in Eq. (2.3)). For a negative disclination, the cylinder region given by $r < R/e$ experiences tensile circumferential stresses, while the region of $r > R/e$ compressive stresses. The tensile and compressive regions reverse for a positive disclination.

The logarithmic divergence of the long-range stresses of wedge disclinations can be disposed of by joining them in dipole and other multipole configurations. For instance, one-axis dipoles and quadrupoles of wedge disclinations are self-screened defect configurations. Their energy depends only on the distance between the disclinations inside the configurations (Romanov and Vladimirov, 1992). Moreover, Shih and Li (1975) obtained the strain energy of a periodic array of disclination dipoles by performing integration on the energy solution of a disclination dipole in isotropic solids. A further review of their work will be given in Section 2.5.

Solutions for the stress fields of a wedge disclination and a disclination dipole in anisotropic solids were obtained by Alshits et al. (1975). However, due to the complexity, the solutions have hardly been applied. Chou and Pan (1973) obtained solutions for a wedge disclination line of special orientations in hexagonal crystals, which are transversely isotropic, using the Green's function for transversely isotropic solids. Yu and Sanday (1994) extended the method to obtain analytic solutions for wedge disclinations of arbitrary orientations in transversely isotropic solids by

employing a certain hexagonal stress vector (Yu et al., 1994) together with the Green's function.

2.1.4.2. Disclinations in Inhomogeneous Solids

Yu and Sanday (1991) investigated straight disclinations in isotropic bimetals using the elastic solutions for the "nuclei of strain". The study represents an advance since the isotropic constants of the two material half spaces could differ, but an isotropic bimaterial is not always adequate because many materials are anisotropic. Belov (1993) investigated the stresses due to wedge disclinations in rotationally inhomogeneous anisotropic media using the consistency method of Kirchner (1989). The solutions are, however, presented in certain forms that require extensive numerical calculations.

Wu (2000) derived the exact theoretical solutions for a disclination dipole located off or on the interface in a transversely isotropic bimaterial. The solutions are, however, restricted to the case where the material c -axis orientations are of special values, i.e., 0° and 90° . Based on these solutions, Wu (2002c) obtained the stress field and strain energy of an infinite periodic array of interfacial wedge disclination dipoles in the same material. Furthermore, Wu (2002b) investigated the stress field of a wedge disclination dipole located at the boundary of a hexagonal bicrystal with arbitrary c -axis orientations. In these works, the solution method is based on the construction of continuous image dislocations (or virtual dislocations) to satisfy continuity conditions across the bicrystal boundary (Weertman, 1996). This leads to a system of four Cauchy integral equations with the image densities as unknown. The equations are solved exactly by using the Hilbert transform of the stresses due to the disclination dipole and the iterative property

of the transform. Numerical results show that the characteristics of the stress distribution depend significantly on the intrinsic crystal anisotropy and the material inhomogeneity. Need to mention that the technique of virtual dislocations was originally introduced by Louat (1962) and then developed by Marcinkowski (1979) to solve surface problems. Romanov and Vladimirov (1981) first used this technique for disclinations near a free surface and then this technique has been broadly used for the solutions of various elasticity problems for defects (Weertman, 1996; Kolesnikova and Romanov, 2004). In this thesis, the term “image dislocation” is used as an alternate one for “virtual dislocation” following the monograph of Weertman (1996).

2.2. Formation Mechanisms of Disclinations in Solids

Disclinations can be formed in crystals in different ways. The most common formation mechanism is the plastic deformation of polycrystals. Plastic deformation leads to the absorption of lattice dislocations by GBs. Lattice dislocations absorbed by GBs change their misorientations and result in the formation of partial disclinations at the junctions of grains (Nazarov and Mulyukov, 2003).

Gutkin et al. (2002) gave a good schematic description for the disclination formation at a GB (Fig. 2.6). Let some gliding dislocations with Burgers vectors $\mathbf{b}_1$ cross a flat GB (Fig. 2.6(a)) and move into the neighbouring grain, in which their Burgers vectors become $\mathbf{b}_2$ (Fig. 2.6(b)). This results in the occurrence of a wall of difference dislocations having Burgers vectors $\delta \mathbf{b} = \mathbf{b}_1 - \mathbf{b}_2$ and interdislocation spacing l at the crossing site. Such a difference dislocation wall can be effectively described as a two-axis dipole of wedge partial disclinations with strengths $\pm \omega = \pm \delta b / l$ (Fig. 2.6(c)).

Fig 2.6. Schematic for the formation of a GB disclination dipole with the strength ω (Gutkin et al., 2002).

Fig 2.7. Generation of a misorientation band by splitting a GB disclination dipole (Gutkin et al., 2002).

Furthermore, Rybin and co-workers from their extensive experimental and theoretical studies of substructure evolution during large plastic deformation concluded that disclinations are accumulated in triple junctions of grains due to their strain incompatibilities (Rybin, 1986; Rybin et al., 1993; Zisman and Rybin, 1996). In fact, junction disclinations due to large plastic deformation have been observed directly by TEM (Motylenko et al., 2004). These triple junction disclinations can have strengths up to 3° (Rybin, 1986; Motylenko et al., 2004).

Junction disclinations are the basic elements of deformed polycrystals and are responsible for the partition of grains (Rybin et al., 1993), which occurs by the

movement of disclinations across the grains, leading to the formation of new boundaries (Nazarov and Mulyukov, 2003). The generation of misorientation bands may explain this phenomenon well. Gutkin et al. (2002) illustrated the splitting of a GB disclination dipole into a misorientation band (Fig. 2.7). Under the action of the internal shear stress caused by the GB disclination dipole and the external shear stress τ , the dislocations nearest to the disclinations glide to them thus forming two dislocation walls, on the edges of which a new disclination dipole is also formed. The misorientation band representing the new disclination configuration is characterized by the parameters given in the figure. TEM observations have demonstrated that microbands are frequently found in plastically deformed crystals and are important defect entities in the substructure evolution at large strain (Klimanek et al., 2001; Klemm et al., 2002).

Another important mechanism of disclination formation is the termination of grain boundaries during the growth of crystal thin films on substrates. For example, during the growth of diamond films a 2° misorientation tilt boundary was observed to terminate inside the film (Jiang and Jia, 1996).

2.3. Disclinations in Nanostructured Materials

Nanostructured materials include nanocrystals, nanoscale films and nanoparticles, in which the constitutive elements have a characteristic size less than 100 nm. Over the past two decades, nanostructured materials have gained much interest of material scientists due to their unique physical and mechanical properties, namely good electrical conductivity, high magnetic permeability, superplasticity, and high strength, ductility and wear resistance (e.g., Gleiter (1989), Gryaznov and Trusov (1993), Valiev et al.

(2000) and Romanov (2003)). These unique properties are mainly determined by two factors. One is the size effect. The other is the presence of high density of interfaces and interface junctions in the material interior.

In bulk nanocrystals produced by severe plastic deformation, GBs are in the metastable, nonequilibrium state (Valiev et al., 2000). Nonequilibrium GBs modeled in terms of disordered arrays of disclinations generate long-range stress fields, which are responsible for improved properties of nanocrystals (Nazarov et al., 1993; Nazarov et al., 1996). The other important sources of internal stresses are junction disclinations in nanocrystals (Romanov, 2003). As discussed in Section 2.2, junction disclinations are essential elements of defect structures at large strains (Rybin et al., 1993), and facilitate the fragmentation and reorientation of grains at the ultrafine scale. Nazarov et al. (1996) studied the root mean square strain, dilation and stored energy of nanocrystals in the framework of disclinations, and found that the disclination contribution to the dilation for ultrafine-grained Al (grain size 100 nm) can reach the order of 10^{-4} .

Experimentally, Murayama et al. (2002) used the high-resolution TEM to observe the atomic structure of partial disclination dipoles in body-centered cubic iron that underwent severe plastic deformation by mechanical milling. They demonstrated that the formation and migration of partial disclinations during deformation allows crystalline solids to rotate and rearrange at the nanometer level.

In addition, the disclination approach has been used in the description of nanoparticles, e.g., pentagonal nanoparticles (Gryaznov and Trusov, 1993; Gryaznov et al., 1999). This approach has also been applied to explain the domain structures in

ferroelectric nanoscale films (Speck et al., 1995; Pertsev and Zembilgotov, 1995; Romanov et al., 1998).

2.4. Modeling of Grain Boundaries by Disclinations

A large number of studies have been devoted to the understanding of structures and energies of GBs, in particular, symmetrical tilt GBs in metals and alloys (Sutton and Baluffi, 1995). These GB studies have been performed using two approaches (Shih and Li, 1975). One is the continuum approach, in which GBs are described by structural defects such as dislocations and disclinations without knowledge of the detailed atomic structures. The other is the atomistic approach which requires knowledge of interatomic forces between atoms in the GB. Based on the two approaches, applications of disclinations in describing GB properties and calculating GB energies have been extensively studied and developed (Nazarov, 2002).

2.4.1. Dislocation Model and Disclination Model

The first theory of the misorientation dependence of the GB energy was proposed by Read and Shockley (1950) for low-angle tilt GBs by means of dislocations (the dislocation model). In their theory, the energy-misorientation relationship was obtained as:

$$\gamma_{gb} = \frac{Gb}{4\pi(1-\nu)} \Theta \ln \frac{e\Theta_m}{\Theta}, \quad (2.4)$$

where γ_{gb} is the energy per unit area of the boundary and e is the exponential constant.

In Eq. (2.4), the misorientation angle Θ can be determined by $\Theta = b/h$ with h being

the GB period, and Θ_m is given by $\Theta_m = b/2\pi r_0$ with r_0 being the core radius of dislocations. The dislocation model, which considers arrays of lattice dislocations, is limited to low-angle GBs because at high-misorientation angles the spacing between dislocations become so small that the dislocation core regions overlap and dislocations cannot be observed, as is reflected by Eq. (2.3) giving physically meaningless negative elastic energy values when $e\Theta_m < \Theta$ at large values of Θ . In attempts to overcome this limitation, the secondary dislocation model was introduced (Brandon, 1966; Bollmann, 1967a, b), in which the structures of high GBs with misorientation angles close to those of special GBs having low reciprocal coincidence site densities Σ are described by a secondary dislocation network superimposed on the special boundaries. However, this model is valid only for small misorientation deviations from those special boundaries. Thus, the early dislocation model failed to describe the GB energy in the whole misorientation range.

Li (1972) proposed that a GB, being a rotational defect, should be described more simply by disclinations based on the reason that the disclination is a rotational defect while a dislocation is a translational defect. In his disclination model, a general GB with misorientation angle Θ , intermediate between Θ_A and Θ_B ($\Theta_A < \Theta < \Theta_B$), is represented as a disclination dipole wall with alternating segments of special boundaries Θ_A and Θ_B . These segments are separated by partial disclinations of strengths $\pm\omega = \pm(\Theta_B - \Theta_A)$. Shih and Li (1975) obtained the elastic energy of a disclination dipole wall as:

$$\gamma_{gb} = \frac{G\omega^2 h}{32\pi^3(1-\nu)} f(\lambda), \quad (2.5)$$

where h is the period of the wall, $\lambda = \pi L_B / h$ with L_B being the length of the special boundary B segment, and

$$f(\lambda) = -16 \int_0^\lambda (\lambda - u) \ln|2 \sin u| du. \quad (2.6)$$

The elastic energy of the disclination dipole wall approaches that given by the dislocation model when the misorientation angle deviates slightly from the special values.

Equation (2.5) has an advantage over Eq. (2.4) in that it produces meaningful values for the elastic energy for any deviation of the misorientation angle from a special boundary because $f(\lambda) > 0$ for any θ . The curve of GB energy against misorientation angle (from 0° to 180°) obtained using Eq. (2.5) showed good agreement with the experimental data for [100] symmetrical tilt boundaries in copper and aluminum and [110] symmetrical tilt boundaries in aluminum (Shih and Li, 1975).

However, the disclination model also has some significant disadvantages (Gertsman et al., 1989). First, the contribution of disclination cores to the GB energy is ignored, and thus the self-consistent determination of the period of the disclination dipole wall is impossible. Second, it is not clear how many special boundaries and which of them should be taken as “favored” for the description of GB properties throughout the interval of misorientations. These solutions cannot be determined from the continuum theory alone. Therefore, a detailed knowledge on the atomic structure of GBs is required.

2.4.2. Structural Unit/ Dislocation Model

Extensive computer simulations made in the early 1980s provided a deep insight into the atomistic structure of high Σ tilt boundaries and their results led to a structural unit model (Sutton and Vitek, 1983a, b, c). This model postulates that structures of all tilt boundaries in a certain misorientation range for the same misorientation axis are composed of mixtures of two structural elements. These structural elements are the “units” of the so-called favored boundaries delimiting the misorientation range. Each favored boundary is composed of a contiguous sequence of one type of these units. The other boundaries (unfavoured) consist of structural units of two favored boundaries taken in a certain proportion and sequence. The set of favoured boundaries for a given misorientation axis can be established by means of computer simulations. Sutton and Vitek (1983a) demonstrated that 0° , 36.87° , 53.13° and 90° misorientations are favored for $[001]$ tilt boundaries in cubic crystals. The structural unit model has been proved by high-resolution electron microscopy studies of GBs in covalent crystals (Thibault, et al., 1993).

Based on the structural unit model, Sutton and Vitek (1983a, b, c) developed a structural unit/dislocation model, in which the minority structural units are regarded as dislocation cores. Using the structural unit/dislocation model, Wang and Vitek (1986) reformulated the Read-Shockley equation to make it applicable to high-angle GBs, and obtained the energy versus misorientation relations for $[001]$ and $[11\bar{1}]$ symmetrical tilt boundaries in copper, which reproduced the results of computer simulations relatively accurately. In their method, the entire misorientation range, however, has to be divided into smaller intervals in order to get meaningful elastic energies from the Read-

Shockley equation. For each interval, the method requires energies and structures of the delimiting boundaries as well as the energy of one additional GB to estimate the dislocation core radius. The total number of required structures is thus fairly large. As Sutton and Balluffi (1995) pointed out, this shortcoming is not a result of the structural unit model but rather due to the logarithmic term in the Read-Shockley equation that imposes a severe constraint on the misorientation range covered.

2.4.3. Disclination-Structural Unit Model

Gertsman et al. (1989) developed the disclination-structural unit model (DSUM), which combines the structural unit model and the disclination model. At the lines where structural units of different types meet, the misorientation angle of a boundary changes from one favored-boundary misorientation angle to another, these lines can therefore be regarded as partial wedge disclinations of strengths $\pm \omega = \pm(\theta_B - \theta_A)$, where θ_A and θ_B are the misorientations of two favoured boundaries. As a result, the boundary is represented by a wall of disclination dipoles in which the minority structural units are considered to be disclination dipoles. In this model, the GB energy is composed of three parts: a weighted sum of the energy of the individual structural units, the elastic energy of the disclination dipole wall, and the energy of the disclination cores. The DSUM has been applied to obtain the GB energy versus misorientation curves for [001] and $[1\bar{1}0]$ symmetrical tilt GBs in aluminum (Gertsman et al., 1989; Valiev et al., 1990). An important feature of the curves is the existence of a large quantity of cusps, corresponding to boundaries with low values of Σ , which are near favored boundaries,

and also to intermediate GBs between favored boundaries. The results agreed well with the experimental data obtained by Hasson and Goux (1971).

Because of the ability of the DSUM to bridge atomic structures and macroscopic-scale GB properties, it serves as a basis for a multiscale modeling approach for predicting GB energies from first principles (Shenderova et al., 1998). In principle, GB energies can be accurately calculated at the atomic scale using the first-principles density-functional methods (Payne, et al., 1987). In practice, however, first-principles calculations can be extremely computationally intensive, especially for systems having long-range stress fields that require a large number of atoms. Consequently, the multiscale modeling approach uses density-functional methods to calculate energies of only a few key structures (structural units). These energies along with elastic properties are then used as input to the DSUM to calculate GB energies in the whole misorientation interval for a given misorientation axis. Shenderova et al. (1998) used this approach to successfully estimate the energies of [001] symmetrical tilt GBs in diamond over the entire misorientation while greatly minimizing the computational efforts.

Recently, the DSUM has also been extended to treat complicated metastable structures with faceted interfaces for [001] and [011] symmetrical tilt GBs in diamond and for [001] and [111] symmetrical tilt GBs in copper (Nazarov et al., 2000a, b). These structures were described in terms of flat and faceted disclination dipole walls and screw dislocation dipole walls. In the elastic energy calculation, the Shih-Li equation was modified by replacing the factor $G/(1-\nu)$ by an energetic factor for edge

dislocations that can be calculated in the anisotropic theory of dislocations (Hirth and Lothe, 1982).

As reviewed above, most of the theoretical and experimental studies reported in the literature are on symmetrical tilt boundaries in cubic bicrystals. Very few atomistic calculations have been performed for hexagonal materials, although the structural unit model developed for cubic metals has been extended to describe GB structures in hcp metals since the 1970s (e.g., Bruggeman et al. (1972)). The studies by Farkas (1994) and Wang and Ye (1997) are two exceptions. Farkas (1994) performed embedded-atom method simulations of several $[1\bar{1}00]$ symmetrical tilt GBs in cobalt and titanium. The structures, energy and boundary expansion of $(11\bar{2}1)$, $(11\bar{2}2)$, $(11\bar{2}3)$, $(11\bar{2}4)$, $(11\bar{2}5)$ and $(11\bar{2}6)$ boundary planes were determined. Wang and Ye (1997) also employed the embedded-atom method to predict the misorientation dependence of the GB energy of $[0001]$ tilt boundaries in titanium. However, simulations of the misorientation dependence of the energy of general $[1\bar{1}00]$, $[0001]$, and $[11\bar{2}0]$ tilt boundaries are limited.

Furthermore, the elastic energy of the disclination dipole wall has been calculated using the isotropic elastic theory in the cited works, except that Nazarov et al., (2000a, b) have made some efforts in taking anisotropy into account. In addition, the material inhomogeneity has not been considered in the elastic energy calculation, even though a symmetrical tilt GB is inhomogeneous due to the different crystallographic orientations of its two constituent components. Wu (2002b) has already demonstrated that the material anisotropy and inhomogeneity may have strong influence on the stress distribution of an interfacial disclination dipole in a hexagonal bicrystal. This suggests

that in order to obtain more accurate estimate for the GB energies anisotropy and inhomogeneity should be considered. However, elastic solutions for a disclination dipole wall in an anisotropic bicrystal are not available as reviewed except those given by Wu (2002c) for the case of two special c -axis orientations 0° and 90° in a hexagonal bicrystal (referred to in Section 2.1.4.2).

Thus, this thesis work aims to develop a DSUM for application to $[1\bar{1}00]$ symmetrical tilt GBs in hcp metals and to derive the elastic solutions of a disclination dipole wall in an inhomogeneous anisotropic hexagonal bicrystal.

2.5. Cracks due to Disclinations

As Eq. (2.2) indicates, disclinations are sources of high stress concentrations. Consequently, a disclination may be unstable and a crack or other defect can nucleate from it. The first model of crack formation at a triple junction disclination was proposed by Rybin and Zhukovskii (1978). The model predicted that microcracks form at fragment contacts with at least one high-angle boundary and open up in a brittle manner along a high-angle boundary, and they are wedge-shaped with the blunt part at the contact. These features of crack formation have been confirmed by numerous experiments (Rybin and Zhukovskii, 1978). Moreover, for a fragment size of $0.5\ \mu\text{m}$, an effective surface energy of $1\ \text{J m}^{-2}$, and a theoretical tensile strength equal to $G/30$ (G is the shear modulus), this model predicted that a wedge disclination with a strength of 1.72° had an equilibrium crack length of about $0.07\ \mu\text{m}$. This prediction is consistent with experimental data (Lyles and Wilsdorf, 1975; Regel et al., 1975). Essentially the same estimate was obtained by Gutkin and Ovid'ko (1994) for unsplit

wedge disclinations based on the method of configurational force (Indenbom, 1962). They also predicted that the splitting of disclinations into ones with smaller strengths resulted in an amorphization of junctions and an increase of the equilibrium crack length.

Accurate estimates of crack length due to disclinations in micron-size cylinders were made by Wu and Zhou (1996). In their work, the stress intensity factors and the opening displacement of a crack in a finite isotropic homogeneous cylinder containing a negative wedge disclination were calculated. The method of crack analysis is based on the modeling of the nucleated crack by initially unknown continuous distributions of infinitesimal edge dislocations. This method is exact in the sense that all boundary conditions were satisfied properly and the stress redistribution due to the crack growth was taken into account intrinsically in the governing equations. It predicted the existence of two equilibrium crack lengths at any value of the disclination strength. The smaller crack is unstable and has a length decreasing with an increase of the cylinder radius and disclination strength, while the larger one is stable and exhibits an opposite dependence on the radius and strength. The crack was assumed to be a Zener crack, proposed by Zener (1948), and has a finite opening displacement at one end (the head) and a zero displacement at the other end (the tip), unlike the Griffith crack which has zero opening displacements at both ends. The Zener crack is a wedge crack. However, in the work of Wu and Zhou (1996) the crack was assumed to grow from the disclination in one direction only. This might be appropriate when the fracture toughness of the material in other directions was higher than that in the assumed growth direction, such as along a GB plane. Examination of the stress field of a wedge

disclination in a cylinder suggests that a real crack is likely to grow in both directions, albeit asymmetrically due to fracture toughness anisotropy. Indeed, Rybin and Zisman (1982) modeled the formation of a doubled-ended crack at wedge disclination dipoles. The possibility of a doubled-ended crack was also discussed by Romanov and Vladimirov (1992).

The formation and growth of cracks have been extensively studied by atomistic computer simulations (Shastry and Farkas, 1996; Cleri et al., 1998, 1999; Farkas, 2000). These simulations, by the use of either molecular statics or molecular dynamics, allow the elucidation of the crack tip processes (cleavage or dislocation emission) and the calculation of the equilibrium crack lengths. However, the role of disclinations in crack formation has never been addressed by atomistic simulations.

Therefore, a primary objective of this thesis work is to study the formation of a double-ended crack from a wedge disclination in a finite cylinder by means of both continuum mechanics theory and atomistic computer simulations. The cylinder will be in the form of a nanowire, as nanostructured materials are of increasing importance in engineering applications and the small system size permits atomistic simulations.

Chapter 3

Elastic Solutions for an Interfacial Disclination Dipole Wall in a Hexagonal Bicrystal

In this chapter, the stress field and strain energy of a disclination dipole wall at the interface of a hexagonal bicrystal are obtained, and the influence of the anisotropy and inhomogeneity of the bicrystal on the elastic field is investigated. The chapter is organized as follows. The problem is defined and the solution method is outlined in Section 3.1. The stress field due to a single disclination dipole is then presented in Section 3.2. Thereafter, the elastic solutions for a disclination dipole wall are obtained in Section 3.3. This is followed by some numerical examples in Section 3.4. Finally, conclusions are provided in Section 3.5.

3.1. Problem Definition and Solution Method

Consider an infinite periodic array of wedge disclination dipoles at the interface of two hexagonal crystals A and B, as shown in Fig. 3.1. Each disclination dipole consists of a positive and a negative disclination with strengths $\pm\omega$. For convenience, let a dipole be centered at the origin of the global frame $x-y-z$ so that the positive disclination is located at $(0, a_d)$ and the negative one at $(0, -a_d)$. Let the period of the dipole wall be h . Accordingly, the dipoles are centered at $(0, Nh)$ with the integer $N \in [-\infty, \infty]$. The c -axis of each crystal is confined to be in the $x-y$ plane and

3.1. The problem of an infinite periodic dipole array on the interface of a hexagonal bicrystal A-B and the decomposition of a single dipole problem into two subproblems. The c -axis orientations θ_A and θ_B are in-plane but otherwise arbitrary. The dislocation images are characterized by the function $F_1(y) = \ln |(y - a_d)/(y + a_d)|$ and its Hilbert transform $H[F_1(y)] = \pi$ for $|y| < a_d$ and 0 for $|y| > a_d$. The parameters Γ_{A1}^c , Γ_{A1}^g , etc. are constants. The single dipole solutions are summed to obtain the solution for the infinite dipole array.

Fig. 3.2. Global and local coordinates for a hexagonal crystal. The c -axis of the crystal is confined to be in the $x-y$ plane and has the orientation θ with respect to x . The c -axis is along x' in the local coordinate with z' coinciding with z .

has the orientation θ (θ_A or θ_B) with respect to x , as shown in Fig. 3.2. In the local crystal frame $x' - y' - z'$ with x' along the c -axis, the hexagonal crystal has the elastic stiffness matrix:

$$\{C'\} = \begin{bmatrix} C'_{11} & C'_{12} & C'_{12} & 0 & 0 & 0 \\ C'_{12} & C'_{33} & C'_{23} & 0 & 0 & 0 \\ C'_{12} & C'_{23} & C'_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C'_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C'_{66} & 0 \\ 0 & 0 & 0 & 0 & 0 & C'_{66} \end{bmatrix}, \quad (3.1)$$

where C'_{11} , C'_{33} , C'_{12} , C'_{23} and C'_{66} are five independent elastic constants in the transversely isotropic matrix, with $C'_{22} = C'_{33}$, $C'_{13} = C'_{12}$, $C'_{55} = C'_{66}$ and $C'_{44} = (C'_{33} - C'_{23})/2$. Note that the above convention for the elastic constants is

different from that used by Nye (1957), which assumes that the z -axis of the global frame is parallel to the c -axis of the hexagonal crystal.

The solutions for the dipole wall are obtained by summing the solutions of all the dipoles in the wall. The single dipole solutions are derived through the decomposition of the bicrystal problem into two homogeneous subproblems A and B, as shown in Fig. 3.1. Each subproblem consists of an infinite crystal (A or B) with the dipole and certain image edge dislocation distributions on the line $x = 0$. The densities of these image dislocations, which are of the climb and glide types, are determined by satisfying the continuity conditions of stress and displacement gradients across the interface. The image climb dislocations have their Burgers vector perpendicular to the interface, while the image glide dislocations have their Burgers vector parallel to the interface. The terms “glide” and “climb” are used only for convenience because the dislocations are virtual; the dislocations do not actually glide or climb.

Wu (2002b) has obtained the solutions of a single disclination dipole in hexagonal bicrystals with the elastic constants obeying the inequality

$$I = |C'_{12}(C'_{12} + 2C'_{66}) - C'_{11}C'_{33}| - 2C'_{66}\sqrt{C'_{11}C'_{33}} < 0. \quad (3.2)$$

Examples of crystals with elastic constants satisfying $I < 0$ are zinc, cadmium and beryllium. However, some hexagonal crystals, such as cobalt and titanium, have their elastic constants satisfying $I > 0$. Therefore, the solutions given by Wu (2002b) are first generalized to be suitable for any hexagonal crystals, i.e., without the limitation of $I > 0$ or $I < 0$, in Section 3.2. Then, the solutions for a disclination dipole wall are obtained in Section 3.3 by summing the generalized solutions of each dipole.

3.2. Single Disclination Dipole in a Hexagonal Bicrystal

The stress field due to a single wedge disclination dipole centered at (0, 0) in a hexagonal bicrystal is given as the sum of the field in the homogeneous crystal (A or B) and the corrective image field, which is added to satisfy the relevant interfacial boundary continuity conditions (Wu, 2000b):

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_{\text{dipole}} + \boldsymbol{\sigma}_{\text{image}} \quad (3.3)$$

Equation (3.3) means that the stress field in crystal A is determined from the homogeneous subproblem of the infinite crystal A, which contains the dipole and the image dislocations on $x = 0$. Similarly, the stress field in crystal B is determined from the subproblem of the infinite crystal B, also containing the dipole and its own image edge dislocations. In each subproblem, the densities of the image dislocations are unknown and can be determined by the continuity conditions

$$\sigma_x^A(0, y) = \sigma_x^B(0, y), \quad \sigma_{xy}^A(0, y) = \sigma_{xy}^B(0, y), \quad (3.4)$$

$$\frac{\partial u_x^A}{\partial y}(0, y) = \frac{\partial u_x^B}{\partial y}(0, y), \quad \frac{\partial u_y^A}{\partial y}(0, y) = \frac{\partial u_y^B}{\partial y}(0, y), \quad (3.5)$$

where the superscripts A and B denote crystals A and B, respectively. Equation (3.4) represents the continuity conditions of normal and shear stresses across the bicrystal interface, while Eq. (3.5) those of normal and tangential displacement gradients. The displacement gradients rather than the displacements are used for the continuity conditions because both of them predict identical stress distribution in the bicrystal although they may result at most in a rigid body displacement difference for the displacement solutions. Furthermore, the expressions of the displacement gradients and

stresses have similar forms, which would reduce the complexity of the integral equations resulting from the continuity conditions.

3.2.1. Single Disclination Dipole in a Hexagonal Crystal

In Eq. (3.3), the stress field σ_{dipole} of a single wedge disclination dipole centered at $(0, 0)$ in a homogeneous hexagonal crystal is obtained as

$$\sigma_{\text{dipole}} = \sum_{i=1}^2 \Lambda(v_i) \times \mathbf{F}(v_i), \quad (3.6)$$

where the stress components in the global frame are given by

$$\sigma_{\text{dipole}} = \begin{bmatrix} \sigma_x \\ \sigma_y \\ \sigma_{xy} \end{bmatrix}_{\text{dipole}}, \quad (3.7)$$

$\Lambda(v_i)$ is the 3×2 matrix of material parameters given by

$$\Lambda(v_i) = \omega \begin{bmatrix} A_1(v_i) & A_2(v_i) \\ A'_1(v_i) & A'_2(v_i) \\ A_3(v_i) & A_4(v_i) \end{bmatrix}, \quad (3.8)$$

and $\mathbf{F}(v_i)$ expresses the functional dependence of the field:

$$\mathbf{F}(v_i) = \begin{bmatrix} F_1(x, y, v_i) \\ F_2(x, y, v_i) \end{bmatrix}, \quad (3.9)$$

where

$$F_1(x, y, v_i) = \frac{1}{2} \ln \frac{[s_\theta x - c_\theta (y - a_d)]^2 + v_i^2 [c_\theta x + s_\theta (y - a_d)]^2}{[s_\theta x - c_\theta (y + a_d)]^2 + v_i^2 [c_\theta x + s_\theta (y + a_d)]^2}, \quad (3.10)$$

$$F_2(x, y, v_i) = \tan^{-1} \left(v_i \frac{c_\theta x + s_\theta (y - a_d)}{s_\theta x - c_\theta (y - a_d)} \right) - \tan^{-1} \left(v_i \frac{c_\theta x + s_\theta (y + a_d)}{s_\theta x - c_\theta (y + a_d)} \right). \quad (3.11)$$

In Eqs. (3.8)-(3.11), $s_\theta = \sin \theta$, $c_\theta = \cos \theta$, and v_i ($i=1, 2$) are the roots of the characteristic equation

$$C'_{11}C'_{66}v^4 + [C'_{12}(C'_{12} + 2C'_{66}) - C'_{11}C'_{33}]v^2 + C'_{33}C'_{66} = 0. \quad (3.12)$$

For $I < 0$, the four roots of Eq. (3.12) form complex conjugates, i.e., $v = \pm v_2 = \pm \bar{v}_1$, where the overhead bar denotes complex conjugation. For $I > 0$, however, the four roots $v = \pm v_1, \pm v_2$ are real and distinct. Furthermore, the parameters in Eq. (3.8) are given by

$$A_1(v_i) = s_\theta^2 [-4C'_{33}J_1 + 8C'_{12}J_2v_i] + c_\theta^2 [-4C'_{12}J_1 + 8C'_{11}J_2v_i], \quad (3.13)$$

$$A_2(v_i) = -2s_\theta c_\theta C'_{66}(4J_1v_i + 8J_2), \quad (3.14)$$

$$A_3(v_i) = -c_\theta s_\theta [4(C'_{33} - C'_{12})J_1 + 8J_2v_i(C'_{11} - C'_{12})], \quad (3.15)$$

$$A_4(v_i) = (s_\theta^2 - c_\theta^2) C'_{66}(4J_1v_i + 8J_2), \quad (3.16)$$

$$A'_1(v_i) = c_\theta^2 [-4C'_{33}J_1 + 8C'_{12}J_2v_i] + s_\theta^2 [-4C'_{12}J_1 + 8C'_{11}J_2v_i], \quad (3.17)$$

$$A'_2(v_i) = 2s_\theta c_\theta C'_{66}(4J_1v_i + 8J_2), \quad (3.18)$$

where

$$J_1 = -\frac{C'_{12} + C'_{11}v_i^2}{8\pi C'_{11}v_i(v_i^2 - v_j^2)}, \quad (3.19)$$

$$J_2 = \frac{(C'_{12} + C'_{11}v_i^2)(C'_{33} - C'_{66}v_i^2)}{16\pi C'_{11}(C'_{12} + C'_{66})v_i^2(v_i^2 - v_j^2)}, \quad (3.20)$$

$i, j = 1, 2$ and $i \neq j$. All these parameters are defined for either crystal A or B, as they depend on the values of the elastic constants C'_{jk} and the orientation θ of each crystal.

The solutions for the disclination dipole in Eq. (3.6) are constructed from the results obtained by Yu and Sanday (1994) for a single wedge disclination in a transversely isotropic solid. Note also that Eq. (3.6) is more general than its counterpart given by Wu (2002b), which includes only ν_1 .

For the later need of applying the interfacial boundary continuity conditions given in Eqs. (3.4) and (3.5), the stresses and displacement gradients along the line $x = 0$ due to a single disclination dipole centered at $(0, 0)$ in a homogeneous hexagonal crystal are given here:

$$\sigma_x(0, y) = \omega \sum_{i=1}^2 A_1(\nu_i) F_1(y), \quad \sigma_{xy}(0, y) = \omega \sum_{i=1}^2 A_3(\nu_i) F_1(y), \quad (3.21)$$

$$\frac{\partial u_x}{\partial y}(0, y) = \omega \sum_{i=1}^2 \Psi_1(\nu_i) F_1(y), \quad \frac{\partial u_y}{\partial y}(0, y) = \omega \sum_{i=1}^2 \Psi_3(\nu_i) F_1(y), \quad (3.22)$$

where

$$F_1(y) = \ln \left| \frac{y - a_d}{y + a_d} \right|, \quad (3.23)$$

$$\Psi_1(\nu_i) = 4s_\theta c_\theta (J_1 + 2J_2 \nu_i), \quad (3.24)$$

$$\Psi_3(\nu_i) = 4(-J_1 c_\theta^2 + 2J_2 s_\theta^2 \nu_i). \quad (3.25)$$

3.2.2. Image Edge Dislocations in a Hexagonal Crystal

3.2.2.1. Individual Edge Dislocation

To derive the corrective image stress field σ_{image} in Eq. (3.3), which is due to image edge dislocations in a homogeneous hexagonal crystal, the knowledge of the elastic field of an individual edge dislocation is first determined.

The stress and displacement gradients due to an edge dislocation located at the origin $(0, 0, 0)$ in a rectangular frame $x_1 - x_2 - x_3$ are given as

$$\sigma_{ij} = 2 \sum_{\alpha=1}^3 \frac{\zeta_{\alpha ij}^{sR} (x_1 + p_{\alpha}^R x_2) + \zeta_{\alpha ij}^{sI} p_{\alpha}^I x_2}{(x_1 + p_{\alpha}^R x_2)^2 + (p_{\alpha}^I x_2)^2} b_s \operatorname{sgn}(p_{\alpha}^I), \quad (3.26)$$

$$\frac{\partial u_k}{\partial x_l} = 2 \sum_{\alpha=1}^3 \frac{\zeta_{\alpha kl}^{sR} (x_1 + p_{\alpha}^R x_2) + \zeta_{\alpha kl}^{sI} p_{\alpha}^I x_2}{(x_1 + p_{\alpha}^R x_2)^2 + (p_{\alpha}^I x_2)^2} b_s \operatorname{sgn}(p_{\alpha}^I), \quad (3.27)$$

where $i, j, k, l = 1, 2, 3$ and $s = 1, 2$. The frame $x_1 - x_2 - x_3$ is taken to be the global frame, i.e., $x_1 \equiv x$, $x_2 \equiv y$, $x_3 \equiv z$. The parameter b_s is the s -th component of the Burgers vector, so that b_x and b_y for $s = 1$ and 2 , respectively, refer to the climb dislocation and glide dislocation. The repeated subscript s indicates summation, $\operatorname{sgn}(\cdot)$ denotes the signum function, and the superscripts R and I denote respectively the real and imaginary parts of a parameter. The complex parameters $\zeta_{\alpha ij}^s$ and $\zeta_{\alpha kl}^s$ and the eigenvalues p_{α} arise from Stroh's sextic formulation (Stroh, 1958). $\zeta_{\alpha ij}^s$ and $\zeta_{\alpha kl}^s$ are given by

$$\zeta_{\alpha ij}^s = \frac{C_{ijkl} [m_l + p_{\alpha} n_l] A_{\alpha k} L_{\alpha s}}{2\pi i}, \quad (3.28)$$

$$\zeta_{\alpha kl}^s = \frac{[m_l + p_{\alpha} n_l] A_{\alpha k} L_{\alpha s}}{2\pi i}, \quad (3.29)$$

where there is no sum on α , C_{ijkl} are the elastic constants of crystal A or B (the contracted form being C_{ij}), and m_l, n_l are the components of orthogonal unit vectors equal to the Kronecker deltas, i.e., $m_l = \delta_{l1}$, $n_l = \delta_{l2}$. Also, $A_{\alpha k}$ and $L_{\alpha s}$ denote the k -th and the s -th elements of the normalized vectors A_{α} and L_{α} , respectively. Together, the

three elements of A_α and L_α constitute the six elements of the eigenvector of the sextic eigenvalue problem for each eigenvalue p_α . The non-italicized symbol i denotes the imaginary number $\sqrt{-1}$.

For enforcing the interfacial boundary continuity conditions, the stresses and displacement gradients along the line $x_1 \equiv x \equiv 0$ due to a climb dislocation or a glide dislocation are needed. They can be obtained by considering the limiting behavior of Eqs. (3.26) and (3.27) as $x_1 \rightarrow 0$. For a climb edge dislocation at $(0, y')$, the stresses and displacement gradients along the line $x = 0$ are

$$\sigma_x(0, y) = \frac{1}{\pi} \frac{b_x D_1^c}{y - y'}, \quad \sigma_{xy}(0, y) = \frac{1}{\pi} \frac{b_x D_2^c}{y - y'}, \quad (3.30)$$

$$\frac{\partial u_x}{\partial y}(0, y) = \frac{b_x}{2} \text{sgn}(x) \delta(y - y') + \frac{1}{\pi} \frac{b_x E_2^c}{y - y'}, \quad \frac{\partial u_y}{\partial y}(0, y) = \frac{1}{\pi} \frac{b_x E_1^c}{y - y'}. \quad (3.31)$$

For a glide edge dislocation,

$$\sigma_x(0, y) = \frac{1}{\pi} \frac{b_y D_1^g}{y - y'}, \quad \sigma_{xy}(0, y) = \frac{1}{\pi} \frac{b_y D_2^g}{y - y'}, \quad (3.32)$$

$$\frac{\partial u_x}{\partial y}(0, y) = \frac{1}{\pi} \frac{b_y E_1^g}{y - y'}, \quad \frac{\partial u_y}{\partial y}(0, y) = \frac{b_y}{2} \text{sgn}(x) \delta(y - y') + \frac{1}{\pi} \frac{b_y E_2^g}{y - y'}. \quad (3.33)$$

In Eqs. (3.30) - (3.33), the parameters D_1^c , D_2^c , E_1^c , E_2^c , D_1^g , D_2^g , E_1^g and E_2^g are given by

$$(D_1^c, D_1^g) = 2\pi \sum_{\alpha=1}^3 \left(\frac{\xi_{\alpha 11}^R P_\alpha^R + \xi_{\alpha 11}^{sl} P_\alpha^l}{|P_\alpha|^2} \text{sgn}(p_\alpha^l) \right), \quad (3.34)$$

$$(D_2^c, D_2^g) = 2\pi \sum_{\alpha=1}^3 \left(\frac{\zeta_{\alpha 12}^{sR} P_{\alpha}^R + \zeta_{\alpha 12}^{sI} P_{\alpha}^I}{|P_{\alpha}|^2} \operatorname{sgn}(P_{\alpha}^I) \right), \quad (3.35)$$

$$(E_1^c, E_1^g) = 2\pi \sum_{\alpha=1}^3 \left(\frac{\zeta_{\alpha 12}^{sR} P_{\alpha}^R + \zeta_{\alpha 12}^{sI} P_{\alpha}^I}{|P_{\alpha}|^2} \operatorname{sgn}(P_{\alpha}^I) \right), \quad (3.36)$$

$$(E_2^c, E_2^g) = 2\pi \sum_{\alpha=1}^3 \left(\frac{\zeta_{\alpha 22}^{sR} P_{\alpha}^R + \zeta_{\alpha 22}^{sI} P_{\alpha}^I}{|P_{\alpha}|^2} \operatorname{sgn}(P_{\alpha}^I) \right), \quad (3.37)$$

where $|P_{\alpha}|^2 = (P_{\alpha}^R)^2 + (P_{\alpha}^I)^2$, $s = 1$ for D_1^c , D_2^c , E_1^c and E_2^c , and $s = 2$ for D_1^g , D_2^g , E_1^g and E_2^g .

3.2.2.2. Image Edge Dislocations

With the knowledge presented in Section 3.2.2.1, one can now determine the densities of image edge dislocations and then the stress field σ_{image} caused by these dislocations.

Assume the distributions of the image dislocations have the densities ρ_A^c , ρ_A^g in the homogeneous crystal A of Subproblem A, and ρ_B^c , ρ_B^g in the homogeneous crystal B of Subproblem B, where the superscripts c and g denote climb and glide dislocations respectively, and the subscripts A and B denote association with crystals A and B respectively. The four unknown densities ρ_A^c , ρ_A^g , ρ_B^c and ρ_B^g can be determined by enforcing the interfacial boundary continuity conditions given in Eqs. (3.4)-(3.5). Continuity of σ_x , σ_{xy} , $\partial u_x / \partial y$ and $\partial u_y / \partial y$ across the interface in the bicrystal problem is enforced by equating these quantities computed on $x = 0^-$ in Subproblem A to those on $x = 0^+$ in Subproblem B. Using Eqs. (3.21)-(3.22) and (3.30)-(3.33) and

integrating the expressions in Eqs. (3.30)-(3.33), the four continuity conditions can be represented by the following four simultaneous Cauchy integral equations:

$$\begin{aligned} & \omega \sum_{i=1}^2 A_{A1}(v_i) \ln \left| \frac{y - a_d}{y + a_d} \right| + \frac{D_{A1}^c}{\pi} \int_{-\infty}^{\infty} \frac{\rho_A^c(y')}{y - y'} dy' + \frac{D_{A1}^g}{\pi} \int_{-\infty}^{\infty} \frac{\rho_A^g(y')}{y - y'} dy' \\ & = \omega \sum_{i=1}^2 A_{B1}(v_i) \ln \left| \frac{y - a_d}{y + a_d} \right| + \frac{D_{B1}^c}{\pi} \int_{-\infty}^{\infty} \frac{\rho_B^c(y')}{y - y'} dy' + \frac{D_{B1}^g}{\pi} \int_{-\infty}^{\infty} \frac{\rho_B^g(y')}{y - y'} dy' \end{aligned} \quad (3.38)$$

$$\begin{aligned} & \omega \sum_{i=1}^2 A_{A3}(v_i) \ln \left| \frac{y - a_d}{y + a_d} \right| + \frac{D_{A2}^c}{\pi} \int_{-\infty}^{\infty} \frac{\rho_A^c(y')}{y - y'} dy' + \frac{D_{A2}^g}{\pi} \int_{-\infty}^{\infty} \frac{\rho_A^g(y')}{y - y'} dy' \\ & = \omega \sum_{i=1}^2 A_{B3}(v_i) \ln \left| \frac{y - a_d}{y + a_d} \right| + \frac{D_{B2}^c}{\pi} \int_{-\infty}^{\infty} \frac{\rho_B^c(y')}{y - y'} dy' + \frac{D_{B2}^g}{\pi} \int_{-\infty}^{\infty} \frac{\rho_B^g(y')}{y - y'} dy' \end{aligned} \quad (3.39)$$

$$\begin{aligned} & \omega \sum_{i=1}^2 \Psi_{A1}(v_i) \ln \left| \frac{y - a_d}{y + a_d} \right| + \frac{E_{A1}^c}{\pi} \int_{-\infty}^{\infty} \frac{\rho_A^c(y')}{y - y'} dy' + \frac{E_{A1}^g}{\pi} \int_{-\infty}^{\infty} \frac{\rho_A^g(y')}{y - y'} dy' - \frac{\rho_A^c(y)}{2} \\ & = \omega \sum_{i=1}^2 \Psi_{B1}(v_i) \ln \left| \frac{y - a_d}{y + a_d} \right| + \frac{E_{B1}^c}{\pi} \int_{-\infty}^{\infty} \frac{\rho_A^c(y')}{y - y'} dy' + \frac{E_{B1}^g}{\pi} \int_{-\infty}^{\infty} \frac{\rho_A^g(y')}{y - y'} dy' - \frac{\rho_B^c(y)}{2} \end{aligned} \quad (3.40)$$

$$\begin{aligned} & \omega \sum_{i=1}^2 \Psi_{A3}(v_i) \ln \left| \frac{y - a_d}{y + a_d} \right| + \frac{E_{A2}^c}{\pi} \int_{-\infty}^{\infty} \frac{\rho_A^c(y')}{y - y'} dy' + \frac{E_{A2}^g}{\pi} \int_{-\infty}^{\infty} \frac{\rho_A^g(y')}{y - y'} dy' - \frac{\rho_A^g(y)}{2} \\ & = \omega \sum_{i=1}^2 \Psi_{B3}(v_i) \ln \left| \frac{y - a_d}{y + a_d} \right| + \frac{E_{B2}^c}{\pi} \int_{-\infty}^{\infty} \frac{\rho_B^c(y')}{y - y'} dy' + \frac{E_{B2}^g}{\pi} \int_{-\infty}^{\infty} \frac{\rho_B^g(y')}{y - y'} dy' - \frac{\rho_B^g(y)}{2} \end{aligned} \quad (3.41)$$

Note that the unknowns are the four image densities. Specifically, the first, second and third terms on the left-hand side of Eq. (3.38) come from the first expressions of Eqs. (3.21), (3.30) and (3.32), respectively, and represent the stresses contributed by the disclination dipole, image climb dislocations, and image glide dislocations, respectively, on $x = 0^-$ in Subproblem A. In contrast, the terms on the right-hand side of Eq. (3.38) represent the contributions to σ_x on $x = 0^+$ in Subproblem B. Equations (3.39)-(3.41)

take similar forms as Eq. (3.38), with the exception that ρ_A^c, ρ_B^c , etc. do not appear within the integrand signs in Eqs. (3.40) and (3.41).

To solve these integral equations, the Hilbert transform of a function $f(y)$ is used, which is defined as

$$H[f(y)] = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{f(y')}{y - y'} dy'. \quad (3.42)$$

The Hilbert transform possesses the following iterative property (Hahn, 1996):

$$H[H[f(y)]] = -f(y), \quad (3.43)$$

which is the key to solving the integral equations above. First, note that the integral terms (without the coefficients) in Eqs. (3.38)-(3.41) are Hilbert transforms of the image densities. Equations (3.38) and (3.39) suggest that the image solutions should be of the form $H[F_1(y)]$, where $F_1(y) = \log|(y - a_d)/(y + a_d)|$, since the integral terms would reduce to $H[H[F_1(y)]]$, which by the iterative property would yield $-F_1(y)$ to match with the first terms of the integral equations. Equations (3.40) and (3.41), on the other hand, contain not only the Hilbert transforms of the densities, but also the densities themselves. This suggests that the image solutions must contain the original function $F_1(y)$ in addition to $H[F_1(y)]$. On the basis of this reasoning, each of the four densities can be written in the form:

$$\rho_A^g(y) = \sum_{i=1}^2 [\Gamma_{A1}^g(v_i)H[F_1(y)] + \Gamma_{A3}^g(v_i)F_1(y)], \quad (3.44)$$

$$\rho_A^c(y) = \sum_{i=1}^2 [\Gamma_{A1}^c(v_i)H[F_1(y)] + \Gamma_{A3}^c(v_i)F_1(y)], \quad (3.45)$$

$$\rho_B^g(y) = \sum_{i=1}^2 [\Gamma_{B1}^g(v_i)H[F_1(y)] + \Gamma_{B3}^g(v_i)F_1(y)], \quad (3.46)$$

$$\rho_B^c(y) = \sum_{i=1}^2 [\Gamma_{B1}^c(v_i)H[F_1(y)] + \Gamma_{B3}^c(v_i)F_1(y)], \quad (3.47)$$

where the sixteen unknown density coefficients $\Gamma_{A1}^g(v_i)$, $\Gamma_{A3}^g(v_i)$, $\Gamma_{A1}^c(v_i)$, $\Gamma_{A3}^c(v_i)$, $\Gamma_{B1}^g(v_i)$, $\Gamma_{B3}^g(v_i)$, $\Gamma_{B1}^c(v_i)$ and $\Gamma_{B3}^c(v_i)$ ($i=1, 2$) can be found by substituting Eqs. (3.44)-(3.47) back into the integral equations. Each integral equation can then be converted into two linear algebraic equations by collecting together the coefficients of the function $F_1(y)$ and those of the function $H[F_1(y)]$ in it, respectively. Consequently, the four integral equations can be converted into eight algebraic ones. However, for the assumed solution forms given in Eqs. (3.44)-(3.47), the system of integral equations can first be split into two systems of integral equations for the different v_1 and v_2 before conversion. This procedure is different from that of Wu (2002b), which considers only v_1 . The four integral equations of each system can thus be converted into eight linear algebraic equations with the eight unknowns $\Gamma_{A1}^g(v_i)$, $\Gamma_{A3}^g(v_i)$, $\Gamma_{A1}^c(v_i)$, $\Gamma_{A3}^c(v_i)$, $\Gamma_{B1}^g(v_i)$, $\Gamma_{B3}^g(v_i)$, $\Gamma_{B1}^c(v_i)$ and $\Gamma_{B3}^c(v_i)$ for each v_i as

$$\begin{aligned} -D_{A1}^c \Gamma_{A1}^c(v_i) - D_{A1}^g \Gamma_{A1}^g(v_i) + D_{B1}^c \Gamma_{B1}^c(v_i) \\ + D_{B1}^g \Gamma_{B1}^g(v_i) + \omega A_{A1}(v_i) - \omega A_{B1}(v_i) = 0 \end{aligned} \quad (3.48)$$

$$\begin{aligned} -D_{A2}^c \Gamma_{A1}^c(v_i) - D_{A2}^g \Gamma_{A1}^g(v_i) + D_{B2}^c \Gamma_{B1}^c(v_i) \\ + D_{B2}^g \Gamma_{B1}^g(v_i) + \omega A_{A3}(v_i) - \omega A_{B3}(v_i) = 0 \end{aligned} \quad (3.49)$$

$$\begin{aligned} -E_{A1}^c \Gamma_{A1}^c(v_i) - E_{A1}^g \Gamma_{A1}^g(v_i) + E_{B1}^c \Gamma_{B1}^c(v_i) + E_{B1}^g \Gamma_{B1}^g(v_i) \\ - \Gamma_{A3}^c(v_i)/2 - \Gamma_{B3}^c(v_i)/2 + \omega \Psi_{A1}(v_i) - \omega \Psi_{B1}(v_i) = 0 \end{aligned} \quad (3.50)$$

$$-E_{A2}^c \Gamma_{A1}^c(v_i) - E_{A2}^g \Gamma_{A1}^g(v_i) + E_{B2}^c \Gamma_{B1}^c(v_i) + E_{B2}^g \Gamma_{B1}^g(v_i) - \Gamma_{A3}^g(v_i)/2 - \Gamma_{B3}^g(v_i)/2 + \omega \Psi_{A3}(v_i) - \omega \Psi_{B3}(v_i) = 0, \quad (3.51)$$

$$D_{A1}^c \Gamma_{A3}^c(v_i) + D_{A1}^g \Gamma_{A3}^g(v_i) - D_{B1}^c \Gamma_{B3}^c(v_i) - D_{B1}^g \Gamma_{B3}^g(v_i) = 0, \quad (3.52)$$

$$D_{A2}^c \Gamma_{A3}^c(v_i) + D_{A2}^g \Gamma_{A3}^g(v_i) - D_{B2}^c \Gamma_{B3}^c(v_i) - D_{B2}^g \Gamma_{B3}^g(v_i) = 0, \quad (3.53)$$

$$E_{A1}^c \Gamma_{A3}^c(v_i) + E_{A1}^g \Gamma_{A3}^g(v_i) - E_{B1}^c \Gamma_{B3}^c(v_i) - E_{B1}^g \Gamma_{B3}^g(v_i) - \Gamma_{A1}^c(v_i)/2 - \Gamma_{B1}^c(v_i)/2 = 0, \quad (3.54)$$

$$E_{A2}^c \Gamma_{A3}^c(v_i) + E_{A2}^g \Gamma_{A3}^g(v_i) - E_{B2}^c \Gamma_{B3}^c(v_i) - E_{B2}^g \Gamma_{B3}^g(v_i) - \Gamma_{A1}^g(v_i)/2 - \Gamma_{B1}^g(v_i)/2 = 0. \quad (3.55)$$

The two systems of linear algebraic equations for v_1 and v_2 respectively can be easily solved. Once the density coefficients $\Gamma_{A1}^g(v_i)$, $\Gamma_{A3}^g(v_i)$, etc. ($i=1, 2$) are solved, the densities ρ_A^c , ρ_B^c , ρ_A^g and ρ_B^g become known. Turning now to Eq. (3.26), the stress field due to the image dislocations can be derived by means of integration. For the climb dislocation density ρ^c (either ρ_A^c or ρ_B^c), replace b_s in Eq. (3.26) by $\rho^c(y')dy'$, while for the glide dislocation density ρ^g , replace b_s by $\rho^g(y')dy'$. Integrating the resultant expressions with respect to y' from $-\infty$ to $+\infty$ yields the solutions for the stress field due to image dislocations as

$$\sigma_{\text{image}} = \sum_{i=1}^2 [\mathbf{I} \times \Gamma(v_i)], \quad (3.56)$$

where the stress components are given by

$$\sigma_{\text{image}} = \begin{bmatrix} \sigma_x \\ \sigma_y \\ \sigma_{xy} \end{bmatrix}_{\text{image}}, \quad (3.57)$$

$\mathbf{I}$ is a 3×4 matrix written as

$$\mathbf{I} = \begin{bmatrix} \text{Im}[I_{111}] & \text{Re}[I_{111}] & \text{Im}[I_{211}] & \text{Re}[I_{211}] \\ \text{Im}[I_{122}] & \text{Re}[I_{122}] & \text{Im}[I_{222}] & \text{Re}[I_{222}] \\ \text{Im}[I_{112}] & \text{Re}[I_{112}] & \text{Im}[I_{212}] & \text{Re}[I_{212}] \end{bmatrix}, \quad (3.58)$$

and $\Gamma(v_i)$ is the vector of image density coefficients

$$\Gamma(v_i) = \begin{bmatrix} \Gamma_1^c(v_i) \\ \Gamma_3^c(v_i) \\ \Gamma_1^g(v_i) \\ \Gamma_3^g(v_i) \end{bmatrix}. \quad (3.59)$$

The elements of $\mathbf{I}$ in Eq. (3.58) express the functional form of the stress dependence and can be written as

$$I_{sjk} = \begin{cases} \sum_{\alpha=1}^3 \text{sgn}(p_\alpha^l) \frac{2\pi(\xi_{\alpha jk}^{sR} - i\xi_{\alpha jk}^{sl})}{p_\alpha^l + ip_\alpha^R} \ln \frac{(y - a_d)p_\alpha^l + i[x + (y - a_d)p_\alpha^R]}{(y + a_d)p_\alpha^l + i[x + (y + a_d)p_\alpha^R]}, & p_\alpha^l x > 0 \\ \sum_{\alpha=1}^3 \text{sgn}(p_\alpha^l) \frac{2\pi(-\xi_{\alpha jk}^{sR} - i\xi_{\alpha jk}^{sl})}{p_\alpha^l - ip_\alpha^R} \ln \frac{(y - a_d)p_\alpha^l - i[x + (y - a_d)p_\alpha^R]}{(y + a_d)p_\alpha^l - i[x + (y + a_d)p_\alpha^R]}, & p_\alpha^l x < 0 \end{cases}, \quad (3.60)$$

3.3. Elastic Solutions for an Interfacial Disclination Dipole Wall

3.3.1. Stress Field

The stress solutions for the dipole wall can be obtained by summing the stress solutions of all the dipoles. As presented in Section 3.2, the stress field due to a single disclination dipole includes two parts, i.e., σ_{dipole} and σ_{image} . Therefore, the summation is first performed on the two parts separately and the two summation results are then added up. The summation starts with replacing y by $y + Nh$ in Eqs. (3.10), (3.11) and (3.60), each of which describes the functional dependence of the stress field.

Subsequently, the two expressions in Eqs. (3.6) and (3.56) for σ_{dipole} and σ_{image} respectively are summed from $N = -\infty$ to ∞ . For convenience, all distance and length variables are normalized by h so that $X = x/h$, $Y = y/h$, $\bar{a}_d = a_d/h$. Exact sums can be derived from the following basic equation (Hirth and Lothe, 1982):

$$\sum_{N=-\infty}^{\infty} \frac{i}{N + P \pm iQ} = \pi i \cot \pi(P \pm iQ), \quad (3.61)$$

where P and Q are some variables. From Eq. (3.61), it can be shown that

$$\sum_{N=-\infty}^{\infty} \left(\frac{1}{N + P + iQ} + \frac{1}{N + P - iQ} \right) = \sum_{N=-\infty}^{\infty} \frac{2(N + P)}{(N + P)^2 + Q^2} = \frac{2\pi \sin[2\pi P]}{\cosh[2\pi Q] - \cos[2\pi P]}, \quad (3.62)$$

$$\sum_{N=-\infty}^{\infty} \left(\frac{i}{N + P + iQ} - \frac{i}{N + P - iQ} \right) = \sum_{N=-\infty}^{\infty} \frac{2Q}{(N + P)^2 + Q^2} = \frac{2\pi \sinh[2\pi Q]}{\cosh[2\pi Q] - \cos[2\pi P]}. \quad (3.63)$$

3.3.1.1. Disclination Dipole Wall in a Hexagonal Crystal

The key to summing σ_{dipole} is the summation performed on Eqs. (3.10) and (3.11). To sum the logarithmic function in Eq. (3.10), which is first expressed in the normalized variables X , $Y + N$ and $\bar{a}_d$, the following procedure is followed. The function is differentiated with respect to Y , and the result after some careful rearrangement can be recast into the form of Eq. (3.62):

$$S_1 = \sum_{N=-\infty}^{\infty} \frac{d}{dY} \left[\ln \{ [s_\theta X - c_\theta (Y + N - \bar{a}_d)]^2 + v_i^2 [c_\theta X + s_\theta (Y + N - \bar{a}_d)]^2 \} \right. \\ \left. - \ln \{ [s_\theta X - c_\theta (Y + N + \bar{a}_d)]^2 + v_i^2 [c_\theta X + s_\theta (Y + N + \bar{a}_d)]^2 \} \right] \quad (3.64)$$

Differentiating the first logarithmic term of Eq. (3.64) yields

$$\begin{aligned} S_1^{(1)} &= \sum_{N=-\infty}^{\infty} \frac{d}{dY} \left[\ln \{ [s_{\theta}X - c_{\theta}(Y + N - \bar{a}_d)]^2 + v_1^2 [c_{\theta}X + s_{\theta}(Y + N - \bar{a}_d)]^2 \} \right] \\ &= \sum_{N=-\infty}^{\infty} \frac{-2c_{\theta}[s_{\theta}X - c_{\theta}(Y + N - \bar{a}_d)] + 2s_{\theta}v_1^2[c_{\theta}X + s_{\theta}(Y + N - \bar{a}_d)]}{[s_{\theta}X - c_{\theta}(Y + N - \bar{a}_d)]^2 + v_1^2[c_{\theta}X + s_{\theta}(Y + N - \bar{a}_d)]^2} . \end{aligned} \quad (3.65)$$

Setting $T = Y + N - \bar{a}_d$, Eq. (3.65) reduces to

$$S_1^{(1)} = \sum_{T=-\infty}^{\infty} \frac{2(T + g_1(v_i)X)}{(T + g_1(v_i)X)^2 + (g_2(v_i)X)^2} , \quad (3.66)$$

where $g_1(v_i)$ and $g_2(v_i)$ are given by

$$g_1(v_i) = \frac{s_{\theta}c_{\theta}(v_i^2 - 1)}{c_{\theta}^2 + s_{\theta}^2v_i^2} , \quad (3.67)$$

$$g_2(v_i) = \frac{v_i}{c_{\theta}^2 + s_{\theta}^2v_i^2} , \quad (3.68)$$

Substituting $T = N + Y - \bar{a}_d$ into Eq. (3.66) results in

$$S_1^{(1)} = \sum_{T=-\infty}^{\infty} \frac{2(N + Y - \bar{a}_d + g_1(v_i)X)}{(N + Y - \bar{a}_d + g_1(v_i)X)^2 + (g_2(v_i)X)^2} . \quad (3.69)$$

In the same way, differentiating the second term of Eq. (3.64) leads to

$$\begin{aligned} S_1^{(2)} &= \sum_{N=-\infty}^{\infty} \frac{d}{dY} \left[\ln \{ [s_{\theta}X - c_{\theta}(Y + N + \bar{a}_d)]^2 + v_1^2 [c_{\theta}X + s_{\theta}(Y + N + \bar{a}_d)]^2 \} \right] \\ &= \sum_{N=-\infty}^{\infty} \frac{2(N + Y + \bar{a}_d + g_1(v_i)X)}{(N + Y + \bar{a}_d + g_1(v_i)X)^2 + (g_2(v_i)X)^2} . \end{aligned} \quad (3.70)$$

Thus,

$$S_1 = S_1^{(1)} - S_1^{(2)} = \sum_{N=-\infty}^{\infty} \frac{2(N+Y-\bar{a}_d + g_1(v_i)X)}{(N+Y-\bar{a}_d + g_1(v_i)X)^2 + (g_2(v_i)X)^2} - \sum_{N=-\infty}^{\infty} \frac{2(N+Y+\bar{a}_d + g_1(v_i)X)}{(N+Y+\bar{a}_d + g_1(v_i)X)^2 + (g_2(v_i)X)^2} \quad (3.71)$$

Setting $P = g_1(v_i)X + Y - \bar{a}_d$, $Q = g_2(v_i)X$ in the first term and $P = g_1(v_i)X + Y + \bar{a}_d$,

$Q = g_2(v_i)X$ in the second term of Eq. (3.71), the use of Eq. (3.62) yields

$$S_1 = \frac{2\pi \sin[2\pi(g_1(v_i)X + Y - \bar{a}_d)]}{\cosh[2\pi g_2(v_i)X] - \cos[2\pi(g_1(v_i)X + Y - \bar{a}_d)]} - \frac{2\pi \sin[2\pi(g_1(v_i)X + Y + \bar{a}_d)]}{\cosh[2\pi g_2(v_i)X] - \cos[2\pi(g_1(v_i)X + Y + \bar{a}_d)]} \quad (3.72)$$

Equation (3.72) is easily integrated with respect to Y as the numerator in each term of the equation is the derivative of the denominator with respect to Y . The integrated result corresponds to the desired expression:

$$\begin{aligned} \int S_1 dY &= \sum_{N=-\infty}^{\infty} \ln \frac{[s_\theta X - c_\theta(Y + N - \bar{a}_d)]^2 + v_i^2 [c_\theta X + s_\theta(Y + N - \bar{a}_d)]^2}{[s_\theta X - c_\theta(Y + N + \bar{a}_d)]^2 + v_i^2 [c_\theta X + s_\theta(Y + N + \bar{a}_d)]^2} \\ &= \ln \frac{\cosh[2\pi g_2(v_i)X] - \cos[2\pi(g_1(v_i)X + Y - \bar{a}_d)]}{\cosh[2\pi g_2(v_i)X] - \cos[2\pi(g_1(v_i)X + Y + \bar{a}_d)]} \end{aligned} \quad (3.73)$$

which is the sum of Eq. (3.10) for an infinite number of dipoles (except for the factor of 1/2). Similarly, the arctangent functions in Eq. (3.11) are summed and differentiated with respect to Y :

$$S_2 = \sum_{N=-\infty}^{\infty} \frac{d}{dY} \left[\tan^{-1} \left(v_i \frac{c_\theta X + s_\theta(Y + N - \bar{a}_d)}{s_\theta X - c_\theta(Y + N - \bar{a}_d)} \right) - \tan^{-1} \left(v_i \frac{c_\theta X + s_\theta(Y + N + \bar{a}_d)}{s_\theta X - c_\theta(Y + N + \bar{a}_d)} \right) \right] \quad (3.74)$$

Evaluation of the first term of Eq. (3.74) yields

$$\begin{aligned}
S_2^{(1)} &= \sum_{N=-\infty}^{\infty} \frac{d}{dY} \left[\tan^{-1} \left(v_i \frac{c_{\theta} X + s_{\theta} (Y + N - \bar{a}_d)}{s_{\theta} X - c_{\theta} (Y + N - \bar{a}_d)} \right) \right] \\
&= \sum_{N=-\infty}^{\infty} \left[\frac{v_i \frac{s_{\theta} (s_{\theta} X - c_{\theta} (Y + N - \bar{a}_d)) + c_{\theta} (c_{\theta} X + s_{\theta} (Y + N - \bar{a}_d))}{(s_{\theta} X - c_{\theta} (Y + N - \bar{a}_d))^2}}{1 + \left(v_i \frac{c_{\theta} X + s_{\theta} (Y + N - \bar{a}_d)}{s_{\theta} X - c_{\theta} (Y + N - \bar{a}_d)} \right)^2} \right]. \quad (3.75)
\end{aligned}$$

Setting $T = Y + N - \bar{a}_d$, Eq. (3.75) reduces to

$$S_2^{(1)} = \sum_{T=-\infty}^{\infty} \left[\frac{g_2(v_i)X}{(T + g_3(v_i)X)^2 + (g_2(v_i)X)^2} \right], \quad (3.76)$$

where $g_3(v_i)$ is given by

$$g_3(v_i) = \frac{s_{\theta} c_{\theta} (v_i^2 + 1)}{c_{\theta}^2 + s_{\theta}^2 v_i^2}. \quad (3.77)$$

Substituting $T = N + Y - \bar{a}_d$ into Eq. (3.76) results in

$$S_2^{(1)} = \sum_{N=-\infty}^{\infty} \frac{g_2(v_i)X}{(N + Y - \bar{a}_d + g_3(v_i)X)^2 + (g_2(v_i)X)^2}. \quad (3.78)$$

In the same way, the second term of Eq. (3.74) is evaluated, yielding

$$\begin{aligned}
S_2^{(2)} &= \sum_{N=-\infty}^{\infty} \frac{d}{dY} \left[\tan^{-1} \left(v_i \frac{c_{\theta} X + s_{\theta} (Y + N - \bar{a}_d)}{s_{\theta} X - c_{\theta} (Y + N - \bar{a}_d)} \right) \right] \\
&= \sum_{N=-\infty}^{\infty} \frac{g_2(v_i)X}{(N + Y + \bar{a}_d + g_3(v_i)X)^2 + (g_2(v_i)X)^2}. \quad (3.79)
\end{aligned}$$

Thus,

$$S_2 = S_2^{(1)} - S_2^{(2)} = \sum_{N=-\infty}^{\infty} \left[\frac{g_2(v_i)X}{(N + g_3(v_i)X + Y - \bar{a}_d)^2 + (g_2(v_i)X)^2} - \frac{g_2(v_i)X}{(N + g_3(v_i)X + Y + \bar{a}_d)^2 + (g_2(v_i)X)^2} \right]. \quad (3.80)$$

Setting $P = g_3(v_i)X + Y - \bar{a}_d$, $Q = g_2(v_i)X$ in the first term and $P = g_3(v_i)X + Y + \bar{a}_d$,

$Q = g_2(v_i)X$ in the second term of Eq. (3.80), the use of Eq. (3.63) yields

$$S_2 = \frac{\pi \sinh[2\pi g_2(v_i)X]}{\cosh[2\pi g_2(v_i)X] - \cos[2\pi(g_3(v_i)X + Y - \bar{a}_d)]} - \frac{\pi \sinh[2\pi g_2(v_i)X]}{\cosh[2\pi g_2(v_i)X] - \cos[2\pi(g_3(v_i)X + Y + \bar{a}_d)]}. \quad (3.81)$$

Equation (3.81) can be integrated with respect to Y with a symbolic manipulator (such as Mathematica) or by residue calculus. The integrated result can be written as

$$\begin{aligned} \int S_2 dY &= \sum_{N=-\infty}^{\infty} \left[\tan^{-1} \left(v_i \frac{c_\theta X + s_\theta(Y + N - \bar{a}_d)}{s_\theta X - c_\theta(Y + N - \bar{a}_d)} \right) - \tan^{-1} \left(v_i \frac{c_\theta X + s_\theta(Y + N + \bar{a}_d)}{s_\theta X - c_\theta(Y + N + \bar{a}_d)} \right) \right] \\ &= \tan^{-1} [\coth[\pi g_2(v_i)X] \tan[\pi(g_3(v_i)X + Y - \bar{a}_d)]] \\ &\quad - \tan^{-1} [\coth[\pi g_2(v_i)X] \tan[\pi(g_3(v_i)X + Y + \bar{a}_d)]] \end{aligned} \quad (3.82)$$

Substituting Eqs. (3.73) and (3.82) into Eq. (3.6) leads to the expressions for the stress components due to the disclination dipole wall:

$$\sigma_{\text{dipole wall}} = \sum_{i=1}^2 \Lambda(v_i) \times \mathbf{V}(v_i), \quad (3.83)$$

where

$$\sigma_{\text{dipole wall}} = \begin{bmatrix} \sigma_x \\ \sigma_y \\ \sigma_{xy} \end{bmatrix}_{\text{dipole wall}}, \quad (3.84)$$

and

$$\mathbf{V}(v_i) = \begin{bmatrix} \ln \frac{\cosh[2\pi g_2(v_i)X] - \cos[2\pi(g_1(v_i)X + Y - \bar{a}_d)]}{\cosh[2\pi g_2(v_i)X] - \cos[2\pi(g_1(v_i)X + Y + \bar{a}_d)]} \\ \tan^{-1}[\coth(\pi g_2(v_i)X) \tan[\pi(g_3(v_i)X + Y - \bar{a}_d)]] \\ - \tan^{-1}[\coth(\pi g_2(v_i)X) \tan[\pi(g_3(v_i)X + Y + \bar{a}_d)]] \end{bmatrix}. \quad (3.85)$$

3.3.1.2. Image Dislocation Wall in a Hexagonal Crystal

The key to summing σ_{image} is the summation performed on Eq. (3.60). To sum the logarithmic function (in normalized variables X , $Y + N$ and $\bar{a}_d$) in Eq. (3.60) for $p_\alpha^I x > 0$, its derivative with respect to Y is summed first:

$$\begin{aligned} S_3 &= \sum_{N=-\infty}^{\infty} \frac{d}{dY} \ln \frac{(Y + N - \bar{a}_d)p_\alpha^I + i[X + (Y + N - \bar{a}_d)p_\alpha^R]}{(Y + N + \bar{a}_d)p_\alpha^I + i[X + (Y + N + \bar{a}_d)p_\alpha^R]} \\ &= \sum_{N=-\infty}^{\infty} \left[\frac{1}{N + \left(\frac{i}{p_\alpha^I + ip_\alpha^R} X + Y - \bar{a}_d \right)} - \frac{1}{N + \left(\frac{i}{p_\alpha^I + ip_\alpha^R} X + Y + \bar{a}_d \right)} \right]. \end{aligned} \quad (3.86)$$

Setting $P \pm iQ = iX/(p_\alpha^I + ip_\alpha^R) + Y - \bar{a}_d$ in the first term and

$P \pm iQ = iX/(p_\alpha^I + ip_\alpha^R) + Y + \bar{a}_d$ in the second term of Eq. (3.61) respectively, Eq. (3.86)

reduces to

$$S_3 = \pi \cot\left[\pi\left(\frac{i}{p_\alpha^I + ip_\alpha^R} X + Y - \bar{a}_d\right)\right] - \pi \cot\left[\pi\left(\frac{i}{p_\alpha^I + ip_\alpha^R} X + Y + \bar{a}_d\right)\right]. \quad (3.87)$$

The integral of Eq. (3.87) with respect to Y is easily performed and the desired result can be written as

$$\int S_3 dY = \ln \frac{\sin[\pi(\frac{i}{p_\alpha^l + ip_\alpha^R} X + Y - \bar{a}_d)]}{\sin[\pi(\frac{i}{p_\alpha^l + ip_\alpha^R} X + Y + \bar{a}_d)]}. \quad (3.88)$$

For $p_\alpha^l X < 0$, i in the above equation is replaced by $-i$. Thus, Eq. (3.60), which is for a single dipole, is summed to obtain the result for a dipole wall:

$$U_{sjk} = \sum_{N=-\infty}^{\infty} I_{sjk} = \begin{cases} \sum_{\alpha=1}^3 \operatorname{sgn}(p_\alpha^l) \frac{2\pi(\xi_{\alpha jk}^{sR} - i\xi_{\alpha jk}^{sl})}{p_\alpha^l + ip_\alpha^R} \ln \frac{\sin[\pi(\frac{i}{p_\alpha^l + ip_\alpha^R} X + Y - \bar{a}_d)]}{\sin[\pi(\frac{i}{p_\alpha^l + ip_\alpha^R} X + Y + \bar{a}_d)]}, & p_\alpha^l X > 0 \\ \sum_{\alpha=1}^3 \operatorname{sgn}(p_\alpha^l) \frac{2\pi(-\xi_{\alpha jk}^{sR} - i\xi_{\alpha jk}^{sl})}{p_\alpha^l - ip_\alpha^R} \ln \frac{\sin[\pi(\frac{-i}{p_\alpha^l - ip_\alpha^R} X + Y - \bar{a}_d)]}{\sin[\pi(\frac{-i}{p_\alpha^l - ip_\alpha^R} X + Y + \bar{a}_d)]}, & p_\alpha^l X < 0 \end{cases}. \quad (3.89)$$

The stress components due to the periodic image wall can now be written as

$$\sigma_{\text{image wall}} = \sum_{i=1}^2 \mathbf{U} \times \Gamma(v_i), \quad (3.90)$$

where

$$\sigma_{\text{image wall}} = \begin{bmatrix} \sigma_x \\ \sigma_y \\ \sigma_{xy} \end{bmatrix}_{\text{image wall}}, \quad (3.91)$$

$$\mathbf{U} = \begin{bmatrix} \text{Im}[U_{111}] & \text{Re}[U_{111}] & \text{Im}[U_{211}] & \text{Re}[U_{211}] \\ \text{Im}[U_{122}] & \text{Re}[U_{122}] & \text{Im}[U_{222}] & \text{Re}[U_{222}] \\ \text{Im}[U_{112}] & \text{Re}[U_{112}] & \text{Im}[U_{212}] & \text{Re}[U_{212}] \end{bmatrix}. \quad (3.92)$$

3.3.1.3. Disclination Dipole Wall in a Hexagonal Bicrystal

The complete stress field σ in A or B of the original problem of the interfacial dipole wall is obtained by adding Eqs. (3.83) and (3.90):

$$\sigma = \sum_{i=1}^2 [\Lambda(v_i) \times \mathbf{V}(v_i) + \mathbf{U} \times \Gamma(v_i)]. \quad (3.93)$$

This expression represents exact closed-form solutions. Note that the derived closed-form results for the integrals of S_1 , S_2 and S_3 with respect to Y in Eqs. (3.73), (3.82) and (3.88) have been verified by direct numerical evaluations of the summations.

The exact solutions of Eq. (3.93) assume the form of the logarithm of hyperbolic and trigonometric functions of complex parameters, while those for a single dipole given in Eqs. (3.10), (3.11) and (3.60) are of the form of the logarithm of algebraic functions. The arctangent functions in Eq. (3.85) can be written as logarithmic functions. As expected, Y appears only inside the trigonometric terms of the solutions, which are therefore periodic in Y . The variable X appears inside the hyperbolic and trigonometric terms in the form of a complex variable, e.g., $g_1(v_i)X$, and the overall solutions are not periodic in X . Furthermore, for the special c -axis orientations of 0° and 90° , $g_2(v_i)$ reduces to v_i and $1/v_i$ respectively, while $g_1(v_i)$ and $g_3(v_i)$ reduce to zero. The dipole wall part of the solutions as expressed by Eq. (3.83) then reduces to precisely those derived earlier for these special cases (Wu, 2002c). For the image wall part of the

solutions, the logarithm function in Eq. (3.89) also reduces to that in the work of Wu (2002c), but the complex pre-factors multiplying the logarithm term differ in form from those in the work of Wu (2002c). This is because the current image dislocation solutions are based on Stroh's complex eigenvalue method, while those in the work of Wu (2002c) are obtained from solutions of partial differential equations of the displacement variables.

A further issue of importance is the long-range behavior of the complete stress field, i.e., the behavior as $X \rightarrow \pm\infty$. The dipole wall part of the solutions tends to zero at large X . However, the image part does not in general. To obtain the limit of the stress field as $X \rightarrow \pm\infty$, consider the limit of Eq. (3.89). First, introduce the parameter

$$\eta = \eta^R + i\eta^I = \frac{i}{p_\alpha^I + i p_\alpha^R} = \frac{p_\alpha}{|p_\alpha|^2}, \quad (3.94)$$

so that the logarithm terms in Eq. (3.89) can be written as

$$\ln \frac{\sin[\pi(\eta^R X + Y - \bar{a}_d \pm i\eta^I X)]}{\sin[\pi(\eta^R X + Y + \bar{a}_d \pm i\eta^I X)]}, \quad (3.95)$$

where the upper and lower signs refer respectively to the expressions for $p_\alpha^I X > 0$ and $p_\alpha^I X < 0$, which correspond to $\eta^I X > 0$ and $\eta^I X < 0$. Expanding Eq. (3.95) in terms of exponential functions and taking the limit results in

$$\lim_{\eta^I X \rightarrow \pm\infty} \ln \frac{e^{i\pi(\eta^R X + Y - \bar{a}_d)} e^{\mp\eta^I \pi X} - e^{-i\pi(\eta^R X + Y - \bar{a}_d)} e^{\pm\eta^I \pi X}}{e^{i\pi(\eta^R X + Y + \bar{a}_d)} e^{\mp\eta^I \pi X} - e^{-i\pi(\eta^R X + Y + \bar{a}_d)} e^{\pm\eta^I \pi X}} = 2\pi\bar{a}_d i, \quad (3.96)$$

which shows that the limit is the same whether $\eta^I X \rightarrow \infty$ or $\eta^I X \rightarrow -\infty$ and is independent of Y and p_α . Hence, U_{sjk} in Eq. (3.89) tends to the limit

$$U_{s/k}^{\infty} = \begin{cases} 4\pi^2 \bar{a}_d \sum_{\alpha=1}^3 \frac{\text{sgn}(p_{\alpha}^I)}{|p_{\alpha}|^2} \left[(\xi_{\alpha jk}^{sI} p_{\alpha}^I + \xi_{\alpha jk}^{sR} p_{\alpha}^R) + i(\xi_{\alpha jk}^{sR} p_{\alpha}^I - \xi_{\alpha jk}^{sI} p_{\alpha}^R) \right], & p_{\alpha}^I X \rightarrow \infty \\ 4\pi^2 \bar{a}_d \sum_{\alpha=1}^3 \frac{\text{sgn}(p_{\alpha}^I)}{|p_{\alpha}|^2} \left[(\xi_{\alpha jk}^{sI} p_{\alpha}^I + \xi_{\alpha jk}^{sR} p_{\alpha}^R) - i(\xi_{\alpha jk}^{sR} p_{\alpha}^I - \xi_{\alpha jk}^{sI} p_{\alpha}^R) \right], & p_{\alpha}^I X \rightarrow -\infty \end{cases}, \quad (3.97)$$

where the lower and upper expressions are complex conjugates of each other. Further simplification can be made by noting that $\text{Im}[U_{s11}^{\infty}]$ and $\text{Im}[U_{s12}^{\infty}]$ actually correspond to the expressions derived in the work of Wu (2002b) for the condition that there should be no net force when an appropriate line integral is taken around a discrete dislocation so that for both $s = 1$ and 2 :

$$\text{Im}[U_{s11}^{\infty}] = \text{Im}[U_{s12}^{\infty}] = 0. \quad (3.98)$$

Consequently, the long-range stress field of the disclination dipole wall is given by

$$\sigma_{\infty} = \sum_{i=1}^2 \mathbf{U}^{\infty} \times \Gamma(v_i), \quad (3.99)$$

where

$$\mathbf{U}^{\infty} = \begin{bmatrix} 0 & \text{Re}[U_{111}^{\infty}] & 0 & \text{Re}[U_{211}^{\infty}] \\ \text{Im}[U_{122}^{\infty}] & \text{Re}[U_{122}^{\infty}] & \text{Im}[U_{222}^{\infty}] & \text{Re}[U_{222}^{\infty}] \\ 0 & \text{Re}[U_{112}^{\infty}] & 0 & \text{Re}[U_{212}^{\infty}] \end{bmatrix}. \quad (3.100)$$

Numerical investigations using Eq. (3.97) show that for the special dissimilar orientations of 0° and 90° in a zinc/zinc bicrystal, the stresses do tend to zero at large X , but for general angles or even for the special angles in a bicrystal made up of dissimilar crystals, they do not. For instance, the long-range stress components in the zinc/zinc bicrystal with the symmetric orientations $\theta_A = 30^\circ$ and $\theta_B = 150^\circ$ are

$(\sigma_x, \sigma_y, \sigma_{xy})_{\pm\infty} = (0.00402, 0.0143, 0)$ GPa, while in the zinc/beryllium bicrystal with $\theta_A = 90^\circ$ and $\theta_B = 0^\circ$ $(\sigma_x, \sigma_y, \sigma_{xy})_{\pm\infty} = (0, 0, -0.00743)$ GPa. These results are similar to those for dislocations in a bicrystal: the stress field of an infinite periodic wall of interfacial dislocations does not vanish in the limit $X \rightarrow \infty$ (Hirth and Lothe, 1982). On the other hand, in isotropic homogeneous materials the stresses of an infinite periodic dislocation wall or disclination dipole wall do vanish at large X . The long-range stresses due to infinite periodic dislocation walls in bicrystals can be relaxed by the imposition of additional elastic solutions (Hirth and Lothe, 1982), and the same may be done for disclination walls. Therefore, the stress field of an infinite periodic disclination dipole wall in a hexagonal bicrystal with complete relaxation at infinity can be obtained by combining Eqs. (3.93) and (3.99):

$$\sigma_{\text{relaxation}} = \sigma - \sigma_\infty = \sum_{i=1}^2 [\Lambda(v_i) \times V(v_i) + (\mathbf{U} - \mathbf{U}^\infty) \times \Gamma(v_i)]. \quad (3.101)$$

3.3.2. Strain Energy Density and Strain Energy

The strain energy density W in a linear elastic solid can be written in the form:

$$W = \frac{1}{2} a'_{jk} \sigma'_j \sigma'_k, \quad (3.102)$$

where a'_{jk} and σ'_j ($j, k = 1, 2, \dots, 6$) are respectively the compliances and stress components in a general coordinate system $x' - y' - z'$. For plane strain about the z' direction, the normal strain $\varepsilon_{z'} = 0$, and the stress components $\sigma'_4(\sigma_{y'z'}) = \sigma'_5(\sigma_{x'z'}) = 0$.

In this two-dimensional case, W can be written as

$$W = \frac{1}{2} \boldsymbol{\sigma}'^T \times \tilde{\mathbf{a}}' \times \boldsymbol{\sigma}', \quad (3.103)$$

where the superscript T denotes the transpose operation, and the stress and plane strain compliance matrices are given by

$$\boldsymbol{\sigma}' = \begin{bmatrix} \sigma'_1 \\ \sigma'_2 \\ \sigma'_6 \end{bmatrix}, \quad \tilde{\mathbf{a}}' = \begin{bmatrix} a'_{11} - \frac{a'^2_{13}}{a'_{33}} & a'_{12} - \frac{a'_{13}a'_{23}}{a'_{33}} & a'_{16} - \frac{a'_{36}a'_{13}}{a'_{33}} \\ & a'_{22} - \frac{a'^2_{23}}{a'_{33}} & a'_{26} - \frac{a'_{36}a'_{23}}{a'_{33}} \\ \text{symmetric} & & a'_{66} - \frac{a'^2_{36}}{a'_{33}} \end{bmatrix}, \quad (3.104)$$

with $\sigma'_1 = \sigma_{x'}$, $\sigma'_2 = \sigma_{y'}$, and $\sigma'_6 = \sigma_{xy'}$. It is convenient to compute W in the local coordinate system of the hexagonal crystal (A or B), where x' lies along the in-plane c -axis direction and makes an angle of θ with respect to the global x -direction (see Fig. 3.1). The compliance components a'_{jk} in Eq. (3.104) can then be written in terms of the five independent elastic constants C'_{jk} :

$$\mathbf{a}' = \begin{bmatrix} \frac{C'_{33} + C'_{23}}{\hat{C}'^2} & \frac{-C'_{12}}{\hat{C}'^2} & \frac{-C'_{12}}{\hat{C}'^2} & 0 & 0 & 0 \\ & \frac{C'_{11}C'_{33} - C'^2_{12}}{\hat{C}'^2(C'_{33} - C'_{23})} & \frac{-C'_{23}C'_{11} + C'^2_{12}}{\hat{C}'^2(C'_{33} - C'_{23})} & 0 & 0 & 0 \\ & & \frac{C'_{11}C'_{33} - C'^2_{12}}{\hat{C}'^2(C'_{33} - C'_{23})} & 0 & 0 & 0 \\ & & & \frac{2}{C'_{33} - C'_{23}} & 0 & 0 \\ \text{symmetric} & & & & \frac{1}{C'_{66}} & 0 \\ & & & & & \frac{1}{C'_{66}} \end{bmatrix}, \quad (3.105)$$

where

$$\hat{C}'^2 = (C'_{33} + C'_{23})C'_{11} - 2C'^2_{12}. \quad (3.106)$$

The stress components in the local frame $x' - y' - z'$ are given by the usual transformation formulas:

$$\boldsymbol{\sigma}' = \mathbf{R} \times \boldsymbol{\sigma}, \quad (3.107)$$

where

$$\mathbf{R} = \begin{bmatrix} c_\theta^2 & s_\theta^2 & 2s_\theta c_\theta \\ s_\theta^2 & c_\theta^2 & -2s_\theta c_\theta \\ -s_\theta c_\theta & s_\theta c_\theta & c_\theta^2 - s_\theta^2 \end{bmatrix}, \quad (3.108)$$

and $\boldsymbol{\sigma}$ is given by either Eq. (3.93) if the long-range stress field is not relaxed or Eq. (3.101) if relaxed. Using Eqs. (3.101) and (3.107), Eq. (3.103), i.e., the strain energy density in crystal A or B, can be written in the form:

$$W = \frac{1}{2} \boldsymbol{\sigma}^T \times \mathbf{R}^T \times \tilde{\mathbf{a}}' \times \mathbf{R} \times \boldsymbol{\sigma}. \quad (3.109)$$

The elastic strain energy γ_s of the dipole wall can be computed by integrating the strain energy density W of Eq. (3.109) over the regions occupied by crystals A and B. The integration is carried out over one normalized period from $Y = -1/2$ to $1/2$, and from $X = -\infty$ to ∞ . It is necessary to exclude the disclination cores from the integration domain as the elastic field is invalid within the cores. To approximately take into account the strain energy in the cores, however, the integration of the elastic field transgresses partially into the core domain, as is done in estimating the core energy of a dislocation. Thus, taking an effective square core of normalized length $\bar{l}_0 = l_0 / h$ around

each of the two disclinations in the period, the total strain energy γ_s (including strain energy inside the cores) can be written as

$$\begin{aligned} \gamma_s = h & \left[\int_{-1/2}^{-\bar{a}_d - \bar{l}_0/2} \int_{-\infty}^0 + \int_{-\bar{a}_d + \bar{l}_0/2}^{-\bar{l}_0/2} \int_{-\infty}^{-\bar{l}_0/2} + \int_{-\bar{a}_d - \bar{l}_0/2}^{\bar{l}_0/2} \int_{-\infty}^0 + \int_{-\bar{a}_d + \bar{l}_0/2}^{\bar{l}_0/2} \int_{-\infty}^{-\bar{l}_0/2} + \int_{\bar{a}_d + \bar{l}_0/2}^{1/2} \int_{-\infty}^0 W_A(X, Y) dX dY \right] \\ & + h \left[\int_{-1/2}^{-\bar{a}_d - \bar{l}_0/2} \int_0^{\infty} + \int_{-\bar{a}_d + \bar{l}_0/2}^{\bar{l}_0/2} \int_{\bar{l}_0/2}^{\infty} + \int_{-\bar{a}_d - \bar{l}_0/2}^{\bar{l}_0/2} \int_0^{\infty} + \int_{-\bar{a}_d + \bar{l}_0/2}^{\bar{l}_0/2} \int_{\bar{l}_0/2}^{\infty} + \int_{\bar{a}_d - \bar{l}_0/2}^{\bar{l}_0/2} \int_{\bar{l}_0/2}^{1/2} + \int_{\bar{a}_d + \bar{l}_0/2}^{\bar{l}_0/2} \int_0^{\infty} W_B(X, Y) dX dY \right]. \end{aligned} \quad (3.110)$$

The disclination core parameter $\bar{l}_0$ is chosen to be 0.02 in the numerical results presented in Section 3.4. Furthermore, all the numerical results in Section 3.4 are based on the stress field without relaxation. Thus, the numerical integration over X in Eq. (3.110) is limited to the ranges $[-R, 0]$ and $[0, R]$ instead of $[-\infty, 0]$ and $[0, \infty]$, where R is taken to be the distance beyond which the stress field has decayed to a constant. Typically, the stress field has decayed to a constant or zero at $X \sim 1.5$ to 2, and R is therefore chosen to be 2.5 in the numerical results.

3.4. Numerical Results

Numerical examples are presented in Figs. 3.3-3.13 for the zinc/zinc (Zn/Zn), zinc/beryllium (Zn/Be) and beryllium/beryllium (Be/Be) bicrystals. The elastic constants of Zn and Be crystals are given in Table 3.1. Orientational inhomogeneity is examined in terms of symmetric and asymmetric orientations in which the c -axes are symmetric or asymmetric with respect to the bicrystal boundary. The numerical results on the elastic fields in Figs. 3.3-3.6 and 3.11 are generated with $\omega = 1^\circ$ and $a_d/h = 0.05$ in a square region $-0.5 < X < 0.5$, $-0.5 < Y < 0.5$ around the dipole centered at $(0, 0)$, while in Figs 3.7-3.10 the stress components at the boundary point

(0, 0.25) are investigated in terms of θ_A and θ_B . In Figs. 3.12 and 3.13 the strain energy of the dipole wall with $\omega = 1^\circ$ and $h = 10$ nm is investigated in terms of a_d/h and θ_A . The parameter values chosen here serve to illustrate some general trends of the model predictions; the appropriate values for ω , a_d and h for any bicrystal system would depend on the crystallographic details. A physical model incorporating the crystallographic structures of symmetric tilt boundaries in hexagonal bicrystals will be developed in Chapter 4.

Table 3.1.
The elastic constants of zinc and beryllium single crystals (Hirth and Lothe, 1982)

	Zinc	Beryllium
C'_{11} (GPa)	61	336.4
C'_{33} (GPa)	161	292.3
C'_{12} (GPa)	50.1	14
C'_{23} (GPa)	34.2	26.7
C'_{66} (GPa)	38.3	162.5

3.4.1. Stress Field in Zn/Zn and Zn/Be Bicrystals

As a reference, Fig. 3.3 plots the stress components σ_x , σ_y and σ_{xy} due to an infinite periodic wedge disclination dipole wall in a homogeneous Zn/Zn crystal for which $\theta_A = \theta_B = 30^\circ$. The image dislocations are predicted to have zero densities in this case. All components are continuous across the line $X = 0$, as an interface does not

exist. In all cases, the distribution has a center of antisymmetry at $(0, 0)$, i.e., $\sigma_x(X, Y) = -\sigma_x(-X, -Y)$ and similarly for σ_y and σ_{xy} . This symmetry is the only one present in a transversely isotropic homogeneous material; if the material is isotropic homogeneous three symmetry elements are present: antisymmetry about $(0, 0)$, and symmetry or antisymmetry about the lines $X = 0$ and $Y = 0$. See the work of Wu (2002c) for the results corresponding to a homogeneous isotropic zinc crystal for which the two isotropic elastic constants are the Voigt averages of the five independent constants.

Figure 3.4 plots the stress components for the case of symmetric orientations $\theta_A = 30^\circ$ and $\theta_B = 150^\circ$ in a Zn/Zn bicrystal. The only symmetry element present is the symmetry of σ_x and σ_y , and the antisymmetry of σ_{xy} , about the interface $X = 0$. This characteristic is intuitive as the c -axis orientations are symmetric about the interface. Comparing Figs. 3.3 and 3.4, the strong influence of orientational inhomogeneity on the distributions is apparent. Although not shown here, the distributions also change significantly as the symmetric orientations θ_A and $\theta_B = 180^\circ - \theta_A$ change. All stress components are continuous across the interface, although the continuity of σ_y is not part of the theoretical formulation. The continuity of σ_y is easily explained: the symmetry of σ_y about the interface must be respected and it would be violated if there were stress jumps across the interface.

Figure 3.5 shows the components for the case of asymmetric orientations $\theta_A = 30^\circ$ and $\theta_B = 70^\circ$ in a Zn/Zn bicrystal. There are no symmetry elements present in the distributions, as expected. The distribution shape is complicated, with kinks at the

Fig. 3.3. Stress distribution in a homogeneous anisotropic zinc crystal (c -axis orientations $\theta_A = \theta_B = 30^\circ$) due to an infinite periodic disclination dipole array of strength $\omega = 1^\circ$ and normalized half arm length $a_d/h = 0.05$. The stress distribution has a center of antisymmetry at $(0, 0)$.

Fig. 3.4. Stress distribution in a zinc/zinc bicrystal (symmetric c -axis orientations $(\theta_A, \theta_B) = (30^\circ, 150^\circ)$) due to an infinite periodic interfacial disclination dipole array of strength $\omega = 1^\circ$ and normalized half arm length $a_d/h = 0.05$. The stress distribution is symmetric or antisymmetric about, and is continuous across, the interface.

Fig. 3.5. Stress distribution in a zinc/zinc bicrystal (c -axis orientations $(\theta_A, \theta_B) = (30^\circ, 70^\circ)$) due to an infinite periodic interfacial disclination dipole array of strength $\omega = 1^\circ$ and normalized half arm length $a_d / h = 0.05$. The stress distribution is asymmetric. The components σ_x and σ_{xy} are continuous, while σ_y is discontinuous, across the interface. The presence of kinks in the distributions is evident.

Fig. 3.6. Stress distribution in a zinc/beryllium bicrystal (c -axis orientations $(\theta_A, \theta_B) = (30^\circ, 30^\circ)$) due to an infinite periodic interfacial disclination dipole wall of strength $\omega = 1^\circ$ and normalized half arm length $a_d / h = 0.05$. The stress distribution is asymmetric. The components σ_x and σ_{xy} are continuous, while σ_y is discontinuous, across the interface.

interface. Comparing Figs. 3.3-3.5, it can be concluded that orientational inhomogeneity has a strong influence on the stress distributions. Furthermore, the continuity of σ_x and σ_{xy} across the interface is predicted, which verifies the success of the image dislocation method. The component σ_y is discontinuous across the interface.

To show the influence of material inhomogeneity alone, Fig. 3.6 plots the stress components in a Zn/Be bicrystal for $\theta_A = \theta_B = 30^\circ$. Comparing this figure with the reference Fig. 3.3 ($\theta_A = \theta_B = 30^\circ$, Zn/Zn bicrystal), it can also be concluded that material inhomogeneity alone exerts a strong influence on the stress distributions. Continuity of σ_x and σ_{xy} across the interface is again successfully predicted, and the discontinuity in σ_y arises from the material inhomogeneity. Similar comments can be made when the bicrystal is both orientationally and materially inhomogeneous. For the physical modeling of the boundary between dissimilar crystals such as Zn and Be, it should be remarked that the mismatch in lattice parameters is generally accommodated by misfit edge dislocations with Burgers vector tangential to the boundary. The elastic solutions for interfacial edge dislocations in hexagonal bicrystals are available; in fact they were recently derived using the image method (Wu et al., 2003)

Figures 3.3-3.6 show that the stresses due to an infinite interfacial disclination dipole wall in a hexagonal bicrystal can be computed with ease in spite of their complex distributions. Moreover, the forces exerted by the disclination dipole wall on other discrete dislocations can also be determined. For instance, the Peach-Koehler equation gives the x - and y -direction forces on an edge dislocation as $F_x = \sigma_{xy} b_x + \sigma_y b_y$,

$F_y = -\sigma_x b_x - \sigma_{xy} b_y$, where b_x and b_y are the components of the Burgers vector of the edge dislocation and σ_x , σ_y and σ_{xy} are the stresses due to the dipole wall.

3.4.2. Dependence of Interfacial Stress on Bicrystal Orientations

Figures 3.7-3.8 plot the dependence of the stress components σ_x and σ_{xy} at the interfacial point $(X, Y) = (0, 0.25)$ on the c -axis orientations θ_A and θ_B in a Zn/Zn bicrystal. The dependences for a Zn/Be bicrystal are plotted in Figs. 3.9 and 3.10. The interfacial point of interest lies between two dipoles. In these figures, σ_x and σ_{xy} are shown as three-dimensional topographical and contour plots. The full range of θ_A and θ_B from 0° to 180° is investigated.

One of the most salient features of Figs. 3.7-3.10 is that the stress topography displays extrema and saddle points. In Fig. 3.7, the maximum and minimum values of σ_x are about -0.030082 GPa and -0.04887 GPa, respectively, and they occur at the four corners ($\theta_A = 0^\circ, \theta_B = 0^\circ$; $\theta_A = 0^\circ, \theta_B = 180^\circ$; $\theta_A = 180^\circ, \theta_B = 0^\circ$; $\theta_A = 180^\circ, \theta_B = 180^\circ$) and the center ($\theta_A = 90^\circ, \theta_B = 90^\circ$) of the square region. For σ_{xy} the maximum and minimum values are about ± 0.00937 GPa and they occur at $\theta_A = 45^\circ, \theta_B = 45^\circ$ and $\theta_A = 135^\circ, \theta_B = 135^\circ$, respectively, see Fig. 3.8. For the Zn/Be bicrystal, the maximum and minimum values of σ_x are about -0.050056 GPa and -0.074504 GPa, respectively, and they occur at the $\theta_A \approx 0^\circ, \theta_B \approx 78.9^\circ$ and $\theta_A \approx 90^\circ, \theta_B \approx 8.4^\circ$, see Fig. 3.9. For σ_{xy} the maximum and minimum values are about

Zn/Zn Bicrystal: $\omega = 1^\circ$, $a_d / h = 0.05$, $X = 0$, $Y = 0.25$

Fig. 3.7. Dependence of the stress component σ_x at the boundary point (0, 0.25) on the c -axis orientations θ_A and θ_B in a Zn/Zn bicrystal. Maxima and minima can be observed. The contours of σ_x are symmetric about the lines $\theta_A + \theta_B = 180^\circ$ and $\theta_A = \theta_B$.

Zn/Zn Bicrystal: $\omega = 1^\circ$, $a_d / h = 0.05$, $X = 0$, $Y = 0.25$

Fig. 3.8. Dependence of the stress component σ_{xy} at the boundary point $(0, 0.25)$ on the c -axis orientations θ_A and θ_B in a Zn/Zn bicrystal. Maxima, minima and saddle points can be observed. The contours of σ_{xy} are antisymmetric about the line $\theta_A + \theta_B = 180^\circ$ and symmetric about $\theta_A = \theta_B$.

Zn/Be Bicrystal: $\omega = 1^\circ$, $a_d / h = 0.05$, $X = 0$, $Y = 0.25$

Fig. 3.9. Dependence of the stress component σ_x at the boundary point $(0, 0.25)$ on the c -axis orientations θ_A and θ_B in a Zn/Be bicrystal. The contours of σ_x appear to be, but are actually not, symmetric about $\theta_A = 90^\circ$.

Zn/Be Bicrystal: $\omega = 1^\circ$, $a_d / h = 0.05$, $X = 0$, $Y = 0.25$

Fig. 3.10. Dependence of the stress component σ_{xy} at the boundary point $(0, 0.25)$ on the c -axis orientations θ_A and θ_B in a Zn/Be bicrystal. The antisymmetry of σ_{xy} contours cannot be observed.

0.004711 GPa and -0.00445 GPa and they occur at $\theta_A \approx 131.4^\circ$, $\theta_B \approx 45.9^\circ$ and $\theta_A \approx 48.7^\circ$, $\theta_B \approx 134.4^\circ$, respectively, see Fig. 3.10.

Another observation is the symmetry for σ_x and antisymmetry for σ_{xy} of the stress components about the line $\theta_A + \theta_B = 180^\circ$ for the Zn/Zn bicrystal. This corresponds to the physical result that the stresses must remain the same when the solid is flipped 180° about the bicrystal boundary. The shear stress changes sign since the shear stress acting at an element after flipping is in the direction opposite to that prior to flipping. A similar line of reasoning can be used to explain the symmetry about $\theta_A = \theta_B$. For the Zn/Be bicrystal, the σ_x and σ_{xy} contours do not possess any symmetry. The σ_x contours appear to be, but are actually not, symmetric about the line $\theta_A = 90^\circ$.

The stress magnitudes depend significantly on the orientations. The range of values of σ_x in the Zn/Zn bicrystal, for instance, is approximately $[-0.05, -0.03]$ GPa, while the range for σ_{xy} is approximately $[-0.0094, 0.0094]$ GPa, see Figs. 3.7 and 3.8. Also, it can be seen that the stresses depend significantly on the material inhomogeneity after comparing the results for the Zn/Zn and the Zn/Be bicrystals.

It should be remarked that results reported in this section are for the interfacial point $(0, 0.25)$. Occurrence of maxima, minima and saddle points is position-dependent, i.e., the values of θ_A and θ_B that give rise to these points vary with the interfacial locations.

3.4.3. Strain Energy in Zn/Zn and Be/Be Bicrystals

Figure 3.11 plots the strain energy density in 10^6 J m^{-3} around a disclination dipole of the periodic wall in a Zn/Zn bicrystal with the c -axis orientations $\theta_A = 30^\circ$ and

$\theta_B = 150^\circ$. As before, $\omega = 1^\circ$ and $a_d = 0.05h$. The following observations can be made. First, the energy density displays peaks around the sites of the disclinations and valleys in between them. Since the strain energy density can be used as a criterion for predicting crack nucleation, the quantitative results here will be useful for crack analysis. Second, for the present case of symmetric orientations, the energy density is, as all three stress components are, continuous across the interface. For general orientations, the energy density, just like σ_y , is discontinuous across the interface. Third, the energy density contours are symmetric about the interface, as expected, but are not symmetric about the line $Y = 0$. This is analogous to the corresponding stress plots of Fig. 3.4.

Figure 3.12 plots the strain energy γ_e of the disclination dipole wall in J m^{-2} versus a_d/h in the range $0 \leq a_d/h \leq 0.25$ for $h = 10 \text{ nm}$ and $\omega = 1^\circ$. Three cases of symmetric orientations in the Zn/Zn bicrystal are considered: $(\theta_A, \theta_B) = (0^\circ, 180^\circ)$, $(30^\circ, 150^\circ)$ and $(60^\circ, 120^\circ)$. Due to the periodicity, the energy curves over the range $0 \leq a_d/h \leq 0.5$ are symmetric about $a_d/h = 0.25$, at which all disclinations (positive or negative) are equally spaced in the infinite wall. The energy increases monotonically with the dipole arm length up to $a_d/h = 0.25$. Except for small values of a_d/h , it is quite strongly dependent on the orientational inhomogeneity. For instance, at $a_d/h = 0.25$ the energy for $(\theta_A, \theta_B) = (60^\circ, 120^\circ)$ is more than three times that for the homogeneous case $(\theta_A, \theta_B) = (0^\circ, 180^\circ)$. This underlines the importance of using a bicrystal model over a homogeneous model for calculations.

Zn/Zn Bicrystal: $\omega = 1^\circ$, $a_d/h = 0.05$

Fig. 3.11. Three-dimensional topographical and contour plots of strain energy density in a zinc/zinc bicrystal (symmetric c -axis orientations $(\theta_A, \theta_B) = (30^\circ, 150^\circ)$) due to an infinite periodic interfacial disclination dipole wall of strength $\omega = 1^\circ$ and normalized half arm length $a_d/h = 0.05$. The density distribution is symmetric about, and is continuous across, the interface.

Fig. 3.12. Dependence of the strain energy of an interfacial disclination dipole wall in a zinc/zinc bicrystal on the dipole arm length for several symmetric c -axis orientations. The disclination strength $\omega = 1^\circ$ and the dipole period $h = 10 \text{ nm}$. The monotonic increase of the energy with the dipole arm length up to $a_d/h = 0.25$ is clearly evident. The dependence of the energy on a_d/h is influenced by the c -axis orientations.

A key question arises as to which orientation pair (θ_A, θ_B) yields the maximum or minimum γ_ϵ for a given a_d/h . Figures 3.13(a) and (b) plot the energy versus the orientation θ_A for the Zn/Zn and Be/Be bicrystals, respectively, using $a_d/h = 0.25$. The figures show that the maximum, minimum and the corresponding orientations are strongly influenced by the bicrystal system. For the Zn/Zn bicrystal, the maximum and minimum γ_ϵ values are about 0.00319 and 0.000863 Jm^{-2} and they respectively occur at $(\theta_A, \theta_B) \approx (47.5^\circ, 132.5^\circ)$ and $(0^\circ, 180^\circ)$. For the Be/Be bicrystal, the maximum and minimum values are about 0.00424 and 0.00314 Jm^{-2} at

Fig. 3.13. Dependence of the strain energy of an interfacial disclination dipole wall in (a) Zn/Zn bicrystal and (b) Be/Be bicrystal on the c -axis orientations (θ_A , $\theta_B = 180^\circ - \theta_A$). The disclination strength $\omega = 1^\circ$, the dipole period $h = 10 \text{ nm}$, and the normalized dipole arm length $a_d/h = 0.25$. The dependence on the orientational inhomogeneity is very significant for the Zn/Zn bicrystal, with the energy attaining a maximum of 0.00319 J m^{-2} at $\theta_A \approx 47.5^\circ$ or 132.5° and a minimum of $0.000863 \text{ J m}^{-2}$ at $\theta_A = 0^\circ$ or 180° , which represents a maximum/minimum ratio of 3.7. For the Be/Be bicrystal, the strain energy attains the maximum of 0.00424 J m^{-2} at $\theta_A \approx 10^\circ$ or 170° .

$(\theta_A, \theta_B) \approx (10^\circ, 170^\circ)$ and $(48^\circ, 132^\circ)$, respectively. Note also that for the Zn/Zn bicrystal, γ_ϵ at $(\theta_A, \theta_B) = (90^\circ, 90^\circ)$ is larger than that at $(0^\circ, 0^\circ)$, while the reverse is true for the Be/Be bicrystal. This shows the influence of elastic anisotropy. Finally, the energy curves are symmetric about $\theta_A = 90^\circ$, which reveals the correct physical result that bicrystals characterized by the orientation pairs $(\theta, 180^\circ - \theta)$ and $(180^\circ - \theta, \theta)$ possess the same strain energy for any θ between 0° and 180° .

The elastic strain energy results of Figs. 3.12 and 3.13 constitute a critical part of the bicrystal boundary energy. They demonstrate that the effect of dissimilarity in orientation or material across the interface can be quantitatively estimated and that the boundary energy can be significantly influenced by the crystallographic orientations.

3.5. Conclusions

An infinite periodic wall of interfacial wedge disclination dipoles in a hexagonal bicrystal with arbitrary in-plane c -axes is investigated by the method of image dislocations. Exact closed-form solutions for the stress and strain energy density are found to be of the form of the logarithm of hyperbolic and trigonometric functions of complex parameters. The long-range stress field of the dipole wall, which generally exists except for special c -axis orientations, is also determined exactly. Numerical results for Zn/Zn, Zn/Be and Be/Be bicrystals show that (i) the fields are highly dependent on the orientational and material inhomogeneities, which emphasizes the importance of using a bicrystal model over a homogeneous model for calculations, and (ii) the strain energy of the dipole wall in a bicrystal with symmetric c -axis orientations

possesses maximum/minimum at specific orientations; both the maximum/minimum and the corresponding orientations vary with the bicrystal system.

Chapter 4

Application of DSUM: Grain Boundaries in Hexagonal Materials

This chapter is organized as follows. The existing knowledge on the disclination-structural unit model (DSUM) for cubic bicrystals is briefly reviewed in Section 4.1. The DSUM is then developed for application in hexagonal bicrystals in Section 4.2. This developed model has two functions. First, it provides realistic physical parameters as input for the mechanics model of the disclination dipole wall presented in Chapter 3, which takes into account the influence of the bicrystal anisotropy and inhomogeneity. Second, it provides a means to incorporate the mechanics model for calculating GB energies of hexagonal bicrystals. For the purpose of comparison, the mechanics model of a disclination dipole wall in homogeneous isotropic crystals is also presented in Section 4.3. Finally, the stress field of the disclination dipole wall and the dependence of GB energy on misorientation are investigated using the DSUM in conjunction with the inhomogeneous anisotropic and homogeneous isotropic mechanics models.

4.1. Disclination-Structural Unit Model for Cubic Bicrystals

The foundations of the DSUM are the structural unit/dislocation model of GBs derived from computer simulations (Sutton and Vitek, 1983a, b, c; Wang et al., 1984) and the disclination model of GBs (Li, 1972; Shih and Li, 1975). Essentially, a general

(intermediate) GB is considered to be made up of alternate segments (structural units) of two favored (delimiting) boundaries with different misorientations; the junctions of these segments represent rotational misfit and are partial disclinations. The GB therefore is represented by a wall of disclination dipoles with strengths $\pm \omega = \pm(\Theta_k - \Theta_j)$, where Θ_j and Θ_k are the misorientations of the delimiting boundaries j and k . The dipole arm length $2a_d$ (spacing between the positive and negative disclinations) and the dipole wall period h can be inferred from the crystallographic structure of the GB. For calculations of the energy of a general GB, the surface energies of a limited number n of delimiting boundaries with misorientations Θ_i , $i = 1, 2, \dots, n$, are determined by the atomistic method. The energy of a GB with misorientation Θ intermediate between Θ_j and Θ_k is then calculated from the surface energies of the delimiting boundaries j and k and the strain energy of the disclination dipole wall modeling the GB (Nazarov et al., 2000a, b).

The DSUM has been applied to cubic bicrystals, particularly face-centered-cubic (FCC) bicrystals. Consider the FCC lattice in Fig. 4.1(a), which shows that there are two crystallographic planes in a period along the $[001]$ direction with different locations of atoms. The atoms in these two planes are distinguished by full circles and crosses. The $[001]$ projection of the atoms is shown in Fig. 4.1(b). The two vectors of $\mathbf{a}_1 = [110]/2$ and $\mathbf{a}_2 = [1\bar{1}0]/2$ along the two edge axes of the square are also indicated. Note that $|\mathbf{a}_1| = |\mathbf{a}_2| = a$, where a is the lattice parameter of FCC crystals. It is convenient to draw the geometry of a $[001]$ symmetric tilt GB, whose tilt axis is $[001]$, on this projection. Let the Miller index of a lattice plane be $(k\ l\ 0)$, of which

Fig. 4.1. (a) Atoms indicated as full circles and crosses on two crystallographic planes of an FCC lattice. The lattice parameter a is as indicated. (b) $[001]$ projection of the FCC lattice with key vectors indicated by the arrows.

Fig. 4.2 (a) Lattice planes A, B, C and D, about each of which a favored boundary can be constructed by reflection. (b) Vectors representing the structural units.

$[k\ l\ 0]$ indicates the vector of the plane normal. A symmetric tilt GB is obtained by mirror reflection of the atoms above this crystallographic plane with respect to it. Figure 4.2(a) shows the $(\bar{1}\ 1\ 0)$, $(\bar{1}\ 2\ 0)$, $(\bar{1}\ 3\ 0)$ and $(0\ 1\ 0)$ lattice planes, denoted by A, B, C and D respectively. The atoms above each plane are reflected about it to obtain the atoms below it, resulting in a symmetric tilt boundary. Therefore, four symmetric tilt boundaries A, B, C and D can be constructed corresponding to the four planes A, B, C

and D. Figure 4.2(b) shows the structural units represented by the vectors $\mathbf{h}_A$, $\mathbf{h}_B$, $\mathbf{h}_C$ and $\mathbf{h}_D$, which join a full circle to the nearest full circle or cross (Sutton and Vitek, 1983a). Apparently, the four GBs A, B, C and D each consist of only one type of structural unit and therefore are favored boundaries (Sutton and Vitek, 1983a; Wang et al., 1984; Sutton and Balluffi, 1995).

Based on the above method to construct a [001] symmetric tilt boundary, the misorientation Θ of the obtained GB can be calculated as twice the angle between the lattice plane, about which mirror reflection takes place, and the edge vector $\mathbf{a}_1$ on the [001] projection. For example, the misorientation of the favored boundary B ($\bar{1}20$) can be obtained as

$$\Theta_B = 2 \tan^{-1} \frac{|\mathbf{a}_2|}{|3\mathbf{a}_1|} = 36.87^\circ. \quad (4.1)$$

In the same way, $\Theta_A = 0^\circ$, $\Theta_C = 53.13^\circ$ and $\Theta_D = 90^\circ$ are obtained for A ($\bar{1}10$), C ($\bar{1}30$) and D (010), respectively.

For a general misorientation, a DSUM can be developed in which the boundary contains two types of structural units. For instance, consider the GB ($\bar{3}70$) with the misorientation angle $\Theta = 43.6^\circ$, which is intermediate between $\Theta_B = 36.87^\circ$ and $\Theta_C = 53.13^\circ$. This boundary can be considered as made up of two B units and one C unit with the period vector of $\mathbf{h} = 2\mathbf{h}_B + \mathbf{h}_C = 5\mathbf{a}_1 + 2\mathbf{a}_2 = [730]/2$, see Fig. 4.3. The line where the two different types of structural units meet represents a disclination, and the minority unit (the C unit) is considered as a disclination dipole, whose arm length

Fig. 4.3. A general GB (dotted line) with a misorientation intermediate between those of the favored B and C boundaries. It can be modeled in terms of B and C structural units in the sequence BBC.BBC. Disclinations occur at the lines where the B and C units meet.

$2a_d$ corresponds to the length of the C unit. The strength of the dipole is given by the difference between the misorientations of the favored boundaries B and C, i.e., $\omega = \pm(\theta_C - \theta_B)$. The dipole period is given by the length of the period vector

$h = 2h_B + h_C$. In a similar manner, other boundaries can be modeled in terms of structural units arranged in certain sequences.

4.2. Disclination-Structural Unit Model for Hexagonal Bicrystals

DSUM for hexagonal bicrystals can be similarly developed as for cubic bicrystals. The thesis work aims to investigate $[1\bar{1}00]$ symmetrical tilt GBs, which are rational in nature. Irrational GBs, for example asymmetrical GBs or interphase boundaries between different HCP crystals, are not considered. As shown below, symmetrical tilt boundaries can always be constructed for any HCP bicrystals, although Θ is dependent on the value of the ratio c/a of the lattice parameters. It should also be noted that exact coincidence site lattices exist in HCP crystals only if $(c/a)^2$ is rational, except for rotations about the $[0001]$ axis. Hence, for $[1\bar{1}00]$ boundaries the Σ values can only be approximated and they depend greatly on c/a . For instance, $\Sigma = 23$ for the $[1\bar{1}00](11\bar{2}6)$ symmetrical tilt boundary in titanium if $(c/a)^2$ is approximated as $5/2$, while $\Sigma = 35$ for the same type of boundary in cobalt if $(c/a)^2$ is taken to be $8/3$ (Farkas, 1994). Calculations of the Σ values are therefore not necessary and are not made here.

Consider the hexagonal lattice of Fig. 4.4, which shows that there are four crystallographic planes in a period along the $[1\bar{1}00]$ direction with different locations of atoms. The atoms in these four planes are distinguished by full squares, full stars, open circles and open triangles. The $[1\bar{1}00]$ projection of the atoms is shown in Fig. 4.5.

Fig. 4.4. Atoms indicated as full squares, full stars, open circles and open triangles on four crystallographic planes of an hcp lattice. The atom positions as viewed along the $[1\bar{1}00]$ direction are shown in Fig. 4.5. The lattice parameters c and a are as indicated.

The two vectors $\mathbf{a} = (1/3)[11\bar{2}0]$ and $-\mathbf{c} = [000\bar{1}]$ along the edge and longitudinal axis of the hexagon are also indicated. Unlike the planes in the FCC lattice, the four planes $(1\bar{1}00)$ in the hexagonal lattice are not equally spaced.

A $[1\bar{1}00]$ symmetrical tilt GB can be constructed by choosing a crystallographic plane passing through the lattice containing the $[1\bar{1}00]$ axis, discarding the atoms on one side of the plane and reflecting the atoms on the other side about this plane. Figure 4.6 shows an example where $\mathbf{H}$ denotes the crystallographic period vector of the symmetrical tilt GB. In general, the period vector $\mathbf{H}$ can be written as the sum of $\mathbf{a}$ and $\mathbf{c}$:

$$\mathbf{H} = \alpha \mathbf{a} + \beta \mathbf{c} = \frac{1}{3}[\alpha \quad \alpha \quad -2\alpha \quad 3\beta], \quad (4.2)$$

Fig. 4.5. The $[1\bar{1}00]$ projection of atoms of the hcp lattice. Delimiting boundaries A, B, C, ..., F with period vectors $H_A, H_B, H_C, \dots, H_F$ are created by removing the atoms below (or above) the boundaries and performing a mirror reflection of the remaining atoms about the boundaries. Each period contains an additional atom in the middle, and the disclination period is one-half of the GB period, i.e., $h_A = H_A / 2$, etc.

where α and β are whole numbers. Let the vector N be parallel to the GB normal. It lies in the plane $(1\bar{1}00)$ and is perpendicular to H . The first part of this statement leads to the following implied relation:

$$N \perp [1\bar{1}00] \Rightarrow N // [h \ h \ k \ l], \quad (4.3)$$

where for HCP crystals $h + h + k = 0$ and hence

Fig. 4.6. A BBC.BBC boundary with disclination dipole period vector $\mathbf{h} = 2\mathbf{h}_B + \mathbf{h}_C$. The dipole arm $2a_d$ is determined by the length of the minority unit (C), and the dipole period is $h = |\mathbf{h}|$. The disclination strength is the difference between the misorientations of the delimiting boundaries B and C, i.e., $\omega = \pm(\Theta_C - \Theta_B)$.

$$\mathbf{N} // [\mathbf{h} \quad \mathbf{h} \quad -2\mathbf{h} \quad \mathbf{l}]. \quad (4.4)$$

Moreover, $\mathbf{N} \perp \mathbf{H}$ implies that

$$[\mathbf{h} \quad \mathbf{h} \quad -2\mathbf{h} \quad \mathbf{l}] \cdot [\alpha \quad \alpha \quad -2\alpha \quad 3\beta] = 0, \quad (4.5)$$

from which $\mathbf{l} = -2\alpha\mathbf{h}/\beta$ and hence

$$\mathbf{N} // \left[\mathbf{h} \quad \mathbf{h} \quad -2\mathbf{h} \quad -2\frac{\alpha}{\beta}\mathbf{h} \right] // \left[1 \quad 1 \quad -2 \quad -2\frac{\alpha}{\beta} \right]. \quad (4.6)$$

The misorientation Θ of the boundary is given by

$$\Theta = 2 \tan^{-1} \left| \frac{\beta}{\alpha} \frac{c}{a} \right|, \quad (4.7)$$

where $a = |\mathbf{a}|$ and $c = |\mathbf{c}|$ are the lattice parameters. The geometrical characteristics of $[1\bar{1}00]$ tilt GBs in HCP bicrystals are thus given by the expressions for the period vector, the boundary normal vector and the misorientation in Eqs. (4.2), (4.6) and (4.7) respectively.

Six short-period boundaries A, B, C, D, E and F are chosen to be the delimiting or favored boundaries in DSUM. The Miller indices of the GB planes are respectively (0001) , $(11\bar{2}6)$, $(11\bar{2}4)$, $(11\bar{2}2)$, $(11\bar{2}1)$ and $(11\bar{2}0)$. The corresponding GB period vectors, illustrated in Fig. 4.5, are

$$\begin{aligned} \mathbf{H}_A &= \mathbf{a} = \frac{1}{3} [1 \quad 1 \quad \bar{2} \quad 0], & \mathbf{H}_B &= 3\mathbf{a} - \mathbf{c} = [1 \quad 1 \quad \bar{2} \quad \bar{1}], \\ \mathbf{H}_C &= 2\mathbf{a} - \mathbf{c} = \frac{1}{3} [2 \quad 2 \quad \bar{4} \quad \bar{3}], & \mathbf{H}_D &= \mathbf{a} - \mathbf{c} = \frac{1}{3} [1 \quad 1 \quad \bar{2} \quad \bar{3}], \\ \mathbf{H}_E &= \mathbf{a} - 2\mathbf{c} = \frac{1}{3} [1 \quad 1 \quad \bar{2} \quad \bar{6}], & \mathbf{H}_F &= -\mathbf{c} = [0 \quad 0 \quad 0 \quad \bar{1}]. \end{aligned} \quad (4.8)$$

The surface energies of the delimiting boundaries B, C, D and E have been determined by the embedded-atom method by Farkas (1994). The geometrical characteristics $\mathbf{H}$ and Θ , the Miller indices and the surface energies (for cobalt and titanium) of these six GBs are summarized in Table 4.1. For any GB with Θ intermediate between those of the two adjacent favored GBs, the period vector can be decomposed into the period vectors of the delimiting ones, i.e.,

Table 4.1.

The Miller indices, the period vector, the misorientation and the surface energy of six special boundaries A, B,..., F of hexagonal bicrystals.

	GB plane Miller indices	GB period vector $\mathbf{H}$	Misorientation Θ (deg)	Surface energy ^a γ_s (J m ⁻²)	
				Cobalt	Titanium
A	(0001)	$\frac{1}{3}[11\bar{2}0]$	0	0	0
B	(11 $\bar{2}$ 6)	$[11\bar{2}\bar{1}]$	$2 \tan^{-1}\left(\frac{c}{3a}\right)$	1.212	0.688
C	(11 $\bar{2}$ 4)	$\frac{1}{3}[22\bar{4}\bar{3}]$	$2 \tan^{-1}\left(\frac{c}{2a}\right)$	1.391	0.693
D	(11 $\bar{2}$ 2)	$\frac{1}{3}[11\bar{2}\bar{3}]$	$2 \tan^{-1}\left(\frac{c}{a}\right)$	0.509	0.259
E	(11 $\bar{2}$ 1)	$\frac{1}{3}[11\bar{2}\bar{6}]$	$2 \tan^{-1}\left(\frac{2c}{a}\right)$	0.229	0.096
F	(11 $\bar{2}$ 0)	$[000\bar{1}]$	180	0	0

^aData obtained by the embedded-atom method (Farkas, 1994).

$$\mathbf{H} = m\mathbf{H}_P + n\mathbf{H}_Q, \tag{4.9}$$

where P and Q denote A, B,..., F. It can be seen from Fig. 4.5 that all delimiting GBs for the $[1\bar{1}00]$ tilt axis are centered, i.e., they contain an additional coincidence atom in the center of the period. Thus, for all delimiting GBs the structural units are characterized by a vector equal to one half of the GB period vector:

$$\mathbf{h} = \mathbf{H} / 2. \tag{4.10}$$

Any intermediate GB also consists of two half periods, i.e., has structures like PQ.PQ, PPQ.PPQ, etc. The displacements of the half periods along the tilt axis are different for

different tilt boundaries, since the center atoms can be located on different crystallographic layers. However, this is not important for the disclination dipole model, which is insensitive to displacements along the tilt axis. Moreover, the structural units of the GB are distributed uniformly within its period, e.g., for $\mathbf{h} = 3\mathbf{h}_P + 2\mathbf{h}_Q$ the sequence is PPQPQ.PPQPQ rather than PPPQQ.PPPQQ. The disclination dipole parameters of strength ω , dipole arm $2a_d$ and dipole period h are determined as follows. Using Fig. 4.6 as an example, which shows a BBC.BBC boundary with the Miller indices $(3\ 3\ \bar{6}\ 16)$ and the period vector $\mathbf{h} = 2\mathbf{h}_B + \mathbf{h}_C$, the disclinations are located at the meeting points of the B and C units projected onto the GB plane. The two disclinations obtained from the projection of the minority structural unit C can be grouped as a disclination dipole, although the alternative of regarding the majority units as the dipole is equally valid. The dipole arm $2a_d$ is thus the distance between the disclinations at the ends of the projection of the minority unit, and the dipole period h is simply the magnitude of the period vector $\mathbf{h}$. The disclination strength is the difference between the misorientations of the delimiting boundaries, i.e., $\pm\omega = \pm(\Theta_C - \Theta_B)$ for the GB shown in Fig. 4.6. For all intermediate GBs between two delimiting GBs, the disclination strength is constant.

According to Nazarov et al. (2000a, b), the energy γ_{gb} of any intermediate boundary can be computed as the sum of the surface energy γ_s of the constituent delimiting favored boundaries P and Q and the total strain energy γ_e of the disclination dipole wall:

$$\gamma_{gb} = \gamma_s + \gamma_e, \quad (4.11)$$

where

$$\gamma_s = \frac{md_p e_p + nd_Q e_Q}{h}, \quad (4.12)$$

d_p and d_Q are the lengths, e_p and e_Q are the surface energies, and m and n are the number of P and Q structural units in the period h .

4.3. Elastic Solutions for a Disclination Dipole Wall

Using DSUM, an infinite disclination dipole wall with strength ω , arm length $2a_d$ and period h is unambiguously obtained for any symmetrical tilt GB with misorientation Θ . To predict the stress field and the strain energy of the dipole wall, two physical facts are considered: the hexagonal crystals are transversely isotropic with five independent elastic constants and the bicrystal is inhomogeneous resulting from the different lattice orientations of the adjoining crystals. Thus, the elastic solutions of an interfacial disclination dipole wall in a hexagonal bicrystal obtained in Chapter 3 will be employed to determine the stress and strain energy of symmetrical tilt GBs.

The elastic solutions in Chapter 3 are applicable for different crystals $A \neq B$ and for different crystal orientations $\theta_A \neq \theta_B$, where A and B are two constituent crystals of a hexagonal bicrystal. However, for symmetrical tilt GBs only the special case of $A = B$ (same crystal type) and $\theta_B = 180^\circ - \theta_A$ (symmetric boundary) is relevant. For this special case, the relationship between the GB misorientation Θ and the crystal orientation θ_A or θ_B can be determined by correlating two figures, i.e., the dipole wall schematic in Fig. 3.1 and the GB schematic in Fig. 4.6. As a result, the correlation is

Fig. 4.7. Relationship between the GB misorientation and the crystal orientation θ_A or θ_B ($\theta_B = 180^\circ - \theta_A$ for the symmetrical tilt GB), referring to Fig. 3.1 and Fig. 4.6. It demonstrates that $\Theta = 2\theta_B$, where $0 \leq \theta_B \leq 90^\circ$.

illustrated in Fig. 4.7, which demonstrates that $\Theta = 2\theta_B$ with $0 \leq \theta_B \leq 90^\circ$. Apparently, the strain energy of crystal B is identical to that of crystal A for symmetrical tilt GBs. Therefore, Eq. (3.110), which is used to calculate the entire strain energy in both crystals A and B, can be simplified as

$$\gamma_\epsilon = 2h \left[\int_{-1/2}^{\bar{a}-\bar{l}_0/2} \int_{-\infty}^0 + \int_{-\bar{a}-\bar{h}_0/2}^{\bar{a}+\bar{l}_0/2} \int_{-\infty}^{-\bar{l}_0/2} + \int_{-\bar{a}+\bar{l}_0/2}^{\bar{a}-\bar{l}_0/2} \int_{-\infty}^0 + \int_{\bar{a}-\bar{l}_0/2}^{\bar{a}+\bar{l}_0/2} \int_{-\infty}^{-\bar{l}_0/2} + \int_{\bar{a}+\bar{l}_0/2}^{1/2} \int_{-\infty}^0 W_A(X, Y) dX dY \right], \quad (4.13)$$

where $\bar{l}_0 = l_0 / h$ is the disclination core parameter.

The mechanics model of a disclination dipole wall in a hexagonal bicrystal takes into account the influence of the bicrystal anisotropy and inhomogeneity. For comparison, the model of a disclination dipole wall in homogeneous isotropic solids is presented here. The stress field of a single disclination in a homogeneous isotropic crystal has been given by de Wit (1973). By superposing the solutions of individual disclinations in the dipole wall, the stress field of the wall can be obtained:

$$\sigma_x, \sigma_y = \frac{G\omega}{2\pi(1-\nu)} \left[\frac{1}{2} \ln \frac{\cosh[2\pi X] - \cos[2\pi(Y - \bar{a}_d)]}{\cosh[2\pi X] - \cos[2\pi(Y + \bar{a}_d)]} \pm \pi X \sinh[2\pi X] \times \left(\frac{1}{\cosh[2\pi X] - \cos[2\pi(Y + \bar{a}_d)]} - \frac{1}{\cosh[2\pi X] - \cos[2\pi(Y - \bar{a}_d)]} \right) \right], \quad (4.14)$$

$$\sigma_{xy} = \frac{G\omega}{2\pi(1-\nu)} \pi X \left(\frac{\sin[2\pi(Y + \bar{a}_d)]}{\cosh[2\pi X] - \cos[2\pi(Y + \bar{a}_d)]} - \frac{\sin[2\pi(Y - \bar{a}_d)]}{\cosh[2\pi X] - \cos[2\pi(Y - \bar{a}_d)]} \right), \quad (4.15)$$

where the upper and lower signs in Eq. (4.14) refer to σ_x and σ_y , respectively, and G is the shear modulus and ν is Poisson's ratio, respectively. The two constants G and ν can be calculated as either the Voigt average of the crystal elastic constants, i.e.,

$$G = \frac{1}{30} (7C'_{33} - 5C'_{23} + 2C'_{11} + 12C'_{66} - 4C'_{12}), \quad (4.16)$$

$$D = \frac{C'_{33} + C'_{11} + 5C'_{23} + 8C'_{12} - 4C'_{66}}{9C'_{33} + 4C'_{11} + 5C'_{23} + 12C'_{12} + 4C'_{66}}, \quad (4.17)$$

or as the Reuss average of the crystal elastic compliances, i.e.,

$$G = \frac{15}{8a'_{33} + 4a'_{11} + 6a'_{66} + 3a'_{44} - 4a'_{23} - 8a'_{12}}, \quad (4.18)$$

$$D = \frac{-2a'_{33} - a'_{11} + a'_{66} + a'_{44} / 2 - 4a'_{23} - 8a'_{12}}{6a'_{33} + 3a'_{11} + 2a'_{66} + a'_{44} + 2a'_{23} + 4a'_{12}}, \quad (4.19)$$

where a'_{ij} ($i, j = 1, 2, 3, \dots, 6$) are given in Eq. (3.105). Equations (4.16)-(4.19) can be deduced from the formulas given by Hirth and Lothe (1982). The strain energy can also be calculated for the homogeneous isotropic model using Eqs. (4.13)-(4.15).

4.4. Stress Field of Dipole Wall and Dependence of Energy on Misorientation

In this section, numerical investigation of the GB energy and the disclination dipole stress field of $[1\bar{1}00]$ symmetrical tilt boundaries in cobalt and titanium bicrystals are carried out using DSUM. The elastic constants and the lattice parameters for cobalt and titanium are listed in Table 4.2.

The stress components of the disclination dipole wall are normalized with respect to the shear modulus G , i.e., $\tilde{\sigma}_x = \sigma_x / G$, $\tilde{\sigma}_y = \sigma_y / G$ and $\tilde{\sigma}_{xy} = \sigma_{xy} / G$. Figures 4.8-4.10 compare these components for the misorientations of $\Theta = 94.46^\circ$ and 156.77° in cobalt, using the value of $G = 84.42 \text{ GPa}$ determined from the Voigt model. The dipole arm and strength for the two misorientations are $\bar{a}_d = 0.21, 0.16$ and $\omega = 38.6^\circ, 34.3^\circ$ respectively. Each figure shows the stress contours in the region $-2.5 \leq X \leq 2.5$ and

Table 4.2.

The elastic constants and lattice parameters of cobalt and titanium crystals. Data for the elastic constants of cobalt and titanium are from Hirth and Lothe (1982) and Fundenberger et al. (1997), respectively. The lattice parameters are from Mehl and Papaconstantopoulos (1996).

	Cobalt	Titanium
C'_{11} (GPa)	358.5	180.7
C'_{33} (GPa)	307	162
C'_{12} (GPa)	103	69
C'_{23} (GPa)	165	92
C'_{66} (GPa)	75.3	46.7
c (nm)	0.407	0.468
a (nm)	0.251	0.295
c/a	1.622	1.586

$-0.5 \leq Y \leq 0.5$, i.e., over one period of the dipole wall in the Y -direction. The stress components determined by the bicrystal model and the homogeneous isotropic model (with the Voigt elastic constants) are also compared in each figure. The homogeneous isotropic model results determined from the Reuss or the Voigt elastic constants do not differ significantly, given the small elastic anisotropy of the cobalt crystal ($C'_{11} / C'_{33} = 1.168$, see Table 4.2).

The bicrystal model results (upper plots of Figs. 4.8-4.10) show that all stress components are continuous across the interface $X = 0$. The interface boundary condition requires the continuity of $\tilde{\sigma}_x$ and $\tilde{\sigma}_{xy}$, but not $\tilde{\sigma}_y$. However, $\tilde{\sigma}_y$ is

Fig. 4.8. Dependence of $\tilde{\sigma}_x = \sigma_x / G$ of the periodic interfacial disclination dipole array on the misorientation of a cobalt bicrystal boundary. The upper and lower plots show the bicrystal and homogeneous isotropic (Voigt) model predictions, respectively. Note the significant distortion of contours in the bicrystal and the complex dependence of the bicrystal stress field on the misorientation.

continuous across the interface since for symmetric boundaries its distribution must be symmetric about the interface. Figures 4.8-4.10 also show that, according to the bicrystal model, both $\tilde{\sigma}_x$ and $\tilde{\sigma}_y$ are symmetric, whereas $\tilde{\sigma}_{xy}$ is antisymmetric, about the interface. The symmetry or antisymmetry is the only symmetry element present in the stress field of symmetrical boundaries.

By examining the differences in the stress distribution of the dipole wall in the bicrystal for $\Theta = 94.46^\circ$ and 156.77° as well as other misorientations, it can be concluded that the stress distribution depends strongly on the details of the GB structure.

Fig. 4.9. Dependence of $\tilde{\sigma}_y = \sigma_y / G$ of the periodic interfacial disclination dipole array on the misorientation of a cobalt bicrystal boundary. Note the continuity of contours across the boundary and the insensitivity of the stress field of the homogeneous crystal to the misorientation.

Suffice to mention here only two points. Firstly, large differences in the position and shape of the zero stress contours occur as Θ changes from 94.46° to 156.77° . The zero-stress contours are distinguished by strong waviness or distortion at $\Theta = 94.46^\circ$ and by relatively gentle curves at $\Theta = 156.77^\circ$ (see Figs. 4.8-4.10). Also, the zero stress contours tend to align in the direction of the boundary as Θ approaches 90° from 0° or 180° . This implies that the non-zero stress contours become more tightly packed around the boundary, i.e., the stress field of high-angle GBs is more localized than that of low-angle boundaries. Secondly, the direction of the shear stress in the bicrystal may change as the misorientation changes, as can be observed in the region around the dipole in the

Fig. 4.10. Dependence of $\tilde{\sigma}_{xy} = \sigma_{xy}/G$ of the periodic interfacial disclination dipole array on the misorientation of a cobalt bicrystal boundary. Note the change in the shear stress direction in the central region of the dipole due to the change in misorientation.

upper plots of Fig. 4.10. This result reflects the effect of elastic anisotropy on the shear stress distribution and is also evident in a homogeneous anisotropic crystal as the c -axis orientation changes. The strong dependence of the stress distribution on misorientation is reasonable as different misorientations give rise to very different GB structures on the atomic scale and consequently different disclination parameters (strength, arm length and period) on the continuum scale.

The homogeneous isotropic model results (lower plots in Figs. 4.8-4.10) are very different from the bicrystal model results. In addition to the symmetry element mentioned above, $\tilde{\sigma}_x$ and $\tilde{\sigma}_y$ are antisymmetric, whereas $\tilde{\sigma}_{xy}$ is symmetric, about

$Y = 0$ in the homogeneous isotropic model. This implies that there is a center of antisymmetry about the origin $(0, 0)$ in the three stress components predicted by the homogeneous isotropic model. The perturbation of the stress distribution caused by anisotropy and inhomogeneity is significant (compare lower and upper plots in the figures), even though the elastic anisotropy of the cobalt crystal is not particularly strong. The following example illustrates the importance of considering inhomogeneity. Figure 4.8 shows that for both misorientations a $\tilde{\sigma}_x = 0$ contour exists on $Y = 0$ according to the homogeneous isotropic model, but $\tilde{\sigma}_x$ is generally non-zero on $Y = 0$ according to the bicrystal model. This means that the interaction between the dipole wall and other defects such as impurities, dislocations and cracks cannot be correctly described using a homogeneous isotropic model. For example, an edge dislocation with Burgers vector (components b_x and b_y) in a stress field would experience x - and y -direction forces $F_x = \sigma_{xy}b_x + \sigma_y b_y$ and $F_y = -\sigma_x b_x - \sigma_{xy}b_y$ according to the Peach-Koehler equations. Thus, an edge dislocation with Burgers vector in the x -direction and situated on the plane $Y = 0$ would not experience a climb force in the y -direction according to the homogeneous isotropic model whereas it would in fact experience a climb force equal to $-\sigma_x b_x$ according to the bicrystal model since σ_x is not always zero on $Y = 0$. Furthermore, only the bicrystal model can capture the dependence of the GB-dislocation interaction on the misorientation, which is expected to be significant since the stress field of the dipole wall depends strongly on misorientation. The lower plots in Figs. 4.8-4.10 show that the homogeneous isotropic model results are quite insensitive to changes in misorientation. An anisotropic but homogeneous model would

Fig. 4.11. Variation of the GB energy with misorientation in cobalt and titanium as calculated by the DSUM. The six favored boundaries with their Miller indices are indicated by the solid arrows at the cusps. Cusps which are less sharp and associated with other short-period boundaries are indicated by the broken arrows. The $(11\bar{2}2)$ boundary demarcates each curve into two parts with average energy in the first part roughly twice that in the second part. The GB energy in cobalt is about twice that in titanium for most misorientations.

similarly fail to predict the stress distribution correctly since the image stress field arising from the inhomogeneity is not taken into account.

Figure 4.11 plots the GB energy γ_{gb} versus the misorientation θ for $[1\bar{1}00]$ symmetrical tilt boundaries in cobalt and titanium. Here, $l_0/h = 0.02$ and the bicrystal model is used. It can be seen that rather sharp cusps appear at the misorientations of the delimiting boundaries $(11\bar{2}6)$, $(11\bar{2}4)$, $(11\bar{2}2)$ and $(11\bar{2}1)$ with the GB period vectors of H_B , H_C , H_D and H_E , respectively. These cusps represent local minima. Also, cusps

which are less sharp are observed at the misorientations corresponding to $(11\bar{2}8)$, $(11\bar{2}5)$, $(11\bar{2}3)$, $(33\bar{6}4)$ and $(33\bar{6}2)$. The structural units of these GBs have short periods consisting of one P-type and one Q-type unit, i.e., $H = H_A + H_B$, $H_B + H_C$, $H_C + H_D$, $H_D + H_E$ and $H_E + H_F$ respectively for the five GBs mentioned above. The solid curves drawn through the data smooth out the cusps, making them appear less sharp. These cusps, especially those on the curve for titanium, are discernibly local minima. It was pointed out by Nazarov et al. (2000b) for cubic materials that the cusps correspond to GBs with relatively short periods, e.g., structural units stacking of the type PQ, PPQ, PQQ, etc., and that the energy curve actually consists of an infinite number of cusps most of which are too small to be detected. These cusps appear because the energy of the disclination dipole wall increases when the misorientation of a short-period GB changes slightly. They have been predicted by atomistic simulations and confirmed by experimental data for cubic materials such as aluminum and copper (Hasson and Goux, 1971; Nazarov et al., 2000b). Figure 4.11 thus predicts that cusps related to short-period GBs are also present in the energy curves of hexagonal materials.

Another salient feature of the energy curves in Fig. 4.11 is that both cobalt and titanium show a high-energy region ($0^\circ < \theta < 116^\circ$) and a low-energy region ($116^\circ < \theta < 180^\circ$). These two regions are delimited by the (0001) , $(11\bar{2}2)$ and $(11\bar{2}0)$ GBs, i.e. the special boundaries A, D and F. The average GB energy in the high-energy region is about twice that in the low-energy region. This is quite unlike the energy curves for cubic materials, e.g. for $[001]$ tilt boundaries there exists only one such region for the entire misorientation range.

Figure 4.11 shows that local energy maxima exist between the cusps. For cobalt, the global maximum of about 1.5 J m^{-2} occurs at $\theta \approx 22.9^\circ$. For titanium, the corresponding values are about 0.9 J m^{-2} and 22.4° . The corresponding GB plane is $(11\bar{2}16)$. The global maxima of about 1.5 and 0.9 J m^{-2} for $[1\bar{1}00]$ symmetrical tilt boundaries in cobalt and titanium respectively can be compared to the maxima of about 1.5 and 1.2 J m^{-2} for $[001]$ and $[111]$ symmetrical tilt boundaries in copper, and to about 5 and 4 J m^{-2} for $[001]$ and $[011]$ symmetrical tilt boundaries in diamond, as determined by DSUM and atomistic simulations (Nazarov et al., 2000b).

The energy curves for cobalt and titanium are similar in shape, as shown in Fig. 4.11. However, for most misorientations the GB energy of cobalt is approximately twice that of titanium. The energy curve of cobalt is also more sensitive to the change in misorientation than that of titanium. The reason for the factor-of-two difference between the cobalt and titanium GB energies is not clear, but the elastic strain energy of the dipole wall in cobalt is about twice that in titanium because the elastic constants of cobalt are roughly twice those of titanium as shown in Table 4.2.

Figure 4.12 illustrates the dependence of the energy-misorientation curve of cobalt on the core parameter l_0/h as computed by the bicrystal model. By increasing the value of l_0/h from 0.02 to 0.08 , the bicrystal model predicts slightly smaller GB energies. A larger value of l_0/h implies that less elastic energy is taken to be equivalent to the core energy so that effectively a smaller core energy will result. The actual value of this parameter can be determined via atomistic simulations, as was done for dislocations (Hirth and Lothe 1982).

Fig. 4.12. Dependence of the GB energy-misorientation relation on the core parameter l_0/h , the normalized length of a square region around each disclination. The total strain energy (elastic strain energy and core energy) of the disclination dipole array is determined by integrating the elastic strain energy density field outside this square region, analogous to the determination of the total strain energy of a dislocation.

Figure 4.13 compares the energy-misorientation curves of cobalt as predicted by the bicrystal model and the isotropic Voigt and Reuss models, assuming $l_0/h = 0.02$. The difference is not very significant, reflecting the small elastic anisotropy ratio ($C'_{11}/C'_{33} = 1.168$) of the cobalt crystal. The small elastic anisotropy limits the inhomogeneity, which in this case is determined by the difference in c -axis orientations of the two crystals adjoining the GB. For titanium, the anisotropy ratio is 1.115 (see Table 4.2), and the bicrystal and isotropic homogeneous solutions do not differ greatly either. For zinc, the ratio is 0.379 and the difference in solutions is expected to be more significant. As shown earlier, however, the difference in the stress field predictions of

Fig 4.13. Effect of bicrystal and isotropic homogeneous assumptions on the energy-misorientation curve for cobalt. The bicrystal calculation considers the elastic anisotropy of the crystals and the inhomogeneity across the boundary, whereas the two homogeneous isotropic calculations employ averaged elastic constants as determined by the Voigt and Reuss methods.

the bicrystal and isotropic homogeneous models is very significant even for the small anisotropy ratio of 1.168.

4.5. Conclusions

The DSUM is applied to hexagonal metals for predicting the stress field and energy of $[1\bar{1}00]$ symmetrical tilt GBs. Six boundaries, namely (0001) , $(11\bar{2}6)$, $(11\bar{2}4)$, $(11\bar{2}2)$, $(11\bar{2}1)$ and $(11\bar{2}0)$, are considered as delimiting boundaries. An intermediate boundary with misorientation between those of two delimiting boundaries, say, P and Q, is constructed from the structural units of these delimiting boundaries distributed as

uniformly as possible, e.g., PQ.PQ, PPQ.PPQ, PQQ.PQQ, PQQP.PQPQP. The disclination parameters are deduced from the structural units of the delimiting boundaries. The bicrystal model for the disclination dipole wall explicitly accounts for the intrinsic elastic anisotropy of the hexagonal crystal as well as the dissimilarity of the lattice orientations across the GB. The GB energy is determined as the sum of the strain energy of the disclination dipole wall and the surface energy of the delimiting boundaries.

Numerical investigations using the bicrystal model for cobalt and titanium show that the misorientation strongly influences the stress field of the disclination dipole wall. Severe distortions of the stress contours result from even small inhomogeneity, which is limited by the degree of crystal elastic anisotropy. The dipole stress field of high-angle boundaries tends to be more localized around the boundaries than that of low-angle boundaries. The homogeneous isotropic models fail to predict the significant dependence of the stress field on the misorientation.

The GB energy-misorientation curve, determined from either the bicrystal or the homogeneous isotropic models, displays cusps at the misorientations of short-period boundaries. The cusps generally represent local minima. Local maxima occur between the cusps, with the global maximum of about 1.5 J m^{-2} for cobalt and about 0.9 J m^{-2} for titanium. These maxima occur at $\theta \approx 23^\circ$ corresponding to the $(11\bar{2}16)$ GB. The energy over the whole misorientation range consists of two regions demarcated by $\theta = 116^\circ$ corresponding to the favored boundary $(11\bar{2}2)$, with the average energy in $0^\circ < \theta < 116^\circ$ roughly twice that in $116^\circ < \theta < 180^\circ$. The GB energy of cobalt is about twice that of titanium for most misorientations. The bicrystal and homogeneous

isotropic model predictions of the GB energy are not significantly different, but this conclusion may be specific to hexagonal materials with relatively weak elastic anisotropy.

Chapter 5

Continuum and Atomistic Studies of a Disclinated Crack in a Bicrystalline Nanowire

This Chapter is organized as follows. A continuum model is introduced to describe a double-ended wedge crack due to a negative disclination in a bicrystalline nanowire in Section 5.1. An atomistic model is then proposed to simulate the same crack in Section 5.2. Thereafter, the results obtained via the two models are presented and compared in Section 5.3 and discussed in Section 5.4. Finally, the key findings of the investigation are summarized in Section 5.5.

5.1. Continuum Model

5.1.1. Problem Description and Boundary Conditions

Consider a negative wedge disclination centered in a homogeneous isotropic cylinder of radius R , as illustrated in Fig. 5.1(a). The disclination has the strength ω , its line coincides with the cylinder axis, and the plane strain condition is assumed. Denote the shear modulus and Poisson's ratio of the cylinder material by G and ν , respectively. Rectangular coordinates (x, y) and polar coordinates (r, ϕ) are defined on a circular cross-section of the cylinder, both originating at the disclination line. A crack of length $2l$ with the disclination at its center is assumed for convenience to lie along the x -axis, although for the isotropic material assumption the crack can be along any

radial direction. Two sets of boundary conditions need to be satisfied in this problem. One is that the outer surface of the cylinder is traction-free with the radial and shear stresses being zero at $r = R$, i.e.,

$$\sigma_r(R, \phi) = 0, \quad \sigma_{r\phi}(R, \phi) = 0. \quad (5.1)$$

The other is that the crack surface is traction-free with the normal and shear stresses being zero at the crack location, i.e.,

$$\sigma_y(x, 0) = 0, \quad \sigma_{xy}(x, 0) = 0, \quad (-l \leq x \leq l). \quad (5.2)$$

5.1.2. Solutions by Superposition

To obtain the solutions for the crack, e.g., its stress intensity factor (SIF), the crack in the original problem of Fig. 5.1(a) is modeled by an initially unknown distribution of infinitesimal edge dislocations in Fig. 5.1(b). The transformed problem in Fig. 5.1(b) is further decomposed into the two additive subproblems of Figs. 5.1(c) and 5.1(d), in which the cylinder is subjected to the internal loading of the disclination and that of the distribution of edge dislocations with unknown densities ρ_x and ρ_y (the subscripts x and y represent two Burgers vector components of the edge dislocations), respectively. The fundamental solutions selected for each subproblem, i.e., the stress field of a disclination in a finite cylinder in Subproblem 1 and that of an eccentrically located dislocation in a finite cylinder in Subproblem 2, automatically satisfy Eq. (5.1). In contrast, Eq. (5.2) is satisfied only after the superposition of the two subproblems, which leads to the solutions for ρ_x and ρ_y . Therefore, the solution method is exact in the sense that all the boundary conditions are satisfied properly and any stress

Fig. 5.1. Decomposition of the original problem into Subproblems 1 and 2. (a) Original problem of a double-ended crack (length $2l$) due to a negative disclination (strength ω) at the center of a cylinder (radius R). (b) Modeling the crack by a distribution of edge dislocations with densities ρ_x and ρ_y . (c) Subproblem 1: the cylinder containing the disclination at its center. (d) Subproblem 2: the cylinder containing the distribution of edge dislocations at the original crack location.

distribution due to crack growth is taken into account intrinsically. Stress redistribution is neglected in almost all previous works on disclinated cracks, i.e., the disclination stress field is assumed to be undisturbed by the crack.

In the subproblem of Fig. 5.1(c), the Airy stress function for a wedge disclination lying along the axis of a cylinder has been given by Romanov and Vladimirov (1992) as

$$\chi^{\nabla} = \frac{1}{2} D \omega (x^2 + y^2) \left[\ln \left(\frac{\sqrt{x^2 + y^2}}{R} \right) - \frac{1}{2} \right], \quad (5.3)$$

where

$$D = \frac{G}{2\pi(1-\nu)}. \quad (5.4)$$

The normal and shear stress components on the plane $y = 0$ due to the disclination are then obtained by differentiating Eq. (5.3), i.e.,

$$\sigma_y^{\nabla}(x, 0) = \frac{\partial^2 \chi^{\nabla}}{\partial x^2} \Big|_{y=0} = D \omega \left(1 + \ln \frac{|x|}{R} \right), \quad (5.5)$$

$$\sigma_{xy}^{\nabla}(x, 0) = \frac{\partial^2 \chi^{\nabla}}{\partial x \partial y} \Big|_{y=0} = 0. \quad (5.6)$$

Equation (5.5) shows that $\sigma_y^{\nabla}(x, 0)$ contains a logarithmic singularity at $x = 0$. The absolute value $|x|$ justifies the assumption of a double-ended crack of length $2l$ wedged open by the disclination at the crack center.

In the subproblem of Fig. 5.1(d), the Airy stress functions for a discrete edge dislocation at the eccentric location $(x, y) = (x', 0)$ have been given by Eshelby (1979) as

$$\chi_x^{\perp} = D b_x(x') \left[-y \ln \left(\frac{q_2}{q_1} \right) + \frac{R^2 y (R^2 - x'^2)}{q_1^2 x'^3} \left(x - \frac{R^2 + x'^2}{2x'} \right) \right], \quad (5.7)$$

$$\chi_y^{\perp} = D b_y(x') \left[(x - x') \ln \left(\frac{q_2 R}{q_1 x'} \right) + \frac{1}{2x'} (r^2 - R^2) (R^2 - x'^2) \left(\frac{xx' - R^2}{q_1^2 x'^2} + \frac{1}{R^2} \right) \right], \quad (5.8)$$

where $b_x(x')$ and $b_y(x')$ are the x - and y -components of the Burgers vector of the discrete dislocation respectively, and r , q_1 and q_2 are given by

$$r^2 = x^2 + y^2, \quad q_1^2 = \left(x - \frac{R^2}{x'}\right)^2 + y^2, \quad q_2^2 = (x - x')^2 + y^2. \quad (5.9)$$

The normal and shear stress components on $y = 0$ due to a discrete dislocation are then obtained by differentiating Eqs. (5.7) and (5.8), i.e.,

$$\sigma_y^\perp(x, 0; x') = \frac{\partial^2(\chi_x^\perp + \chi_y^\perp)}{\partial x^2} \Big|_{y=0} = b_y(x') G_y^\perp(x, y; x') \Big|_{y=0}, \quad (5.10)$$

where

$$G_y^\perp(x, y; x') \Big|_{y=0} = D \left[\frac{1}{x - x'} + \frac{-3R^6 x - R^2 x^3 x'^2 + (R^2 + x^2)(3R^4 x' - 2R^2 x'^3 + x x'^4)}{R^2 (R^2 - x x')^3} \right], \quad (5.11)$$

and

$$\sigma_{xy}^\perp(x, 0; x') = \frac{\partial^2(\chi_x^\perp + \chi_y^\perp)}{\partial x \partial y} \Big|_{y=0} = b_x(x') G_{xy}^\perp(x, y; x') \Big|_{y=0}, \quad (5.12)$$

where

$$G_{xy}^\perp(x, y; x') \Big|_{y=0} = D \left[\frac{1}{x - x'} + \frac{2R^4 x' - R^4 x - R^2 x x'^2 - (R^2 - x^2) x'^3}{(R^2 - x x')^3} \right]. \quad (5.13)$$

The above stress components contain a singularity arising from $1/(x - x')$. Note that $b_y(x')$ and $b_x(x')$ are present in $\sigma_y^\perp(x, 0; x')$ and $\sigma_{xy}^\perp(x, 0; x')$ respectively so that the expressions for the two stress components are decoupled. The stress components for a

distribution of dislocations can be obtained by replacing $b_x(x')$ and $b_y(x')$ in Eqs. (5.12) and (5.10) with $\rho_x(x')dx'$ and $\rho_y(x')dx'$ respectively and then taking integration with respect to x' from $x' = -l$ to $x' = l$.

To satisfy Eq. (5.2), the normal and shear stresses at the crack location in the two subproblems are superimposed and set equal to zero, i.e.,

$$\int_{-l}^l \sigma_y^\perp(x, 0; x') dx' + \sigma_y^\nabla(x, 0) = 0, \quad (5.14)$$

$$\int_{-l}^l \sigma_{xy}^\perp(x, 0; x') dx' + \sigma_{xy}^\nabla(x, 0) = 0, \quad (5.15)$$

where $-l \leq x \leq l$. Equations (5.14) and (5.15) are two decoupled singular integral equations with the unknown density functions $\rho_x(x')$ and $\rho_y(x')$. Referring to Eqs. (5.6) and (5.13), we can easily determine that Eq. (5.15) has the solution $\rho_x(x') = 0$. This leaves only $\rho_y(x')$ in Eq. (5.14) unsolved. Substituting Eqs. (5.5) and (5.10) (with $b_y(x')$ replaced by $\rho_y(x')dx'$) into Eq. (5.14) yields

$$D \int_{-l}^l \left(-\frac{1}{x' - x} + \frac{-3R^6 x - R^2 x^3 x'^2 + (R^2 + x^2)(3R^4 x' - 2R^2 x'^3 + x x'^4)}{R^2 (R^2 - x x')^3} \right) \rho_y(x') dx' \\ + D \omega \left(1 + \ln \frac{|x|}{R} \right) = 0, \quad -l \leq x \leq l. \quad (5.16)$$

The symmetry of the crack about the origin implies that the dislocation distribution for modeling the crack should be antisymmetric about the origin, i.e., $\rho_y(x') = -\rho_y(-x')$.

Thus, after some manipulation Eq. (5.16) can be recast into

$$\begin{aligned}
& \int_0^l \frac{\rho_y(x')}{x' - x} dx' + \int_0^l \left(\frac{1}{x' + x} + \frac{3R^6 x + R^2 x^3 x'^2 - (R^2 + x^2)(3R^4 x' - 2R^2 x'^3 + xx'^4)}{R^2(R^2 - xx')^3} \right. \\
& \quad \left. - \frac{3R^6 x + R^2 x^3 x'^2 - (R^2 + x^2)(-3R^4 x' + 2R^2 x'^3 + xx'^4)}{R^2(R^2 + xx')^3} \right) \rho_y(x') dx' \\
& = \omega \left(1 + \ln \frac{x}{R} \right), \quad (0 \leq x \leq l).
\end{aligned} \tag{5.17}$$

Equation (5.17) is a Cauchy singular integral equation, and its right side consists of a logarithmic singularity at $x = 0$. It is expected that the density function $\rho_y(x')$ will have singularities at $x' = 0$ and l which correspond to the disclination location and the crack tip location respectively. To solve this equation, the numerical method of Gerasoulis (1982) is used. His method has been successfully adapted to the solutions of similar singular integral equations (Lo, 1978; He and Hutchinson, 1989; Wu and Zhou, 1996; Niu and Wu, 1997). We can summarize the numerical method as follows. First, Eq. (5.17) is normalized to the interval $[-1, 1]$ by writing

$$x' = \frac{l}{2}(1+t), \quad x = \frac{l}{2}(1+s), \tag{5.18}$$

where $-1 \leq s, t \leq 1$. Then, the dislocation density $\rho_y(t)$ is written as the product of a weight function $w(t)$ and an unknown function $k_y(t)$, i.e.,

$$\rho_y(t) = w(t)k_y(t), \tag{5.19}$$

where

$$w(t) = \frac{1}{\sqrt{1-t^2}}. \tag{5.20}$$

Next, the interval $[-1, 1]$ is divided into $2M$ intervals and $k_y(t)$ is approximated by piecewise quadratic polynomials with $2M + 1$ unknowns at the boundary points of the $2M$ intervals. The integral equation is then converted into a system of $2M$ linear algebraic equations with the $2M + 1$ unknowns. An additional equation $k_y(-1) = 0$ to ensure solution uniqueness is used (Lo, 1978; He and Hutchinson, 1989). Note that the weight $w(t)$ correctly captures the inverse square root singularity of $\rho_y(t)$ at $t = 1$ ($x' = l$, crack tip position), but it might not correctly capture the singularity at $t = -1$ ($x' = 0$, disclination position). However, as investigated in the two aforementioned works for kinked cracks, the actual order of singularity used in the calculations does not significantly affect the results. The $2M + 1$ equations are solved for $k_y(t)$ at the same number of boundary points, after which the unknown density $\rho_y(t)$ can be determined via the quadratic polynomials.

Once $\rho_y(t)$ and hence $\rho_y(x')$ is known, the stress field in the nanowire containing the disclinated crack, i.e., that shown in Fig. 5.1(a), can be determined. For instance, the stress component $\sigma_y(x, y)$ is the sum of the corresponding components in the subproblems of Fig. 5.1(c) and Fig. 5.1(d):

$$\sigma_y(x, y) = \sigma_y^\nabla(x, y) + \int_{-l}^l G_y^\perp(x, y; x') \rho_y(x') dx', \quad (5.21)$$

where $\sigma_y^\nabla(x, y)$ and $G_y^\perp(x, y; x')$ are determined from the second order derivatives of the Airy stress functions, as were similarly done for the special case of $y = 0$ in Eqs. (5.5) and (5.10).

The disclinated crack is a mode I crack since $\sigma_{xy}^{\nabla}(x, 0) = 0$ according to Eq. (5.6).

The mode I SIF of the crack can be determined from the following equation as x approaches the crack tip from outside the crack, i.e.,

$$K_I = \lim_{x \rightarrow l} [\sqrt{2\pi(x-l)} \sigma_y(x, 0)], \quad (5.22)$$

where $\sigma_y(x, 0)$ is the total stress component obtained by superposition. This stress takes exactly the same form as the left side of Eq. (5.16). Only the singular term of the stress at $x = l$, however, is of relevance in Eq. (5.22). From Eq. (5.16), the relevant singular term is:

$$\sigma_y^{\perp}(x, 0) = D \int_{-l}^l \frac{\rho_y(x')}{x-x'} dx'. \quad (5.23)$$

The combination of Eqs. (5.22) and (5.23) leads to the following expression for K_I :

$$\begin{aligned} K_I &= \lim_{x \rightarrow l} \left[D \sqrt{2\pi(x-l)} \int_{-l}^l \frac{\rho_y(x')}{x-x'} dx' \right] \\ &= \lim_{x \rightarrow l} \left[D \sqrt{2\pi(x-l)} \int_0^l \left(\frac{\rho_y(x')}{x-x'} \right) dx' + D \sqrt{2\pi(x-l)} \int_{-l}^0 \left(\frac{\rho_y(x')}{x-x'} \right) dx' \right], \\ &= \lim_{x \rightarrow l} \left[D \sqrt{2\pi(x-l)} \int_0^l \frac{\rho_y(x')}{x-x'} dx' \right], \end{aligned} \quad (5.24)$$

where the second term in the second line drops out because the term $1/(x-x')$ is never singular as $x \rightarrow l$ and $-l \leq x' \leq 0$. Converting to dimensionless variables using Eq. (5.18) and substituting from Eqs. (5.19) and (5.20), Eq. (5.24) can be rewritten as

$$\begin{aligned}
K_I &= \lim_{s \rightarrow 1} \left[D \sqrt{\pi l (s-1)} \int_{-1}^1 \frac{k_y(t)}{(s-t)\sqrt{1-t^2}} dt \right] \\
&= \lim_{s \rightarrow 1} \left[D \sqrt{\pi l (s-1)} \oint \frac{k_y(t)}{2(s-t)\sqrt{1-t^2}} d\Gamma \right]
\end{aligned} \tag{5.25}$$

In Eq. (5.25), Γ is a clockwise contour around the crack and the contour integral can be evaluated (Muskhelishvili, 1953). Omitting the details of this contour integration, the final result after taking the limit is

$$K_I = D \left(\frac{\pi^3 l}{2} \right)^{\frac{1}{2}} k_y(1). \tag{5.26}$$

Furthermore, the opening displacement $[u_y(x, 0)] = u_y(x, 0^+) - u_y(x, 0^-)$ in the y -direction of the mode I crack can be obtained directly from the dislocation density $\rho_y(x')$:

$$[u_y(x, 0)] = - \int_l^x \rho_y(x') dx', \quad (-l \leq x \leq l). \tag{5.27}$$

5.2. Atomistic Model

5.2.1. Atomistic Simulation Technique - Molecular Statics

The formation and growth of cracks have been extensively studied by atomistic computer simulations (Shastry and Farkas, 1996; Cleri et al., 1998, 1999; Farkas, 2000), in which either molecular statics or molecular dynamics has been used.

Molecular statics, which is used in the present simulation, is a technique designed to determine the lowest-energy configuration of a given system containing a defect. In the initial configuration of simulation, a three-dimensional simulation cell is constructed

and the initial positions of the atoms defined by type and mass within the cell are specified according to the crystallographic properties of the material studied in the system. Meanwhile, the atomic interaction within the cell is described by an interaction potential and a cut-off distance, beyond which atoms are no longer considered to interact, is provided. The boundary conditions are also applied to the cell. During molecular static relaxation, the presence of a defect induces forces on the atoms, which are allowed to move in order to relax the system to a minimum energy configuration. The molecular statics relaxation is carried out at zero absolute temperature and therefore no vibrations due to thermal activation are taken into account. In order to take temperature into consideration, molecular dynamics has to be used.

5.2.2. Atomistic Simulation Configurations

To construct the initial configurations of the atomistic simulations, cylinders containing a negative wedge disclination are first prepared. A partial wedge disclination inserted into a perfect crystal delineates a lattice plane and a tilt GB (Romanov and Vladimirov, 1992), which can however have significantly different cleavage energies. To avoid this large difference, the disclination is inserted into a bicrystalline cylinder consisting of two FCC crystals with common $[001]$ axis initially delimited by a symmetric tilt GB with the reciprocal coincidence site density $\Sigma = 5$, plane $(\bar{1}30)$ and misorientation angle $\theta = 53.13^\circ$ (Fig. 5.2(a)). The tilt axis of the boundary is parallel to the cylinder axis. In this case, the insertion of a disclination will delineate two $[001]$ tilt GBs: $\Sigma = 5$ $\theta_1 = 53.13^\circ$ on the right-hand side and a boundary with misorientation angle $\theta_2 < \theta_1$ on the left-hand side. To construct this system following the definition of

Fig. 5.2. Schematic of constructing an initial configuration in the atomistic model. (a) An FCC bicrystal with [001] 53.13° tilt GB. (b) Two FCC bicrystals with [001] 36.87° (left) and [001] 53.13° (right) tilt GBs, respectively. (c) A bicrystalline nanowire containing a 16.26° wedge disclination, constructed from the two bicrystals in (b), along the central axis. Note that black and gray solid circles distinguish atoms lying on two successive (001) lattice planes.

disclinations, one should make a cut along one (say, left) side of the initial bicrystal and open a wedge with the angle $\omega = \Theta_1 - \Theta_2$ by an appropriate elastic deformation of the cylinder. This wedge should then be filled in by material through the adding of atoms whose arrangement continues the deformed lattice of the initial system on both sides of the cut (i.e. initial GB plane). After this filling, along the cut plane one will obtain a GB with the misorientation angle $\Theta_2 = \Theta_1 - \omega$. The atomic structure of this GB in general can be far from well-relaxed, and very much different from the structure of the GB $\Sigma = 5 (\bar{1}30)$ on the right-hand side of the cylinder. To avoid this non-equilibrium structure of the GB, the disclination is introduced in the following simpler, but essentially equivalent way.

First, two [001] bicrystals with misorientation angles θ_1 and θ_2 are prepared by separate simulations using the same interatomic potential. These are cut along the {110} lattice planes as shown in Fig. 5.2(b) and the resulting wedges are brought into contact at a common origin. The {110} lattice planes of the two bicrystals will then be misoriented by the angle $\omega/2 = (\theta_1 - \theta_2)/2$ and the lattices will overlap. To remove this overlap and match the lattice planes and thus finish the construction of the disclination, each atom of the system is displaced by a vector calculated on the basis of isotropic elasticity theory for wedge disclinations (de Wit, 1972). Eventually one obtains a disclinated cylinder shown in Fig. 5.2(c). Varying the misorientation angle θ_2 of the left bicrystal, one can vary the strength ω of the disclination.

In the particular case presented in Fig. 5.2 the second GB is of the type $\Sigma = 5$ (210) $\theta_2 = 36.87^\circ$. The GBs $\Sigma = 5$ ($\bar{1}20$) and ($\bar{1}30$) are two of the four favored GBs for the tilt axis [001], each of which is composed of a contiguous sequence of one type of structural units. In Fig. 5.2 the structural units of these boundaries are outlined. The other two favored GBs for this axis are the crystal lattice planes ($\bar{1}10$) ($\theta = 0^\circ$) and (010) ($\theta = 90^\circ$) (Sutton and Vitek, 1983a; Wang et al., 1984; Sutton and Balluffi, 1995). The structural units of the boundaries ($\bar{1}10$), ($\bar{1}20$), ($\bar{1}30$), and (010) are denoted by the letters A, B, C, and D, respectively (Bachurin et al., 2003). The atomic structures of all other GBs with this axis are described in the structural unit model (Sutton and Vitek, 1983a; Sutton and Balluffi, 1995). According to this model, each GB whose misorientation angle is intermediate between the misorientation angles of two adjacent favored GBs (for example, B and C), consists of the structural units of these

Table 5.1
Geometrical characteristics of the modeled GBs and disclinations

No.	Structural Unit Sequence	n/m	Θ , deg	ω , deg	b , Å
First GB					
C		1/2	53.13	0	N.A.
Second GB					
1	BBC	2/5	43.60	9.53	0.32
2	BBBCBBCBBCBBC. BBBCBBCBBCBBC	17/43	43.14	9.99	0.02
3	BBBCBBC. BBBCBBC	9/23	42.74	10.39	0.14
4	BBBC. BBBC	5/13	42.08	11.06	0.19
6	(3B)C(3B)C(4B)C	8/21	41.71	11.42	0.03
7	(3B)C(4B)C. (3B)C(4B)C	11/29	41.54	11.59	0.05
8	BBBBBC	3/8	41.11	12.02	0.10
9	(6B)C	4/11	39.97	13.16	0.01
10	(10B)C	6/17	38.88	14.25	0.04
11	B.B	1/3	36.87	16.26	0.55
12	A(10B)	5/16	34.71	18.42	-0.02
13	A(3B).A(3B)	3/11	30.51	22.61	-0.07

The letters A, B, and C denote the structural units of the GBs $\Sigma = 0/0^\circ$, $\Sigma = 5/36.87^\circ$, and $\Sigma = 5/53.13^\circ$, which are favored boundaries for the tilt axis [001] (Bachurin et al., 2003). n and m are two integers determining the geometry of the boundaries; the misorientation angle is defined as $\Theta = 2 \arctan(n/m)$. Minimum possible value of the net dislocation Burgers vector is also presented.

boundaries taken in a certain proportion and arrangement. The structural unit sequences per GB period characteristic of the GBs chosen to construct disclinations with varying strengths are presented in Table 5.1. The geometry of each GB in this table is characterized by two integers m and n the meaning of which is clear from Fig. 5.3, in which the left GB is a symmetric tilt boundary characterized by $m = 13$ and $n = 5$. The period vector of the boundary can be represented through the crystallographic vectors of

Fig. 5.3. Detailed schematic of the construction of a junction disclination from two bicrystals. The left GB is a $\Sigma = 97$ ($\Theta = 42.08^\circ$) GB with parameters $m = 13$ and $n = 5$. The left half-period of this GB is shown as decomposed into structural units (indicated by closed polygons) in the BBBC stacking, of which atoms α , β , ξ , and ζ occupy the possible positions for locating a disclination line. When two bicrystals are brought into contact to form the disclination, the open circles of the left bicrystal are replaced by the gray atoms of the right bicrystal. The junction line will coincide with the crossed chain of atoms.

one of the grains as $\mathbf{H} = m\mathbf{u}_1 + n\mathbf{u}_2$, where $\mathbf{u}_1 = (a_0/2)[110]$ and $\mathbf{u}_2 = (a_0/2)[1\bar{1}0]$ with a_0 denoting the lattice parameter. The reciprocal coincidence site density of the boundary is calculated as $\Sigma = (m^2 + n^2)$ if $m^2 + n^2$ is odd, and $\Sigma = (m^2 + n^2)/2$ if $m^2 + n^2$ is even. In this case, $\Sigma = 97$, and the misorientation angle is calculated as $\Theta = 2\arctan(n/m) = 42.08^\circ$. The right half-period of the boundary is represented in a non-relaxed geometrical model, whereas the left one in the structural unit model. The structure described in the structural unit model is obtained from the geometrical one by combining each pair of atoms which are too close to each other near the GB plane into one atom (these pairs are enclosed by ellipses in Fig. 5.3) and subsequent atomic

relaxation. In the structural unit model this GB is represented by the sequence BBBC.BBBC. The dot in this sequence means that the period of the boundary consists of two half-periods with the same stacking of units which are displaced with respect to each other by $a_0/2$ along the tilt axis [001]. Such boundaries contain two coinciding atoms in one period in the geometrical model and are called centered GBs (Sutton and Vitek, 1983a). The boundaries with one coinciding atom per period are called non-centered GBs. Sutton and Vitek (1983a) showed that [001] tilt GBs were centered, if both integers m and n characterizing their geometry were odd. If one of these numbers is even and the other is odd, the GB is non-centered.

When bringing the two bicrystals into contact, one should bear in mind that in general they have different volume expansions. The volume expansion e of a GB is defined as the difference between the volumes of a bicrystal containing the boundary and an ideal crystal, both having the same number of atoms, per unit area of the boundary (Sutton and Balluffi, 1995). In terms of atomistic simulations, e is equal to a relative rigid-body shift of adjoining crystals in the direction normal to the GB plane during relaxation from an initial structure constructed by the use of the geometrical coincidence site lattice model. The difference of volume expansions will result in an edge dislocation with a Burgers vector normal to the GB plane that shares a line with the disclination. In order to study the effects caused purely by disclinations, the Burgers vector of this dislocation must be set to a minimum value. This can be done on the basis of the concept of geometrically necessary junction dislocations recently introduced for triple junctions by Nazarov et al. (2003).

This concept as applied to the junction of two boundaries under consideration is illustrated also in Fig. 5.3, which shows the construction of a disclination with the strength $\omega = 11.06^\circ$. As the right half-period of the left GB is not decomposed into structural units, one can see that atoms on different $\{110\}$ planes, two of which are marked by broken lines, are differently dislocated from the GB plane. The junction can be located at a line crossing an atom of any of the types denoted by the Greek letters α , β , ξ and ζ . In Fig. 5.3 it will be located at a ζ -type position. When welding the two bicrystals, atoms on the surface of the left bicrystal depicted by open circles must be superposed with gray atoms of the right bicrystal and deleted (in fact, these circles illustrate empty sites). As one can see from the figure, this will involve not only a rotation corresponding to the disclination but also a translation normal to the GB plane to a distant Δb equal to the distance between the two closely spaced atoms on the edge of the left bicrystal. This translation forms a geometrically necessary dislocation whose Burgers vector magnitude Δb oscillates with the position of the junction. For a junction located at an α -type position $\Delta b = 0$. In addition, volume expansions of both bicrystals will occur during relaxation as indicated by double arrows in the figure. Therefore, the net Burgers vector magnitude of the junction disclination will be equal to $b = \Delta b + e_2 - e_1$. Varying Δb this Burgers vector can be made as close to zero as possible.

Table 5.1 summarizes the characteristics of GBs used to construct disclinations and the strength values of the resulting disclinations, which are used for simulations in the present work. For convenience, the negative signs for the disclination strengths are

dropped here and elsewhere. The minimum Burgers vector magnitudes of the accompanying dislocations are also presented in the table.

Disclinations constructed by the proposed method can be considered as junction disclinations, since they form a junction of two GBs having different misorientation angles. Elastically, they are equivalent to disclinations introduced either in a perfect crystal or in a tricrystal or any other aggregate provided that the properties of the crystals are isotropic. On the atomic level, they will be similar to triple junction disclinations. Therefore, the results obtained in the present work can be extended to predict some properties of triple junction disclinations.

In the simulations, disclinations are inserted into cylinders with an initial radius of $R = 25 \text{ nm}$. The systems constructed contain about 2.6×10^5 atoms. They serve as ready initial configurations for one series of the simulations, in which the behavior of growing cracks is studied. In the other series of simulations, initial cracks are inserted into the disclinated cylinder. The crack is opened by a simple construction of an approximate displacement field for atoms in the region $|x| < l_s$, $|y| < y_s \approx l_s$ such that there are no too closely spaced atoms. This allows us to avoid instabilities at the start of simulations. For small values of the disclination strength smaller initial cracks are inserted and they have the shape of a double-ended wedge of half-length l_s . For large values of the disclination strength long elliptic cracks are inserted with the long half-axis length l_s . In all cases l_s is chosen to be slightly larger than the crack half-length predicted by the continuum calculations for given values of ω . These structures with initial cracks are designed to study the behavior of closing cracks.

Starting from the initial configurations described above, the structures of disclinated cylinders are simulated by molecular statics, i.e., by energy relaxation at zero absolute temperature. Interatomic forces are described by the embedded-atom method (Foiles et al., 1986). A potential of this method for Ni is used. It is fitted to the lattice period $a_0 = 3.52 \text{ \AA}$, and the elastic constants $C_{11} = 233 \text{ GPa}$, $C_{12} = 154 \text{ GPa}$, and $C_{44} = 128 \text{ GPa}$. The cut-off distance of the original potential is equal to $r_c = 4.8 \text{ \AA}$. The above values of the elastic constants are also used to calculate Voigt averages for the shear modulus and Poisson ratio: $G = 92.6 \text{ GPa}$ and $\nu = 0.281$. These values are used to calculate the crack characteristics in the continuum mechanics approach.

Relaxation is performed by the code XMD - Molecular Dynamics for Metals and Ceramics (2005) authored by J. Rifkin at the University of Connecticut. This method adds some distance to the cut-off distance r_c , so that $r_c = 5.8 \text{ \AA}$. Due to this, the minimum simulation cell size along the $[001]$ direction compatible with the minimum image convention (Allen and Tildesley, 1987) is equal to $H_z = 4a_0 = 14.08 \text{ \AA} > 2r_c$. Fixed periodic boundary conditions are applied in this direction, since we consider the disclination under the plane-strain condition. In the other two directions the system has finite sizes, i.e., the cylinder has a free lateral surface.

5.3. Results

5.3.1. Numerical Estimates by Continuum Model

The SIFs are calculated for a disclinated crack in a bicrystalline cylinder with $R = 25 \text{ nm}$. The GB cleavage energy $2\gamma_f$ is calculated for the two boundaries

Fig. 5.4. Variation of the model I SIF with the normalized half crack length l/R for different disclination strengths ω . The nanowire radius is $R = 25$ nm. The critical disclination strength for crack formation is $\omega = 11.56^\circ$, estimated from the curve tangential to the straight line $K_{IC} = 0.756 \text{ MPa m}^{1/2}$. For $\omega > 11.56^\circ$, the K_{IC} line intersects the curves at two locations, which correspond to two equilibrium crack lengths.

$\Sigma = 5 (\bar{1}20)$ and $(\bar{1}30)$ by the atomistic method described in Section 5.2. For both boundaries the value $2\gamma_f = 2.22 \text{ J m}^{-2}$ is found. This value is used for the estimate of the critical SIF: $K_{IC} = \sqrt{4\gamma_f G / (1-\nu)} = 0.756 \text{ MPa m}^{1/2}$. Figure 5.4 plots the dependence of the SIF on the normalized half-crack length l/R for some of values of ω shown in Table 5.1.

Analyzing Fig. 5.4 one can come to the following conclusions. For $\omega < 11.56^\circ$, the SIFs are less than the critical SIF for all crack lengths. This means that below the value

Fig. 5.5. Dependence of the critical disclination strength for crack formation on the nanowire radius.

$\omega_c \approx 11.6^\circ$, referred to as the critical disclination strength, no crack can exist in the cylinder of the given radius. When $\omega > \omega_c$ there are two values of the equilibrium crack length. The shorter crack is unstable, while the longer crack is stable. With increasing disclination strength the unstable crack length decreases, while the stable crack length increases.

The critical disclination strength is a physical characteristic, which is important for the failure prediction of materials containing disclinations. This characteristic depends on the screening radius of the long-range stresses of the defect (in this case, the radius of the cylinder). This dependence is illustrated in Fig. 5.5, which shows a linear relationship in log-log scale with a slope of -0.5 . It can be interpolated with good accuracy by the relationship

$$\log \omega_c = \log 55.7 - 0.5 \log R, \quad \text{or} \quad \omega_c \approx \frac{55.7}{\sqrt{R}}, \quad (5.28)$$

where R is substituted in nm and ω_c is in degrees. As one can see from this relationship, the critical strength of disclination slowly decreases with the increasing radius of the cylinder.

5.3.2. Results of Atomistic Simulations

The simulations show that small-strength disclinations have a stable structure with a non-broken core, which does not differ significantly from the initial structure. To compare the atomistic model with an elastic continuum model of the disclination, maps of the normal stress $\sigma_y(x, y)$ and hydrostatics pressure $\sum_{i=1}^3 \sigma_{ii}(x, y)/3$ are calculated using both methods for a disclination with the strength $\omega = 11.06^\circ$ accompanied by a $0.19 \text{ \AA}$ edge dislocation (Figs. 5.6 (a) to (d)). In the atomistic model the product of the stress at a given atomic site with the local atomic volume at this site is calculated (Vitek and Egami, 1987). The stress is determined from this product by simply dividing it by the atomic volume of the ideal Ni lattice, $V_a = 10.9 \text{ \AA}^3$. Thus, atomic level stresses are calculated approximately. Comparing the stress maps, one can make two important conclusions. First, there is a significant influence of the anisotropy on the stress distribution. Second, stress values in the far-field compare well, but near the disclination line stresses in the atomistic model increase more slowly than those in the elastic one.

When the strength of the disclination increases, a greater disorder is observed in its core. At a certain value of the strength the disclination is no longer stable: it opens a crack along the GBs on both of its sides. With a further increase of the disclination

Fig. 5.6. Normal stress σ_y and hydrostatic stress $\sum_{i=1}^3 \sigma_{ii}(x,y)/3$ maps of a nanowire containing an 11.06° wedge disclination and a $0.19 \text{ \AA}$ edge dislocation. The results in (a) and (c) are calculated by the continuum model, while those in (b) and (d) by the atomistic model. The nanowire has a radius of 25 nm, but the maps only represent the inner part of the nanowire with a radius of 15 nm. The stress scale in the order of increasing intensity is: < 0 , $0 - 1$, $1 - 2.5$, $2.5 - 5$, $5 - 7$, $7 - 10$, ≥ 10 GPa.

strength the length of the crack also increases. Figure 5.7 shows the sequence of relaxed structures obtained with a crack-free initial structure. The critical disclination strength ω_c , at which the disclination initiates a crack, cannot be exactly determined from the

Fig. 5.7. Atomic structures near a negative wedge disclination with the strength equal to (a) 9.99° , (b) 10.39° , (c) 11.06° , (d) 13.16° , and (e) 22.61° obtained by relaxation from initial structures containing no cracks. Atoms on all (001) planes are represented by black circles. The studied nanowire has a radius of 25 nm and its center coincides with the center of each figure.

atomistic computations. For $\omega = 9.99^\circ$ one sees a very small crack, while for $\omega = 10.39^\circ$ no definite crack is observed, and at $\omega = 11.06^\circ$ a crack is open again. This non-monotonic behavior is most probably due to an interplay between the disclination strain energy release and the GB cleavage energy. The latter depends on the GB period. Generally, a shorter period GB has a lower energy and correspondingly higher cleavage energy. The left GB corresponding to $\omega = 9.99^\circ$ has a longer period than that

corresponding to $\omega = 10.39^\circ$ and hence a smaller GB cleavage energy (compare GB periods $h = a_0 \sqrt{(n^2 + m^2)}/2$ and the stacking of structural units for boundaries No.2 and No. 3 in Table 5.1). At $\omega > 11.06^\circ$ there are no stable disclinations: cracks will always nucleate. Consequently, the approximate value for the critical disclination strength at $R = 25$ nm obtained from the above data is $\omega_c \approx 11.1^\circ$.

The cracks illustrated in Fig. 5.7 correspond to the stable cracks studied in Section 5.1. In qualitative agreement with the results of the continuum model, the equilibrium length of these cracks increases with the strength of the disclination. However, the crack sizes determined from the atomistic simulations are nearly twice less than those predicted by the continuum approach for the same strength values (Fig. 5.4). Analysis of the atomic structures near cracks shows that the cracks do not open in a purely brittle matter. At the disclination strength equal to and slightly above ω_c there is significant atomic disorder near the crack tips (Figs. 5.7(a)-(c)). At larger values of the disclination strength one observes the nucleation of a small crack ahead of the main crack (see the left side of Fig. 5.7(d)). Such a behavior has been observed earlier by Farkas (2000) in the simulations of crack propagation under load in a NiAl ordered alloy. At even larger disclination strength there is a significant relaxation of the disclination stress field by the emission of dislocations from the crack. For example, these dislocations are seen as black spots in Fig. 5.7(e) where a crack grown from the $\omega = 22.61^\circ$ disclination is illustrated. The dislocation seen on the upper part of Fig. 5.7(e) is visualized via a magnified view shown in Fig. 5.8. A further analysis shows that the dislocation has the Burgers vector $\mathbf{b} = (a_0/2)[0\bar{1}\bar{1}]$, which has a projection equal to $a_0/2$ on the (001)

Fig. 5.8. Magnified view of Fig. 5.7 (e), showing the emission of a dislocation from a disclinated crack during atomistic simulations.

plane. Corresponding (100) extra half-planes are easily detected in the figure for each dislocation. It should be remarked that disclination splitting, disclination migration and disclination core amorphization are the other possible channels for energy relaxation in disclinated nanowires (Mikhailin and Romanov, 1986; Zhigilev et al., 1988; Gryaznov et al., 1991).

5.3.3. Comparison of Continuum and Atomistic Model Results

In general, all cracks have the shape of a double-ended wedge as predicted by the continuum analysis. However, in many cases the cracks predicted by the atomistic method have asymmetric shapes: it usually propagates a longer distance along one of the GBs than along the other, although the GB cleavage energies calculated by a

Fig. 5.9. Dependence of the stable crack length on the disclination strength as calculated by the continuum model (open squares) and the atomistic model (crosses). The studied nanowire has a radius of 25 nm.

simulation of these GBs have very similar values: $2\gamma_f = 2.22 \text{ J m}^{-2}$ for $\Sigma = 5 / 53.1^\circ$ and $2\gamma_f = 2.23 \text{ J m}^{-2}$ for $\Sigma = 5 / 36.89^\circ$. In all these cases dislocation emission is observed mainly in the direction of the short wing of the crack. This indicates a significant trapping effect of the dislocation emission on the crack growth.

In order to exclude the dislocation emission, simulations with a starting structure containing an initial crack are also carried out for the same values of the disclination strength as described in Section 5.2. In this case the tips of equilibrium cracks always have an ordered atomic structure. The results of these simulations are presented in Fig. 5.9, along with the data of continuum mechanics calculations. In this case a crack open near a disclination with the strength $\omega = 11.06^\circ$ is closed back. At higher values of

ω the cracks are not closed. This confirms that the critical disclination strength is $\omega_c \approx 11.1^\circ$. As one can see from Fig. 5.9, stable crack lengths calculated by the atomistic simulations are now very similar to the values obtained from the continuum model calculations. At ω slightly larger than ω_c , there is a significant scatter of the values of the crack length calculated by the atomistic simulations around the continuum model predictions. At larger ω the crack length increases monotonically. At $\omega = 13.16^\circ$ the agreement between the two calculations is very close, while at $\omega = 22.61^\circ$ the atomistic model result is approximately 15% less than the continuum model result. The discrepancy increases at large ω when $l \rightarrow R$.

Figure 5.10 plots the distribution of the normal stress σ_{yy} around the disclinated crack of half-length $l = 0.38R$ in a nanowire of radius $R = 25$ nm. The disclination strength is $\omega = 13.16^\circ$. The left and right parts of the figure show the predictions of the continuum and atomistic models, respectively. It can be seen that the overall agreement is satisfactory, given the fact that the continuum model assumes isotropic homogeneous medium while the atomistic model does not. Dependences of the stress on distance from the crack tips and the stress concentrations near the tips as predicted by the two models are also very similar.

Figure 5.11 overlays the crack profile predicted by Eq. (5.27) onto that predicted by the atomistic simulation (with a starter crack) for the case of $\omega = 13.16^\circ$ and $R = 25$ nm. A very good agreement between the predictions of the two approaches is found. The largest crack opening displacement is estimated to be about 1.34 nm, and the half-crack length is $l = 0.38R$. Some disagreement, barely noticeable, arises from the slight asymmetry of the crack predicted by the atomistic model.

Fig. 5.10. Comparison of the maps of the normal stress σ_y , which are calculated from the continuum model (a) and the atomistic model (b) respectively, in a nanowire of radius $R = 25 \text{ nm}$ containing a disclination of strength $\omega = 13.16^\circ$. The nucleated crack due to the disclination reaches a half length of $l = 0.38R$ in both models. The stress scale in the order of increasing intensity is: < 0 , $0-1$, $1-2.5$, $2.5-4$, $4-5.5$, $5.5-9$, $\geq 9 \text{ GPa}$.

Fig. 5.11. Overlay of the crack profile (dotted line) predicted by the continuum model onto that predicted by the atomistic model for the same case presented in Fig. 5.10. The two crack profiles show very good agreement. The largest crack opening displacement is about 1.34 nm .

5.4. Discussions

In the continuum fracture mechanics approach, the stability of a pre-existing crack under the given conditions is a key characteristic to be investigated. For instance, at $K_I = K_{IC}$ a Griffith crack in an infinite medium subjected to a remote load normal to the crack is unstable, while it is stable if subjected to a normal line load acting at the crack surface. In a disclinated cylinder, Wu and Zhou (1996) were the first to show that there are two equilibrium crack lengths, one for an unstable crack and the second for a stable longer crack. The unstable crack length was shown to decrease with an increase of the radius of the cylinder, i.e. the screening distance of the disclination long-range stresses, while the stable crack length depends on the cylinder radius in the opposite manner.

A new result of the present work, fundamentally different from the earlier studies of disclinated cracks, is that there exists a critical disclination strength ω_c below which the disclination is stable with no crack formation while above which a crack can nucleate. This is predicted directly for the first time via atomistic simulations, and supported by the continuum model, which predicts that the critical $K_I = K_{IC}$ condition can never be reached for any crack length for $\omega < \omega_c$, see Fig. 5.4. This introduces a new concept of critical disclination strength in the theory of fracture related to disclinations. The concept is important in that it determines the influence of disclinations on the strength of materials. As shown by the present comparison, continuum mechanics calculations can predict this characteristic with good accuracy even for screening distances for the disclination stress field lying on the nanometer scale ($\omega_c \approx 11.1^\circ$ versus 11.6° by

atomistic calculation for $R = 25 \text{ nm}$). In addition to the results on the applications of the DSUM to the calculations of GB energies (Shenderova et al., 1998; Nazarov et al., 2000), the current work demonstrates that continuum mechanics models can have a good predictive capability on the nanoscale.

For $\omega \geq \omega_c$, the continuum model predicts unstable cracks less than a few nanometers in length. These predictions may be considered unphysical, and inaccurate at best, since the continuum theory is based on the linear elastic assumption without taking the disclination core structure into consideration. In the atomistic simulations starting from initial structures, which are nonequilibrium in nature since their displacement fields are given by linear elastic isotropic theory, the high internal strain within the disclination core would likely initiate a crack that extends unstably until it reaches its longer stable length. Any shorter unstable crack, even if it physically exists, will not be easily captured by the atomistic simulations due to the possibly unstable nature (as suggested by the continuum theory) and the nonequilibrium initial structures. Indeed, the atomistic simulations can only capture the stable cracks, also predicted by the continuum theory. From the current continuum and atomistic investigations, we cannot yet make definite conclusions on the existence of the nanometer-size unstable cracks.

Stable crack length above ω_c has been shown to increase with the disclination strength by both approaches. However, there are discrepancies between the results of continuum mechanics predictions and atomistic simulations. They are particularly large for the first method of simulation starting from structures without an initial crack. These discrepancies warrant several explanations.

First, continuum mechanics calculations are performed in the isotropic theory of linear elasticity. The significance of elastic anisotropy is demonstrated in Fig. 5.6, which shows the different shapes of the stress field calculated via the isotropic theory and via the atomistic theory that is essentially anisotropic. However, the errors due to this factor are not expected to be too large in certain situations. For example, recent studies of brittle fracture in iron have shown that critical loadings for cleavage calculated for different crack orientations from anisotropic theory differ by no more than 10% from each other (Shastry and Farkas, 1996). Therefore, an error of the order of 10% may also be expected when calculating this parameter using isotropic theory. Nevertheless, as one can see from Fig. 5.4, a small error of 10% in estimating the critical SIF can significantly change the equilibrium crack length prediction.

Second, fracture is not purely brittle in the atomistic simulations. In the first method of simulation, the crack tip regions have a disordered atomic structure even when ω is slightly above ω_c (Figs. 5.7 (a)-(c)). A part of the disclination strain energy is spent on this disordering and the crack stops at a length smaller than that predicted for ideal brittle fracture. At higher disclination strength values this disorder is retained. Moreover, some additional features appear. In some cases, a small crack can nucleate ahead of the main crack and separated from it by an un-cleaved region (Fig. 5.7(d)). At even larger strength, a significant part of the disclination strain energy is spent via another channel of relaxation: dislocation emission (Fig. 5.7(e)). This phenomenon is very common for fracture in metals (Cleri et al., 1998, 1999). Furthermore, even if brittle fracture can occur in real Ni bicrystals at certain given conditions, empirical potentials may not make such a prediction. Recent studies in silicon, for example, have shown that most of

the empirical potentials predict ductile fracture, often in contradiction with experiments indicating brittle fracture (Bernstein and Hess, 2003).

The third factor that can significantly influence the equilibrium crack length prediction is lattice trapping, which is caused by a periodicity of the lattice. A crack in the lattice overcomes a periodic energy barrier that can arrest its motion. This is similar to the trapping of lattice dislocations by the Peierls barrier. It is well known that due to the lattice trapping a crack can be stable and cannot advance up to a load $K_I^+ > K_{IC}$, or can be stable and cannot heal down to a load $K_I^- < K_{IC}$ (Pérez and Gumbsch, 2000). Therefore, for a real crack in the discrete lattice there may be a dead zone corresponding to a certain interval with boundaries below and above the equilibrium length predicted by the continuum theory.

The agreements between the predictions of the two approaches are much better, however, when the atomistic simulations are carried out using the second method, i.e., by introducing an initial crack. At intermediate values of the disclination strength $\omega = 14^\circ - 16^\circ$ the difference in predictions is about 15%. At ω slightly above the critical value there is some scatter of the simulation results around the continuum predictions. In this region, most probably, the discreteness of the structure of the left GB, which changes non-monotonically with the misorientation angle, plays an important role. At high ω the cracks have a length comparable to the cylinder diameter. In the atomistic model, there is a significant surface tension that is not taken into account in the mechanics model. This surface tension induces a bulk compression, which is non-uniform due to crack perturbation, that might have a larger influence on the length of longer cracks than on that of shorter ones. This is because a longer crack, being closer to

the cylinder boundary, interacts strongly with the surface tension and also redistributes the stress significantly compared to a shorter crack. This can explain the increase of discrepancies between the results at large disclination strengths.

It is also noteworthy that the atomistic and continuum approaches yield reasonably consistent predictions in the crack opening displacement and the stress distribution in the nanowire containing the disclinated crack. This is in spite of the fact the nanowire is not only elastically anisotropic but also bicrystalline in the atomistic model, while it is purely isotropic and monocrystalline in the continuum model. Continuum solutions for such a finite anisotropic and inhomogeneous medium containing a wedge disclination or even an edge dislocation, are not presently available.

In view of the above discussion, the consistency between the results of atomistic simulations and continuum mechanics calculations can be considered quite satisfactory in terms of the predictions of the critical disclination strength, the stable crack length, the crack opening displacement, and the stress field in the nanowire. The obtained results can be used to estimate the critical strength of disclinations in deformed polycrystalline metals. The screening distance R for the stress fields of the disclinations will be of the order of the grain size d , i.e., one may take $R \approx d$. Thus, by Eq. (5.28) $\omega_c \approx 5.6^\circ$ for $d = 100$ nm and $\omega_c = 3.9^\circ$ for $d = 200$ nm. These estimates are applicable to submicrocrystalline metals prepared by severe plastic deformation (Valiev et al., 2000). In polycrystals, disclinations are coupled into dipoles and quadrupoles. Taking such n -pole configurations into account, the estimated critical strength may further decrease. With this note, the above estimates are indeed consistent with the results of experimental measurements (Motylenko et al., 2004), which show the

existence of disclinations with strengths up to 3° in the nodes of cell-blocks in deformed polycrystals. Further research on the critical behavior of disclinations in multipole configurations is necessary to shed light on this issue.

5.5. Conclusions

In this chapter, the atomistic and continuum models are used for the first time to investigate a double-ended disclinated crack in a cylindrical nanowire of nickel. The continuum model for fracture takes into account the stress redistribution due to crack generation in a finite isotropic cylinder. The atomistic model is based on constructing a certain initial structure for the wedge disclination in a bicrystalline cylinder, which may or may not contain an initial crack, and the subsequent relaxation via molecular statics.

For a cylinder radius of 25 nm, the results of both the atomistic and continuum models show general agreement in the predicted critical disclination strength, the stable crack length, the crack opening profile, and the stress distribution in the cylinder. The key physical results are (1) the existence of a critical value (11.1° to 11.6° for the cylinder radius of 25 nm) for the disclination strength below which a crack cannot nucleate, (2) the decrease of the critical disclination strength with the inverse square root of the cylinder radius, (3) the increase of the stable equilibrium crack length with the disclination strength. These results highlight certain fundamental characteristics of disclinated solids with implications on the reliability of nanostructured materials. Moreover, critical disclination strengths in the range of 4° to 6° are predicted for nanocrystalline materials prepared by severe plastic deformation for grain sizes in the range of 200 nm to 100 nm.

Chapter 6

Conclusions and Recommendations

Three major contributions can be identified in this research. These are described in Sections 6.1, 6.2 and 6.3. On the basis of the accomplished work, recommendations for future research are made in Section 6.4.

6.1. Mechanics Model for Inhomogeneous Anisotropic Bicrystals

The mechanics model of an interfacial disclination dipole wall in a hexagonal bicrystal with arbitrary in-plane c -axes was established by the method of image dislocations.

- 1) Exact closed-form solutions for the stress and strain energy density are shown to be of the form of the logarithm of hyperbolic and trigonometric functions of complex parameters.
- 2) The long-range stress field of the dipole wall is determined exactly. The strain energy of the dipole wall is calculated by numerical integration of the density field.
- 3) The numerical results show that the stress, strain energy density and strain energy all depend significantly on the orientational and material inhomogeneities, which emphasizes the importance of using an anisotropic bicrystal model over a homogeneous model for calculations.

- 4) For bicrystals with symmetric c -axis orientations, it is also shown that the strain energy of a dipole wall can be a strong function of the orientations, with the maximum and minimum at specific orientations that depend on the bicrystal materials.

6.2. DSUM for Hexagonal Materials

The physical model of a DSUM for hexagonal materials was developed and applied for predicting the stress field and energy of $[1\bar{1}00]$ symmetrical tilt GBs.

- 1) The developed DSUM provides realistic physical parameters as input for the mechanics model of the disclination dipole wall. It therefore provides a means to incorporate the inhomogeneous anisotropic mechanics model for calculating GB energies of hexagonal bicrystals. The GB energy is determined as the sum of the strain energy of the disclination dipole wall and the surface energy of the delimiting boundaries.
- 2) Numerical investigations show that the misorientation strongly influences the stress field of the GB. Severe distortions of the stress contours result from a small inhomogeneity, which is limited by the degree of crystal elastic anisotropy. The stress field of high-angle boundaries tends to be more localized around the boundaries than that of low-angle boundaries.
- 3) The GB energy-misorientation curve displays cusps at the misorientations of short-period boundaries. The cusps generally represent local minima. Local maxima occur between the cusps, with the global maximum of about 1.5 J m^{-2}

for cobalt and about 0.9 J m^{-2} for titanium. These maxima occur at $\theta \approx 23^\circ$ corresponding to the $(11\bar{2}16)$ GB. The energy over the whole misorientation range consists of two regions demarcated by $\theta = 116^\circ$ corresponding to the favored boundary $(11\bar{2}2)$, with the average energy in $0^\circ < \theta < 116^\circ$ roughly twice that in $116^\circ < \theta < 180^\circ$. The GB energy of cobalt is about twice that of titanium for most misorientations.

6.3. Atomistic and Continuum Models for Disclinated Cracks

The atomistic and continuum models were used for the first time to investigate a double-ended disclinated crack in a bicrystalline nanowire. The continuum model for fracture takes into account the stress redistribution due to crack generation in the nanowire. The atomistic model is based on constructing an initial configuration of the nanowire containing a wedge disclination and the subsequent relaxation via molecular statics.

- 1) The concept of critical disclination strength is proposed, i.e., the value above which the disclination is unstable and an equilibrium crack can grow from it.
- 2) The critical disclination strength is about 11.1° to 11.6° for a nanowire of 25 nm radius.
- 3) For a nanowire of 25 nm radius, the results of both the atomistic and continuum models show general agreement in the predicted critical disclination strength, the stable crack length, the crack opening profile, and the stress distribution in the nanowire.

- 4) The critical disclination strength decreases with the inverse square root of the nanowire radius. The stable equilibrium crack length increases with the disclination strength.
- 5) Critical disclination strengths in the range of 4° to 6° are predicted for nanocrystalline materials prepared by severe plastic deformation for grain sizes in the range of 200 nm to 100 nm.

6.4. Recommendations for Future Research

Some further research work can be carried out in the following areas.

- 1) The study of polycrystalline and nanocrystalline film-substrates is of significance due to their wide applications. To study a film-substrate system, the disclination dipole wall may be used to model the interface of the system.
- 2) The DSUM can be developed for materials with a general crystal structure, e.g., cubic, hexagonal and tetragonal.
- 3) Triple junction disclinations are commonly found in polycrystalline and nanocrystalline materials. Atomistic simulations and/or continuum modeling may therefore be used to study the mechanism of crack formation at such junctions.
- 4) Further research may take into account the influence of temperature and mechanical loadings on crack formation due to disclinations. Brittle fracture is assumed in the present atomistic simulations at zero absolute temperature. At high temperatures, however, ductile rather than brittle fracture dominates.

List of Publications

Wu, M. S., Nazarov, A. A., and Zhou, K. (2004). Misorientation dependence of the energy of $[1\bar{1}00]$ symmetrical tilt boundaries in hcp metals: prediction by the disclination-structural unit model. *Philosophical Magazine*, 84, 785-806.

Zhou, K., Nazarov, A. A., and Wu, M. S. (2006). Continuum and atomistic studies of a disclinated crack in a bicrystalline nanowire. *Physical Review B*, 73, 045410-1-045410-11.

Zhou, K., and Wu, M. S. (2005). Exact solutions for periodic interfacial wedge disclination dipoles in a hexagonal bicrystal. *Mathematics and Mechanics of Solids*. (Accepted in 2003, first published on Jan 12, 2005 as doi: 10.1177/1081286504040400)

References

- Allen, M.P., and Tildesley, D.J. (1987). *Computer simulations of liquids*. Oxford: Clarendon Press.
- Alshits, V.I., Indenbom, V.L., and Kossecka, E. (1975). Disclination field in elastic anisotropic media. *Physica Status Solidi B*, 70, K25-K28.
- Anthony, K.-H. (2002). Crystal disclinations versus continuum theory. *Solid State Phenomena*, 87, 15-46.
- Bachurin, D.V., Murzaev, R.T., and Nazarov, A.A. (2003). Atomistic computer and disclination simulation of [001] tilt boundaries in nickel and copper. *Physics of Metals and Metallography*, 96, 555-561.
- Belov, A. Yu. (1993). Scaling regimes and anomalies of wedge disclination stresses in anisotropic rotationally inhomogeneous media. *Philosophical Magazine A*, 68, 1215-1231.
- Bernstein, N., and Hess, D.W. (2003). Lattice trapping barriers to brittle fracture, *Physical Review Letters*, 91, 025501/1-025501/4.
- Bollmann, W. (1967a). On the geometry of grain and phase boundaries. I. General theory. *Philosophical Magazine*, 16, 363-381.
- Bollmann, W. (1967b). On the geometry of grain and phase boundaries. II. Applications of general theory. *Philosophical Magazine*, 16, 383-399.
- Brandon, D.G. (1966). Structure of high-angle grain boundaries. *Acta Metallurgica*, 14, 1479-1484.

- Bruggeman, G.A., Bishop, G.H., and Hartt, W.H. (1972). In: Hu, H. (Ed.), *The nature and behavior of grain boundaries*. New York: AIME.
- Chou, T.W., and Pan, Y.C. (1973). Elastic energies of disclinations in hexagonal crystals. *Journal of Applied Physics*, 44, 63-65.
- Cleri, F., Phillpot, S.R., and Wolf, D. (1999). Atomistic simulations of intergranular fracture in symmetric-tilt grain boundaries. *Interface Science*, 7, 45-55.
- Cleri, F., Phillpot, S.R., Wolf, D., and Yip, S. (1998). Atomistic simulations of materials fracture and the link between atomic and continuum length scales. *Journal of the American Ceramic Society*, 81, 501-516.
- de Wit, R. (1972). Partial disclinations. *Journal of Physics C*, 5, 529-534.
- de Wit, R. (1973). Theory of disclinations: III. Continuous and discrete disclinations in isotropic elasticity. *Journal of Research of the National Bureau of Standards*, 77A, 359-368.
- Eshelby, J.D. (1979). Boundary problems. In: Nabarro, F.R.N. (Ed.), *Dislocations in solids* (vol. 1, pp. 169-221). Amsterdam: North-Holland.
- Farkas, D. (1994). Grain-boundary structures in hexagonal materials: coincident and near coincident grain boundaries. *Metallurgical and Materials Transactions A*, 25, 1337-1346.
- Farkas, D. (2000). Fracture mechanisms of symmetrical tilt grain boundaries. *Philosophical Magazine Letters*, 80, 229-237.
- Foiles, S.M., Baskes, M.I., and Daw, M.S. (1986). Embedded-atom-method functions for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys. *Physical Review B*, 33, 7983-7991.
- Friedel, J. (1964). *Dislocations* (pp.27). Reading, MA: Addison-Wesley.

- Fundenberger, J.J., Philippe, M.J., Wagner, F., and Esling, C. (1997). Modelling and prediction of mechanical properties for materials with hexagonal symmetry (zinc, titanium and zirconium alloys). *Acta Materialia*, 45, 4041-4055.
- Gerasoulis, A. (1982). The use of piecewise quadratic polynomials for the solution of singular integral equations of Cauchy type. *Computers and Mathematics with Applications*, 8, 15-22.
- Gertsman, V.Yu., Nazarov, A.A., Romanov, A.E., Valiev, R.Z., and Vladimirov, V.I. (1989). Disclination-structural unit model of grain boundaries. *Philosophical Magazine A*, 59, 1113-1118.
- Gleiter, H. (1989). Nanocrystalline materials. *Progress in Materials Science*, 33, 223-315.
- Gryaznov, V.G., Heydenreich, J., Kaprelov, A.M., Nepijko, S.A. Romanov, A.E., and Urban, J. (1999). Pentagonal symmetry and disclinations in small particles. *Crystal Research and Technology*, 34, 1091-1119.
- Gryaznov, V.G., Kaprelov, A.M., Romanov, A.E., and Polonskii, I.A. (1991). Channels of relaxation of elastic stresses in pentagonal nanoparticles. *Physica Status Solidi B*, 167, 441-450.
- Gryaznov, V.G., and Trusov, L.I. (1993). Size effects in micromechanics of nanocrystals. *Progress in Materials Science*, 37, 289-401.
- Gutkin, M.Yu., Mikaelyan, K.N., Romanov, A.E., and Klimanek, P. (2002). Disclination models of misorientation band generation and propagation. *Physica Status Solidi A*, 193, 35-52.
- Gutkin, M.Yu., and Ovid'ko, I.A. (1994). Disclinations, amorphization and microcrack generation at grain boundary junctions in polycrystalline solids. *Philosophical Magazine A*, 70, 561-575.
- Hahn, S.L. (1996). *Hilbert transforms in signal processing*. Boston: Artech House.

Hasson, G.C., and Goux, C. (1971). Interfacial energies of tilt boundaries in aluminium. Experimental and theoretical determination Source. *Scripta Metallurgica*, 5, 889-894.

He, M.Y., and Hutchinson, J.W. (1989). Kinking of a crack out of an interface. *Journal of Applied Mechanics, Transactions ASME*, 56, 270-278.

Heinig, N.F., Redwing, R.D., Nordman, J.E., and Larbalestier, D.C. (1999). Strong to weak coupling transition in low misorientation angle thin film $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ bicrystals. *Physical Review B*, 60, 1409-1417.

Hirth, J. P., and Lothe, J. (1982). *Theory of dislocations*. New York: Wiley.

Indenbom, V.L. (1962). On fracture criteria in dislocation theories of strength. *Soviet Physics, Solid State*, 33, 1506-1511.

Jiang, X., and Jia, C.L. (1996). The coalescence of [001] diamond grains heteroepitaxially grown on (001) silicon. *Applied Physics Letters*, 69, 3902-3904.

Kirchner, H.O.K. (1989). Elastically anisotropic angularly inhomogeneous media I. A new formalism. *Philosophical Magazine B*, 60, 423-432.

Klemm, V., Klimanek, P., and Motylenko, M. (2002). TEM identification of disclinations in plastically deformed crystals. *Solid State Phenomena*, 87, 57-72.

Klimanek, P., Klemm, V., Romanov, A.E., and Seefeldt, M. (2001). Disclinations in plastically deformed metallic materials. *Advanced Engineering Materials*, 3, 877-884.

Kolesnikova, A.I., and Romanov, A.E. (2004). Virtual circular dislocation-disclination loop technique in boundary value problems in the theory of defects. *Journal of Applied Mechanics*, 71, 409-417.

Li, J.C.M. (1972). Disclination model of high angle grain boundaries. *Surface Science*, 31, 12-26.

Lo, K.K. (1978). Analysis of branched cracks. *Journal of Applied Mechanics, Transactions ASME*, 45, 797-802.

Louat, N. (1962). Solution of boundary value problems in plane strain. *Nature*, 196, 1081-1082.

Lyles, R.L., and Wilsdorf, H.G.F. (1975). Microcrack nucleation and fracture in silver crystals. *Acta Metallurgica*, 23, 269-277.

Marcinkowski, M.J. (1979). *Unified theory of the mechanical behavior of matter*. New York : Wiley

Mehl, M.J., and Papaconstantopoulos, D.A. (1996). Applications of a tight-binding total-energy method for transition and noble metals: elastic constants, vacancies, and surfaces of monatomic metals. *Physical Review B*, 54, 4519-4530.

Mikhailin, A.I., and Romanov, A.E. (1986). Amorphization of a disclination core. *Soviet Physics -Solid State*, 28, 337-338.

Mori, T., Oliver, E.C., Daymond, M.R., and Withers, P.J. (2004). An analysis of lattice strain due to disclination dipole wall in Fe-Pd martensite. *Journal of Neutron Research*, 12, 39-44.

Motylenko, M., Klemm, V., Klimanek, P., Pavlovitch, T., and Straube, H. (2004). Characterization of the cell block structure and disclination configurations in plastically deformed metals by electron diffraction. *Journal of Alloys and Compounds*, 378, 93-96.

Murayama, M., Howe, J.M., Hidaka, H., and Takaki, S. (2002). Atomic-level observation of disclination dipoles in mechanically milled, nanocrystalline Fe. *Science*, 295, 2433-2435.

Muskhelishvili, N.I. (1953). *Some basic problems of the mathematical theory of elasticity*. Groningen: Noordhoff.

- Nazarov, A.A. (2002). Modelling of grain boundary structures by means of dislocations. *Solid State Phenomena*, 87, 193-204.
- Nazarov, A.A., Bachurin, D.V., Shenderova, O.A., and Brenner, D.W. (2003). On the origin and energy of triple junction defects due to the finite length of grain boundaries. *Interface Science*, 11, 417-424.
- Nazarov, A.A., and Mulyukov, R.R. (2003). Nanostructured materials. In: Goddard, W.A., Brenner, D.W., Lyshevski, and S., Iafrate, G. (Eds.), *Handbook of nanoscience, engineering, and technology* (pp. 22-1–22-41). Boca Raton: CRC Press.
- Nazarov, A.A., Romanov, A.E., and Valiev, R.Z. (1993). On the structure, stress field and energy of nonequilibrium grain boundaries. *Acta Metallurgica et Materialia*, 41, 1033-1040.
- Nazarov, A.A., Romanov, A.E., and Valiev, R.Z. (1996). Random disclination ensembles in ultrafine-grained materials produced by severe plastic deformation. *Scripta Materialia*, 34, 729-734.
- Nazarov, A.A., Shenderova, O.A., and Brenner, D.W. (2000a). Elastic models of symmetrical $\langle 001 \rangle$ and $\langle 011 \rangle$ tilt grain boundaries in diamond. *Physical Review B*, 21, 928-936.
- Nazarov, A.A., Shenderova, O.A., and Brenner, D.W. (2000b). On the disclination-structural unit model of grain boundaries. *Materials Science and Engineering A*, 281, 148-155.
- Niu, J., and Wu, M.S. (1997). Strong interactions of morphologically complex cracks. *Engineering Fracture Mechanics*, 57, 665-687.
- Nye, J.F. (1957). *Physical properties of crystals: their representation by tensors and matrices*. Oxford: Clarendon Press.

-
- Payne, M.C., Bristowe, P.D., and Joannopoulos, J.D. (1987). Ab initio determination of the structure of a grain boundary by simulated quenching. *Physical Review Letters*, 58, 1348-1351.
- Pérez, R, and Gumbsch, P. (2000). Directional anisotropy in the cleavage fracture of silicon. *Physical Review Letters*, 84, 5347-5350.
- Pertsev, N.A., and Zembilgotov, A.G. (1995). Energetic and geometry of 90° domain structures in epitaxial ferroelectric and ferroelastic films. *Journal of Applied Physics*, 78, 6170-6180.
- Read, W.T., and Shockley, W. (1950). Dislocation models of crystal grain boundaries. *Physical Review*, 78, 275-289.
- Regel, V.R., Leksovskii, A.M., and Sakiev, S.N. (1975). The kinetics of the thermofluctuation induced micro- and macrocrack growth in plastic metals. *International Journal of Fracture*, 11, 841-850.
- Romanov, A.E. (2003). Mechanics and physics of disclinations in solids. *European Journal of Mechanics, A/Solids*, 22, 727-741.
- Romanov, A.E., Lefevre, M.J., Speck, J.S., Pompe, W., Streiffer, S.K., and Foster, C.M. (1998). Domain pattern formation in epitaxial rhombohedral ferroelectric films. II. Interfacial defects and energetics. *Journal of Applied Physics*, 83, 2754-2765.
- Romanov, A.E., and Vladimirov, V.I. (1981). Straight disclinations near a free surface. I. Stress fields. *Physica Status Solidi A*, 63, 109-118.
- Romanov, A.E., and Vladimirov, V.I. (1992). Disclinations in crystalline solids. In: Nabarro, F. R. N. (Ed.), *Dislocations in solids* (vol. 9, pp. 191-402). Amsterdam: North-Holland.
- Rybin, V.V. (1986). *Large plastic deformations and fracture of metals*. Moscow: Metallurgy (in Russian).
-

- Rybin, V.V., and Zhukovskii, I. M. (1978). Disclination mechanism of microcrack formation. *Soviet Physics Solid State*, 20, 1056-1059.
- Rybin, V.V., and Zisman, A.A. (1982). Microcrack formation under conditions of developed plastic strain. *Strength of Materials*, 14, 1584-1590.
- Rybin, V.V., Zisman, A.A., and Zolotarevsky, N.Yu. (1993). Junction disclinations in plastically deformed crystals. *Acta Metallurgica et Materialia*, 41, 2211-2217.
- Shastry, V., and Farkas, D. (1996). Molecular statics simulation of fracture in α -iron. *Modelling and Simulation in Materials Science and Engineering*, 4, 473-492.
- Shenderova, O.A., and Brenner, D.W. (2002). Atomistic simulation of grain boundaries, triple junctions and related disclinations. *Solid State Phenomena*, 87, 205-214.
- Shenderova, O.A., Brenner, D.W., Nazarov, A.A., Romanov, A.E., and Yang, L.H. (1998). Multiscale modeling approach for calculating grain-boundary energies from first principles. *Physical Review B*, 57, R1381-R1384.
- Shenderova, O.A., Brenner, D.W., Omeltchenko, A., Su, X., Yang, L. H., and Nazarov, A.A. (2000). Properties of polycrystalline diamond: Multiscale modeling approach. *Molecular Simulation*, 24, 197-207.
- Shih, K.K., and Li, J.C.M. (1975). Energy of grain boundaries between cusp misorientations Source. *Surface Science*, 50, 109-124.
- Speck, J.S., Daykin, A.C., Seifert, A., Romanov, A.E., and Pompe, W. (1995). Domain configurations due to multiple misfit relaxation mechanisms in epitaxial ferroelectric thin films. III. Interfacial defects and domain misorientations. *Journal of Applied Physics*, 78, 1696-1706.
- Stroh, A.N. (1958). Dislocations and cracks in anisotropic elasticity. *Philosophical Magazine*, 3, 625-646.

Sutton, A.P., and Balluffi, R.W. (1995). *Interfaces in crystalline materials*. Oxford: Clarendon Press.

Sutton, A.P., and Vitek, V. (1983a). On the structure of tilt grain boundaries in cubic metals. I. Symmetrical tilt boundaries. *Philosophical Transactions of the Royal Society of London A*, 309, 1-36.

Sutton, A.P., and Vitek, V. (1983b). On the structure of tilt grain boundaries in cubic metals. II. Asymmetrical tilt boundaries. *Philosophical Transactions of the Royal Society of London A*, 309, 37-54.

Sutton, A.P., and Vitek, V. (1983c). On the structure of tilt grain boundaries in cubic metals. III. Generalizations of the structural study and implications for the properties of grain boundaries. *Philosophical Transactions of the Royal Society of London A*, 309, 55-68.

Thibault, J., Putaux, J.L., Jacques, A., George, A., Michaud, H.M., and Baillin, X. (1993). Structure and characterization of the dislocations in tilt grain boundaries between $\Sigma = 1$ and $\Sigma = 3$: a high resolution electron microscopy study. *Materials Science and Engineering A*, A164, 93-100.

Tsurekawa, S., Tanaka, T., and Yoshinaga, H. (1994). Grain boundary structure, energy and strength in molybdenum Source. *Materials Science and Engineering A*, 176, 341-348.

Valiev, R.Z., Islamgaliev, R.K., and Alexandrov, I.V. (2000). Bulk nanocrystalline materials from severe plastic deformation. *Progress in Materials Science*, 45, 103-189.

Valiev, R.Z., Vladimirov, V.I., Gertsman, V.Yu., Nazarov, A.A., and Romanov, A.E. (1990). Disclination-structure model and energy of grain boundaries in metals with the FCC lattice. *Physics of Metals and Metallography*, 69, 30-37.

Vitek V., and Egami T. (1987). Atomic level stresses in solids and liquids. *Physica Status Solidi B*, 144, 145-156.

- Wang, G.J., Sutton, A.P., and Vitek, V. (1984). Computer Simulation study of $\langle 001 \rangle$ and $\langle 111 \rangle$ tilt boundaries: the multiplicity of structures. *Acta Metallurgica*, 32, 1093-1104.
- Wang, G.J., and Vitek, V. (1986). Relationships between grain boundary structure and energy. *Acta Metallurgica*, 34, 951-960.
- Wang, Y.C., and Ye, H.Q. (1997). On the tilt grain boundaries in hcp Ti with [0001] orientation. *Philosophical Magazine A*, 75, 261-272.
- Watanabe, T., and Tsurekawa, S. (1999). The control of brittleness and development of desirable mechanical properties in polycrystalline systems by grain boundary engineering. *Acta Materialia*, 47, 4171-4185.
- Weertman, J. (1996). *Dislocations based fracture mechanics*. Singapore: World Scientific.
- Wu, M.S. (2000). Exact solutions for a wedge disclination dipole in a transversely isotropic bimaterial. *International Journal of Engineering Science*, 38, 1811-1835.
- Wu, M.S. (2001). Characteristics of a disclinated Zener crack with cohesive end zones. *International Journal of Engineering Science*, 39, 1459-1485.
- Wu, M.S. (2002a). Characteristics of a Zener crack wedged open by a disclination dipole. *Solid State Phenomena*, 87, 277-300.
- Wu, M.S. (2002b). Interfacial wedge disclination dipole in a hexagonal bicrystal with arbitrary in-plane c-axis orientations. *Mathematics and Mechanics of Solids*, 7, 541-567.
- Wu, M.S. (2002c). Stress and strain energy of a periodic array of interfacial wedge disclination dipoles in a transversely isotropic bicrystal. *International Journal of Engineering Science*, 40, 873-897.

- Wu, M.S., Huang, H., and Feng, R. (2003). Closed-form solutions for interfacial edge dislocations in anisotropic bicrystals by the image method. *Mechanics of Materials*, 35, 913-930.
- Wu, M.S., and Zhou, H. (1996). Analysis of a crack in a disclinated cylinder. *International Journal of Fracture*, 82, 381-399.
- XMD - Molecular Dynamics for Metals and Ceramics. (2004). Retrieved August 5, 2004, from Website: <http://xmd.sourceforge.net/about.html>.
- Xu, C.K., Xue, L., Yin, C.R., and Wang, G.H. (2003). Formation and photoluminescence properties of AlN nanowires. *Physica Status Solidi A*, 198, 329-335.
- Yu, H.Y., and Sanday, S.C. (1991). Disclinations in bimetals. *Physica Status Solidi A*, 126, 355-365.
- Yu, H.Y., and Sanday, S.C. (1994). Dislocations and disclinations in transversely isotropic elastic solids. *Philosophical Magazine A*, 70, 725-738.
- Yu, H. Y., Sanday, S. C., and Chang, C. I. (1994). Elastic inclusions and inhomogeneities in transversely isotropic solids. *Proceedings of the Royal Society of London, Series A*, 444, 239-252.
- Zener, C. (1948). The micro-mechanism of fracture. In: *Fracturing of metals* (pp. 3-31). American Society for Metals.
- Zhigilev, L.V., Mikhailin, A.I., and Romanov, A.E. (1988). Molecular dynamical simulation of two-dimensional disclinations. *Physics of Metals and Metallography*, 66, 56-63.
- Zisman, A.A., and Rybin, V.V. (1996). Basic configurations of interfacial and junction defects induced in a polycrystal by deformation of grains. *Acta Materialia*, 44, 403-407.