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AN INVESTIGATION OF DISLOCATION MOVEMENT THROUGH METALLIC GRAIN BOUNDARIES

The Ohio State University

Ph.D. 1987

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An Investigation of Dislocation Movement through Metallic Grain Boundaries

Dissertation

Presented in Partial Fulfillment of the Requirements for the Degree Doctor of Philosophy in the Graduate School of the Ohio State University

By

Zhiyong Shen, B.S., M.S.

The Ohio State University

1987

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To My Parents
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CHAPTER I

INTRODUCTION

Microscopically, polycrystalline metal deformation proceeds by dislocation movement within individual grains and across the boundaries between neighboring grains. In this study, slip propagation through grain boundaries in polycrystalline metals is investigated at the individual dislocation level. The dislocations and grain boundaries involved in the slip propagation are fully characterized and the parameters obtained are used in stress calculations. It is then possible to clarify processes already known and to develop a model to explain newly-observed slip propagation events. The results obtained from static and dynamic electron microscopy and stress field calculations are used for the further understanding of the initial stages of polycrystalline metal deformation. The most important objectives in this study are as follows:

1. Determine what type of detailed motions of lattice dislocations take place at or near the grain boundary when stress is applied.

2. Using both crystallographic analyses and stress calculations, determine the factors which control
dislocation-grain boundary interaction events.

3. Establish a criterion for selection of the slip system of the emitted dislocation in cases of dislocation transmission across the grain boundary.

4. Develop a model which will explain the observed dislocation-grain boundary interaction events in dynamic in-situ electron microscopy straining experiments.

1.1 Relations between dislocation-grain boundary interactions and mechanical properties of polycrystalline metals

Grain boundaries in polycrystalline metals play an important role in controlling mechanical properties of the materials. The yield stress, for example, has been found to be directly affected by the density of grain boundaries in the metal [1]. For plastic deformation to occur in polycrystalline metals, strain has to propagate from grain to grain. A variety of microscopic mechanisms were proposed to explain the Hall-Petch relationship [1], which states that the yield stress of a polycrystalline metal is inversely proportional to the square root of its grain size. These mechanisms involve dislocation and grain boundary interactions, and have been discussed by various authors [3-12]. A fundamental process in the deformation of polycrystalline metals is the propagation of slip across
grain boundaries [13-15]. This study is aimed at investigating these interactions at the individual dislocation level and thereby offering mechanistic explanations for the slip propagation processes. The method used is a combination of the direct observations using electron microscopy and the stress analysis of the dislocation-grain boundary interactions. The details of the observed dislocation movement through grain boundaries are discussed in the light of the crystallographic and stress calculations.

1.2 Stress field calculations and their applications in dislocation-grain boundary interactions

Anisotropic elastic stress solutions for dislocations parallel to grain boundaries have been formulated by Tucker [16] and Tewary [19] using different mathematical approaches. These mathematical methods can be used to calculate the stress field of dislocation-grain boundary interactions. Consequently, studies of such interactions can be related to the bulk properties of the metal by comparing the stress levels involved in microscopic and macroscopic studies. The stress level at the area of intensive dislocation activities can be used to understand actual interaction processes and to relate them to macroscopic properties of materials.
1.3 Static TEM studies and dynamic HVEM in-situ straining techniques

The role of slip propagation across grain boundaries in polycrystalline metal deformation has been studied by a variety of techniques. Among others, etch pitting [21], slip line analysis [22,23] and transmission electron microscopy (TEM) [24] have been used. TEM studies of the interaction between dislocations and grain boundaries provides direct and detailed information about the initial stage of the yielding in polycrystalline metals. Here both static observations and dynamic in-situ experiments were conducted to achieve the best results. Static TEM experiments have the advantages of being easily controlled, providing more detailed information from a large area of the specimen, and allowing stable imaging conditions. Moreover, it is always possible to obtain enough data to characterize the grain boundary and dislocation configurations completely in the course of the experiment. Dynamic in-situ straining, on the other hand, enables us to observe dislocation-boundary interactions in motion and to capture those critical stages of the strain propagation process in the sample which are of importance to our understanding. However, it has the disadvantage of being difficult to control. Thus these two procedures can complement each
other for our study of the slip propagation processes.

1.4 Difficulties in reaching the goals and measures to overcome them

The prominent obstacles encountered in such a study are mostly related to (1) dynamic nature of the dislocation-grain boundary interaction events, (2) preparation of samples which will likely to yield results in in-situ straining experiments, and (3) searching for sample areas which show dislocation activation. The difficulties which arise and the steps taken to overcome them are outlined below:

1. Samples with uniform thin areas which can be expected to exhibit dislocation-grain boundary interaction events upon the initiation of deformation are needed. It was found that miniature tensile samples with regular center holes and uniform thin areas were less likely to fail prematurely during in-situ straining [89]. Caution and care were exerted to ensure samples which will behave as expected during the dynamic experiments, that is, the sample deforms uniformly without premature tearing or cracking before dislocation activation can be observed. Moreover, samples prepared using the identical procedures are also examined in the static TEM experiments to investigate the same dislocation-grain boundary configurations as would result
from a dynamic study.

2. Individual interaction events must be observed in such a way that the details can be resolved and classified. Video tape recordings are made during the dynamic straining process. Micrographs are taken whenever possible.

3. Dislocation-grain boundary configurations must be completely characterized so that quantitative results can be obtained. In addition to standard TEM analyzing techniques [58,60], stress calculations are used to study quantitatively the interaction events. The stress level indicates how the kinds of interactions observed are related to the bulk deformation process.
2.1 Grain boundary strengthening in the initial stages of polycrystalline metal deformation

Among the ways by which polycrystalline metals can be strengthened, grain boundary hardening is the only mechanism which increases the strength of the material without sacrificing toughness [2]. While grain boundaries also affect many other processes of the metal such as fracture, segregation and fatigue [1], this literature survey will be limited to their contributions to the material strength.

Hall [3] and Petch [4] were the first to formulate an inverse square root relationship between the yield strength and grain diameter in metals as follows:

\[ \sigma_y = \sigma_0 + k_y d^{-1/2} \]  \hspace{1cm} (2.1)

where \( \sigma_y \) is the yield stress, \( \sigma_0 \) is a constant related to the contribution of the lattice friction, \( k_y \) is a constant and \( d \) is the grain diameter. Petch [4] was the first to suggest that the above equation was consistent with a model of slip propagation by dislocation pileup activation at grain boundaries.

It was shown later that the relationship does not have
such a simple form and various alternate forms have been proposed [1]. However an empirical relation between yield or flow stress and the grain size of polycrystalline metals can still be represented as follows: [1]:

$$\sigma_y = \sigma_0 + Kd^n$$  \hspace{1cm} (2.2)

where \(\sigma_y\), \(\sigma_0\), \(K\), and \(d\) have the same meaning as in equation \(2.1\); \(n\) is a material constant. The parameter \(n\) can range from \(-1/3\) to \(-1\) for different materials [4-6].

Although other variations of the above equation have been derived [30-33], the common feature is that materials are strengthened by grain boundaries. Henceforth reference will be made to the above equation \(2.2\) as the Hall-Petch type relation.

To explain Hall-Petch type relationships, various dislocation and grain boundary interaction models were proposed [34-40]. The major models assume dislocation-grain boundary interactions as the limiting mechanism of slip propagation in polycrystalline metals. Most of them are based on grain boundaries acting as barriers or sources of moving dislocation arrays. It was shown by Dong and Thompson [41] that the slip obstruction effect of grain boundaries decreases as the strain increases. Therefore the initial stages (small strain) of the polycrystalline deformation investigated in this study can be used to reveal the role of grain boundaries in such deformation processes.

When grain boundaries act as barriers to the movement
of dislocation pileups, then the Hall-Petch equation with $n=-1/2$ can be derived [34-37]. The grain boundary stops the movement of the leading dislocation of an array of mobile dislocations, while other dislocations still attempt to move toward the boundary under the applied stress. This causes the stress to build up at the head of the pileup. The stress concentration is directly proportional to the number of dislocations in the pileup, and the number of dislocations is proportional to the square root of the pileup length [45], which is related in these models to the grain size.

When grain boundaries are the source of the dislocation emission, it is again possible to obtain the Hall-Petch relationship [38-40]. The yield stress of a material is approximately proportional to the square root of the dislocation density [41] while the dislocation density in turn is proportional to the inverse of the grain size.

These are simplified versions of the real processes. A variety of other types of dislocation-grain boundary interactions are also important in the deformation of polycrystals. Among them are dislocations which enter the grain boundary and form grain boundary dislocations [42,43], and dislocation sources near the grain boundary [44].

However, the quantitative evidence provided in these models are mainly obtained by optical microscopy, which reveals only the slip planes. It is necessary to obtain the
dislocation Burgers vector in order to fully determine the slip systems involved. Furthermore, despite the dynamic nature of the process, these models were based on studies of static observations. Better tools are needed to investigate further the relationship between dislocation-grain boundary interactions and the grain boundary strengthening effect. Direct observations of the above-mentioned dislocation-grain boundary interactions will greatly advance our understanding of polycrystalline strengthening mechanisms.

2.2 Details of slip propagation process in polycrystalline metals

The materials selected for this study were 304 stainless steel which has a face centered cubic crystal structure and molybdenum which has a body centered cubic crystal structure.

In austenitic stainless steels, the relatively low stacking fault energy means that planar slip, in which the dislocations remain in planar arrays and do not cross-slip, is the favored deformation mode at room temperatures [45]. Grain boundaries can act as barriers to dislocation motion and cause a dislocation pileup, the tip of which is a source of stress concentration. Since the pileup produces a force at the tip which is proportional to the applied stress and the number of dislocations in the pileup, it can initiate
yielding on the other side of the boundary [45], and the strain can thereby propagate from one grain to another. Microscopically, this may be accomplished by one of several different mechanisms, such as those shown in Figure 2.1. In Figure 2.1(a) new dislocations are nucleated on the other side of the boundary under the pileup stress concentration. In Figure 2.1(b), direct dislocation transmission across the grain boundary takes place activated by the stress concentration at the dislocation pileup tip. In Figure 2.1(c) the pileup dislocation are simply absorbed into the grain boundary. In Figure 2.1(d), the pileup dislocations absorbed by the grain boundary are emitted in the neighboring grain. In cases (b)-(d) a residual dislocation is retained in the grain boundary and may make steady-state operation impossible.

In each of the above-mentioned processes the grain boundaries strengthen the material by making microstrain propagation more difficult than in single crystals [47-52].
Figure 2.1 Models of Slip Propagation via dislocation movement

(a) Nucleation at Boundary

(b) Pass-through

(c) Boundary Absorption

(d) Absorption and Emission
Livingston and Chalmers [53] showed that in the case of slip propagation, the slip systems subsequently activated can be predicted by the geometry of the dislocation-grain boundary configuration. They found [53] that slip is propagated from one grain to the slip system in another grain with the maximum transmission factor $N$:

$$N = e_1 \cdot e_2 \cdot g_1 \cdot g_2 + e_1 \cdot e_2 \cdot g_1 \cdot g_2$$  \hspace{1cm} (1.3)

where $e$ is a unit normal to the slip plane, $g$ is a unit vector along the dislocation Burgers vector. Subscripts indicates the grain involved. Grain 1 is the grain with the dislocation pileup and grain 2 is the neighboring grain.

The geometry is shown in Figure 2.2. $N$ is proportional to the resolved shear stress on the grain 2 slip system due to the dislocation pileup in grain 1. This shear stress activates slip in grain 2.

![Figure 2.2: Geometry for Transmission Factor [15]](image-url)
Several types of slip propagation across metal grain boundaries have been studied using transmission electron microscopy. In these studies [54-58], correlations are made between the slip propagation and detailed crystallographic analysis.

Clark and Wagoner [54] studied the process of dislocation absorption into and dislocation transmission across high angle grain boundaries in 304 stainless steel. They found that both direct dislocation transmission across the grain boundary and dislocation absorption into the grain boundary are possible in this material. For the transmission case, a local stress of 130 MPa acting at the first dislocation position of the pileup was obtained.

Bamford et al. [55] again used both stress and crystallographic analyses to reveal the details of dislocation transmission in 70-30 brass and found that details of slip propagation via dislocation transmission across high angle grain boundaries can be predicted using crystallographic and stress analysis. They concluded [55] that in most cases of dislocation transmission across grain boundaries, a residual dislocation will be left at the grain boundary. The activated slip systems in the neighboring grain have the highest resolved stress and the residual dislocation has the smallest magnitude [55].

King and Chen [56] studied the interactions between
lattice partial dislocations and grain boundaries and found that there are energy barriers inside grain boundaries for dislocation absorption and transmission processes. They concluded that such barriers are weaker for grain boundaries with a Σ value which is an integer multiple of 3. However, this theory has not been confirmed by experiments.

Valiev et al. [57] demonstrated that the boundaries act as sources and sinks for dislocations in their in-situ deformation of thin foils of magnesium and Grade MA8 alloy, which is a wrought magnesium alloy [59]. Orlov et al. [58] found that lattice dislocations cross a high angle grain boundary more easily in one direction than the other. The evidence for this was discovered when much higher dislocation densities were shown on one side of grain boundaries than on the other side in electron microscope pictures. Orlov [58] et al. proposed that this phenomenon arose from the asymmetric nature of general high angle grain boundaries in polycrystalline metals.

From the above literature, in many instances it is possible that activated slip systems across in the neighboring grain can be predicted by crystallographic and stress field data.

Molybdenum has a higher endurance to irradiation damage because of its large atomic mass [60]. Moreover, its higher elastic modulus makes molybdenum samples more responsive to the imposed strain [61], i.e., dislocations begin to move
with relatively small strains compared to those needed to activate dislocation movement in stainless steel [89]. Therefore it is easier to observe dislocation movement when the stress is applied to the sample during straining.

2.3 Mathematical methods of dislocation stress field calculations

In order to study and characterize observed dislocation-grain boundary interactions, various stress analysis methods are available. While it has been suggested that isotropic elastic calculations can be used for this problem and offer an approximate illustration of certain aspects of the interactions between dislocations and grain boundaries [62], it is more appropriate to use the anisotropic elastic solutions derived by Stroh [18], Eshelby [17], Tucker [16] and others [63,64,66-69]. These solutions are based on complex variable analysis to calculate the dislocation stress field in an anisotropic bicrystal with the dislocations parallel to the interface. The method was used by Yoo and Loh to calculate displacement in anisotropic crystals [63,64]. Wagoner applied Tucker's solution to dislocation pileup configurations and their interactions with the grain boundaries in cubic metals [66]. He found that for dislocations parallel to the grain boundary in iron, elastic interactions with some grain boundaries could
facilitate dislocation adsorption while in other boundaries the same elastic effect may effectively block slip transmission. Wagoner pointed out [66] that full anisotropic elastic solutions are required to obtain accurate dislocation spacings in pileups near grain boundaries, furthermore, the number of pileup dislocations required for slip transmission through a grain boundary may depend strongly on boundary and crystal orientation. Wagoner's numerical adaptation [66] of Tucker's complex variable analysis [16] forms the basis of the first calculation procedure in this paper.

To cross check the validity of the computed stress field data, a Green's function method formulated by Tewary et al. [19] was also used in the stress analysis. With some modifications, this method can handle dislocations which are not parallel to the interface [70], a more realistic procedure in view of the experimental results. Moreover, Green's function methods can be readily extended to incorporate contributions from other defects such as a crack [71]. Since the dislocation and grain boundary interaction process is an idealized model, considering many other crystal defects observable in electron microscopy experiments, the Green's function method is perhaps more suited to further this type of studies.

Since the dislocation spacings are much greater than the atomic distances, nonlinear core fields are not
significant, according to Kuan and Hirth [72]. Therefore core fields are not included in the calculations.

2.4 TEM studies and dynamic HVEM in-situ straining experiments

Using transmission electron microscopy (TEM) techniques, dislocation-grain boundary interaction events can be resolved down to the individual dislocation level [73,74]. This enables observation and analysis of phenomena which are fundamental to the grain boundary role in the deformation process. Dislocation and grain boundary parameters which are required in the anisotropic stress computation can be obtained using stereographic projection procedures [75-77]. Moreover, the accuracy of crystal orientation data can be improved by using Kikuchi line analysis programs developed by Heilman et al [79].

Various techniques of dynamic experiments in electron microscopy have been presented by Butler and Hale [80], Murr [81], and Fujita [82]. Murr [84] used high voltage electron microscopy (HVEM) to study dislocation and grain boundary interactions in 304 stainless steel and pointed out that HVEM would be very promising in revealing detailed mechanisms of such interactions which are fundamental to the understanding of the basics of the slip propagation process. Although he could not observe any evidence of interior
dislocation sources for the dislocation pileups, he pointed out that characterization of dislocation pileups and grain boundary dislocation emission need further theoretical and experimental clarification. Campany et al. [85] performed similar experiments using single crystal molybdenum. They observed that [85] the basic problem to be encountered in dynamic in-situ straining experiments are: (i) the ability of the straining system to provide smooth controllable deformation so that the sample can be observed while under stress, (ii) the double tilting stage which makes crystallographic characterization possible, (iii) the ability to produce suitable specimens for stressing and (iv) the ability to record dynamic events at adequate resolution. Kurzydlowski et al. [83] used the dislocation pile-up configuration to estimate the stress level involved during in-situ straining experiments of stainless steel samples. They observed that slip propagation from grain to grain via dislocation movement is the most important process during the initial stages of deformation.

Fujita et al. [88] studied dislocation behavior in the vicinity of grain boundaries in FCC metals by in-situ HVEM deformation experiments and found that dislocation movement across grain boundaries became more difficult as the misorientation of the crystals increased.

In-situ TEM straining studies of Varin [86], and Styczynska [87] again revealed that grain boundaries can act
as both sources and sinks of the dislocations.

Sample preparation is essential for the success of the dynamic in-situ straining experiment [81,89]. The sample preparation procedures developed by Hardiman [89] were used in this study.

2.5 Burgers vector determination by image simulation

In some cases, especially for dynamic in-situ straining experiments, the Burgers vectors of dislocations cannot be determined by imaging alone due to limitations of sample tilting using HVEM sample holder [89]. The image simulation technique can then be used to solve any ambiguity that exists [78].

Computer programs for generating two-beam calculated electron micrographs were adapted from those developed by Head et al. [78]. The intensity variations in the incident and diffracted beams can be expressed as follows [78]:

\[
\frac{dT}{dz} = \pi i \left( \frac{1}{T_0} + \frac{1}{S_0} \right) T + \pi i \left( \frac{1}{T_0} + \frac{1}{S_0} \right) S \exp(2\pi i(sz + g \cdot R))
\]

\[
\frac{dS}{dz} = \pi i \left( \frac{1}{T_0} + \frac{1}{S_0} \right) S + \pi i \left( \frac{1}{T_0} + \frac{1}{S_0} \right) T \exp(-2\pi i(sz + g \cdot R))
\]

\[<2.3>\]

where \(T\) and \(S\) are the amplitudes of the electron waves in the directions of the incident and diffracted beams respectively; \(g\) is the diffracting vector; \(z\) is the
direction of the incident beam; $R$ is the displacement field at depth $z$ in the beam direction; $s$ is a parameter which measures the deviation of the crystal orientation from the exact Bragg position; $\xi_o$ and $\xi_g$ are the extinction distances in the directions of the incident and diffracted beams.

The displacement field represented by $R$ of a lattice dislocation in an anisotropic material is calculated using Stroh's method [18]. The integration of the equations (2.3) along $z$ with all the necessary parameters listed above gives enough information to construct a calculated dislocation image.

The input data necessary for the image simulation are the foil normal, the beam direction, the dislocation line direction. The Burgers vector identification involves generating computed micrographs with several different Burgers vectors until the computed images match the experimental images. In the next chapter, this procedure will be illustrated through the analysis of a dislocation pileup.

2.6 Summary of the literature review

It is possible to make some generalized comments from information that can be learned from the literature survey:

1. Grain boundary hardening is an important strengthening mechanism in polycrystalline metals.
2. **Macroscopic studies of the origin of grain boundary strengthening** can rationalize the empirical relationship between grain size and strength using widely different mechanisms.

3. **Transmission electron microscopy** can reveal more detailed pictures of polycrystalline strengthening. It was observed that dislocation-grain boundary interactions were the underlying process which leads to the strengthening. When the grain boundaries and dislocations are fully characterized, the nature and the mode of such interactions can be revealed.

4. Deformation in polycrystalline metals proceeds by slip propagation from one grain to another. Microscopically, it is the process of dislocation movement around and across the grain boundary that leads to slip propagation. As described by Livingston and Chalmers [53] the activation of slip systems during slip propagation can be predicted from the geometry of the crystals involved. However, the effect of the grain boundary is not accounted for in their work, which may be important to our studies.

5. Anisotropic elastic stress calculations can be used to obtain quantitative results for the dislocation-grain boundary interaction processes and help to establish models for the observed phenomena. It has been shown that while dislocation movement across grain boundaries has been investigated previously, there has been no association with
the stress values involved in such processes.

6. Dynamic in-situ HVEM straining experiments can ultimately resolve the ambiguities of the studies based on static observations alone.
3.1. Mathematical Methods

The boundary value problem to be solved is that for a bicrystal with a welded interface. The two crystals on both sides of the interface are assumed to extend to infinity. Furthermore, only elastic stress fields of dislocations and their linear superimpositions are considered. The coordinate system used in the calculations is shown schematically in Figure 3.1.

The equation of elastic equilibrium can be written in terms of displacements $u_i$ (i=1,2 or 3) [45]:

$$c_{ijkl}u_{k,j,l} = 0 \quad <3.1>$$

where $c_{ijkl}$'s are elastic constants and the subscript ".," denotes differentiation with respect to the following coordinate. In this and all the following formulae in this chapter, summation is implied over repeated Latin subscripts. No summation is indicated by Greek subscripts unless explicitly written out.

Two numerical methods used in the analysis are respectively based on two mathematical methods: Tucker's complex variable analysis and Green's function technique. In
the following sections an outline is provided for each method.

![Diagram](image)

Crystal A (UHP)

Grain Boundary

Crystal B (LHP)

Figure 3.1. Geometry and Problem Coordinates for Stress Analysis

3.2. Tucker's Complex Variable Analysis [16]

The following is a summary of Tucker's formulation to solve equation \( \langle 3.2 \rangle \), subject to boundary conditions suitable to the dislocation/grain boundary problem.

Since in our problem, stress and displacement components are assumed to be independent of \( x_3 \), solutions to \( \langle 2 \rangle \) can be expressed as analytic functions of the complex variables \( z = x_1 + px_2 \) in the form [17]:

\[
    u_i = A_i f(z) \quad \langle 3.2 \rangle
\]
By substituting \( \langle 3.2 \rangle \) into \( \langle 3.1 \rangle \), it has been shown by Eshelby et al \[17\] that \( \langle 3.2 \rangle \) is the solution provided that:

\[
| c_{11k1} + p(c_{12k1} + c_{11k2}) + p^2c_{22k2} | = 0 \quad \langle 3.3 \rangle
\]

The sextic equation \( \langle 3.3 \rangle \) can only have complex roots, occurring in conjugate pairs \[18\]. We pick three \( p_\alpha (\alpha=1,2 \text{ or } 3) \) with \( \text{Im}(p_\alpha) > 0 \). Then the displacements are:

\[
u_1 = \Sigma_{\alpha} A_{i\alpha} f_\alpha (z_\alpha) \quad \langle 3.4 \rangle
\]

where \( A_{i\alpha} \) and \( f_\alpha \) are the forms of \( A_i \) and \( f \) which correspond to the particular solution \( p_\alpha \) and \( z_\alpha = x_1 + p_\alpha x_2 \).

The strains can be found by differentiating displacement:

\[
\varepsilon_{kl} = (u_{k1} + u_{1,k})/2
\]

then stresses can be obtained using Hooke's law \[45\]:

\[
\sigma_{ij} = c_{ijkl} \varepsilon_{kl} \quad \langle 3.5 \rangle
\]

The analytical functions, \( f_\alpha \), are of the form:

\[
\begin{align*}
f^g_{\alpha}(z^g_\alpha) &= f^g_{0\alpha}(z^g_\alpha) + \Sigma_{\beta=1}^{3} \Sigma_{h=1}^{m} g_{i\alpha li} j^{g}_{ij} k^{g}_{j\beta} \bar{f}^{g}_{0\beta}(z^g_\alpha) \\
&\quad + \Sigma_{\beta=1}^{3} \Sigma_{h=1}^{m} g_{i\alpha li} \delta_{ij} k^{h}_{j\beta} \bar{f}^{h}_{0\beta}(z^g_\alpha)
\end{align*}
\quad \langle 3.6 \rangle
\]

where

\[
L_{1\alpha} = (c_{i1k1} + p_\alpha c_{i2k2})A_{k\alpha}
= -(p_\alpha c_{i1k1} + c_{i1k2})A_{k\alpha}
\]
the matrices can be calculated as follows:

\[ M = L^{-1} \quad W = AM \]

\[ j^{g,h} = [W^{g,h}]^{1/2} \]

\[ h^{g,h} = [W^{g,h}]^{1/2} \]

\[ G = H^{-1} \]

\( \delta_{ij} \) is the Kronecker delta, while \( g \) and \( h \) are general superscripts denoting individual crystals such that if \( g=1 \) (crystal A in Figure 3.1) then \( h=2 \) (crystal B) and vice versa. The stresses can now be calculated:

\[ \sigma_{11} = -\sum a_{1\alpha} \frac{\partial}{\partial x_2} [f_\alpha(z_\alpha)] \quad \langle 3.7 \rangle \]

\[ \sigma_{12} = \sum a_{1\alpha} \frac{\partial}{\partial x_1} [f_\alpha(z_\alpha)] \quad \langle 3.8 \rangle \]

The stress field around the pileup-boundary region was computed. Since both sides of the grain boundary are stressed by the dislocation under an applied stress, the forces exerted at both sides of the boundary at the pileup tip are calculated. Then the forces on each allowable slip system in the grain with emitted dislocations are calculated and used as a criterion for the most favorable slip system. Forces were calculated using the Peach-Koehler equation [45]:

\[ \frac{F}{L} = (b \cdot \sigma) \times f \quad \langle 3.9 \rangle \]

where \( F/L \) is the force per unit length exerted on the emitted dislocation, \( b \) and \( f \) are the Burgers vector and line direction of the emitted dislocations, and \( \sigma \) is the stress field of the dislocation pileup. In order to compare the
boundary term effect with that of the dislocation stress field, forces are calculated for three different cases: without boundary term (i.e., same crystal orientation across the boundary), pileup side with boundary term and emission side with boundary term. These constitute three criteria to determine which slip system in the emitted grain the dislocations choose based on the stress analyses.

3.3. Green's Function Method [19]

The Green's function [20] solution for a bimaterial solid can be obtained by solving the elastic equilibrium equation for a line force subject to the welded interface constraints. First, the following equation is solved by using the Fourier transformation for \( G \) subject to the same boundary conditions as prescribed for \( u \):

\[
Z_{ij}(x)G_{jk}(x,x') = -\delta_{ik}\delta(x-x') \tag{3.10}
\]

where \( Z_{ij}(x)=\partial^2/\partial x_i \partial x_j \), \( \delta \) is the Kronecker's delta and \( \delta(x-x') \) is the Dirac delta function. Next, the solution of equation (3.1) is given in terms of \( G \).

In the following formulae, superscript \( A, B \) denotes upper and lower crystal respectively. UHP is the upper half plane and LHP is the lower half plane.

Green's functions, their derivatives, and dislocation force functions \( F_i \), which are defined as the force field of a lattice dislocation located in \( x' \), for different cases are
explained as follows:

1. $G^{(\alpha)}_{ij}(x,x')$ will be summed over $\alpha$ alone. $G^{(\alpha)}_{ij}(x,x')$ is its derivative with respect to $z_\alpha (z_\alpha = x_1 + p_\alpha x_2)$, equivalent to $\frac{\partial}{\partial z} G^{(\alpha)}_{ij}(x,x')$

2. $G^{(\alpha,\beta)}_{ij}(x,x')$ will be summed over $\alpha$ and $\beta$. $G^{(\alpha,\beta)}_{ij}(x,x')$ is derivative with respect to $z_\alpha$, as described above.

Case 1: $x$ and $x'$ in UHP ($x_2 > 0, x'_2 > 0$)

$$G^{(\alpha)}_{ij}(x,x') = -\frac{1}{\pi} \gamma^A(p_\alpha^A) \ln[z_\alpha^A - z_\alpha^A']$$

$$G^{(\alpha,\beta)}_{ij}(x,x') = -\frac{1}{\pi} \gamma^B(p_\alpha^B) Q_\beta^B \ln(z_\alpha^B - z_\beta^B)$$

Dislocation Force Functions:

$$F_i(\alpha) = b_k L^A_2(p_\alpha^A) \quad \text{and} \quad F_i(\beta) = b_k L^A_2(p_\beta^A)$$

Case 2: $x$ in LHP, $x'$ in UHP ($x_2 < 0, x'_2 > 0$)

$$G^{(\alpha,\beta)}_{ij}(x,x') = -\frac{1}{\pi} \gamma^B(p_\alpha^B) Q_\beta^B \ln(z_\alpha^B - z_\beta^B)$$

$$F_i(\beta) = b_k L^B_2(p_\beta^B)$$

Case 3: $x$ in UHP, $x'$ in LHP ($x_2 > 0, x'_2 < 0$)

$$G^{(\alpha,\beta)}_{ij}(x,x') = \frac{1}{\pi} \gamma^A(p_\alpha^A) Q_{\beta}^B \ln(z_\alpha^B - z_\beta^B)$$

$$F_i(\beta) = b_k L^B_2(p_\beta^B)$$

Case 4: $x$ and $x'$ in LHP ($x_2 < 0, x'_2 < 0$)

$$G^{(\alpha)}_{ij}(x,x') = -\frac{1}{\pi} \gamma^B(p_\alpha^B) \ln(z_\alpha^B - z_\alpha^B)$$

$$G^{(\alpha,\beta)}_{ij}(x,x') = \frac{1}{\pi} \gamma^B(p_\alpha^B) Q_{\beta}^B \ln(z_\alpha^B - z_\beta^B)$$

$$F_i(\alpha) = b_k L^B_2(p_\alpha^B) \quad \text{and} \quad F_i(\beta) = b_k L^B_2(p_\beta^B)$$
Definition of the Matrices:

\[ \Lambda_{ij}(p_\alpha) = c_{ijkl} q_k q_l \]

where \( c_{ijkl} \) is the elastic constant tensor

\( p_\alpha = \) Roots of the equation \(| \Lambda_{ij} | = 0 \), \(| \Lambda_{ij} | \) is the determinant of \( \Lambda_{ij} \). For superscript A or B, we have:

\[ \Gamma_{ij}(p_\alpha) = \text{cofactor matrix of } \Lambda_{ij}(p_\alpha) \]

\[ \gamma_{ij}(p_\alpha) = \frac{i \Gamma_{ij}(p_\alpha)}{a(p_\alpha-p_\alpha)^\beta \beta - \alpha (p_\alpha-p_\beta)(p_\alpha-p_\beta)} \]

\[ \gamma_{s} = \sum_{\alpha} \gamma_{s}^{A,B}(p_\alpha) \]

\[ \sigma_{ij}^{A,B}(p_\alpha) = L_{ik}^{A,B}(p_\alpha) \gamma_{kj}(p_\alpha) \] and \( L_{ik}^{A,B}(p_\alpha) = c_{ikjl} + c_{ijkl} p_\alpha \)

\[ \sigma_{s} = \sum_{\alpha} \sigma_{s}^{A,B}(p_\alpha) \]

\[ M = \gamma^{A-1}_{s}(\sigma^{A}_{s} - \sigma^{A}_{s} A-1)_{s} - \gamma^{A-1}_{s} \]

\[ N = \sigma^{A-1}_{s}(\sigma^{A}_{s} - \sigma^{A}_{s} A-1)_{s} - \gamma^{A-1}_{s} \]

\[ Q^{I}_{\beta} = M[\sigma^{A}_{s}(p_\beta) - \sigma^{A}_{s} A-1(p_\beta)] \]

\[ Q^{II}_{\beta} = N[\sigma^{A}_{s}(p_\beta) - \sigma^{A}_{s} A-1(p_\beta)] \]

\[ Q^{III}_{\beta} = M[\sigma^{B}_{s}(p_\beta) - \sigma^{B}_{s} B-1(p_\beta)] \]

\[ Q^{IV}_{\beta} = N[\sigma^{B}_{s}(p_\beta) - \sigma^{B}_{s} B-1(p_\beta)] \]

\[ L_{ik}^{A}(p_\alpha) = c_{ijkl} + c_{ijkl} p_\alpha \]

\[ L_{ik}^{B}(p_\alpha) = c_{ijkl} + c_{ijkl} p_\alpha \]

When the forces produced from the dislocation are used, then the displacement field at \( x \) of an dislocation at \( x' \) can be calculated as follows:

\[ u_{j}(x,x') = \sum_{\alpha} F_{i}(\alpha) G_{ij}(\alpha)(x,x') + \sum_{\alpha \beta} F_{i}(\beta) G_{ij}(\alpha,\beta)(x,x') \]
A simple differentiation of the displacement field will yield strain and stress fields of a dislocation in the anisotropic bicrystal. The resulting formulae are as follows:

**Displacement Gradients:**

\[
u_{ij}^{(a)}(\mathbf{x}, \mathbf{x}') = F_i^j(\alpha)G_{ij}^{(a)}(\mathbf{x}, \mathbf{x}') + \sum_{\beta} F_i^j(\beta)G_{ij}^{(\alpha, \beta)}(\mathbf{x}, \mathbf{x}') \tag{3.20}\]

**Stresses:**

\[
\sigma_{ij} = \sum_{\alpha} L_{ik}^{A_j(p^A)} u_k^{(\alpha)} \text{ for } x \text{ in UHP } (x_2 \geq 0) \tag{3.21}
\]

\[
\sigma_{ij} = \sum_{\alpha} L_{ik}^{B_j(p^B)} u_k^{(\alpha)} \text{ for } x \text{ in LHP } (x_2 \leq 0) \tag{3.22}
\]

Again, the stress field of a dislocation pileup is obtained by summing over all the dislocations.

Although identical results were obtained using either method, both were adopted because of several advantages in doing so. First this provides a thorough check of both the algorithm and the programming for two methods. It would be most unlikely that two different procedures get the same answer with hidden errors. Secondly in the further studies of similar problems involving other types of defects than grain boundaries and dislocations, one will be superior to the other in terms of expandability and adaptability.

### 3.4. Computer Programs

The pileup tip stress field was calculated for
experimentally-observed pileup configurations. The magnitude of stress involved in the slip propagation helps to understand boundary-dislocation events and support suggested slip propagation models. All the programs are written in Vax Fortran [65].

The program uses "problem coordinates", the coordinate system shown schematically in Figure 3.1. \( x_3 \) is along the dislocation line direction, \( x_2 \) is the grain boundary plane normal and \( x_1, x_2, x_3 \) form a right-handed system. Since all the dislocation and grain boundary parameters were measured in terms of crystal coordinates, they are first converted into the problem coordinates before being used in the calculation. In the calculation, strain and displacement components are assumed to be independent of the third axis of the problem coordinates, which is parallel to dislocation lines. The elastic equilibrium equation is solved to give a planar distribution of the displacement fields, from which strain and stress fields are subsequently obtained. The stress field at the pileup tip is the linear summation of all the stress fields of the individual dislocations in the pileup.

The stress calculation program listed in Appendix A using Tucker's complex variable analysis is adapted from the original program developed by Wagoner [66].

The stress calculation program using Green's function method is listed in Appendix B. When the test calculation
for three different cases (a mixed dislocation in the upper half plane, in the lower half plane and in the boundary) are compared with the results from Tucker's method a perfect match was obtained. This provides a check on the correctness of both the programs. Figure 3.2 shows the path along which the stress profiles plotted in Figures 3.3-3.6 were calculated. Figures 3.3 - 3.5 are a series of calculation results plottings for comparison of the two methods for different cases, all the results being identical for the two calculation methods outlined above. Figure 3.6 shows a typical stress contour plot for a mixed dislocation located at the origin. Identical results are again obtained using the two methods.

\[ X_2 \text{ (Path of Stress Profile)} \]

\[ \perp (10,10) \text{ Fig. 3.3} \]

\[ \perp (10,0) \text{ Fig. 3.4} \]

\[ \perp (10,-10) \text{ Fig. 3.5} \]

Figure 3.2. Spatial path for stress profile calculations
Figure 3.3. Stress Profile for Dislocation in UHP

Figure 3.4. Stress Profile for Dislocation in LHP
Figure 3.5. Stress Profile for Dislocation in Boundary

Figure 3.6. A Typical Anisotropic Elastic Stress Contour Plot for a Dislocation in a Bicrystal
CHAPTER IV
EXPERIMENTAL PROCEDURES

4.1 Sample Preparations

Disc samples 3 mm in diameter were made from 304 stainless steel for static TEM experiments. Miniature tensile specimens used in HVEM straining experiments were made both from 304 stainless steel and molybdenum.

304 stainless steel sheets with the dimension 0.040" by 12" by 12" were supplied by Republic Steel. Table 4.1 shows its composition.

Table 4.1. Composition of 304 Stainless Steel

<table>
<thead>
<tr>
<th>C</th>
<th>Mn</th>
<th>P</th>
<th>S</th>
<th>Si</th>
<th>Ni</th>
<th>Cr</th>
<th>Fe</th>
</tr>
</thead>
<tbody>
<tr>
<td>.055</td>
<td>1.41</td>
<td>.019</td>
<td>.011</td>
<td>.35</td>
<td>8.15</td>
<td>18.11</td>
<td>Balance</td>
</tr>
</tbody>
</table>

First the sheet was cold rolled to 0.2 mm thick foils. Then the foils were solution treated at 1080°C for 1 hour in argon atmosphere and water quenched to room temperature to avoid sensitization.

Pure molybdenum in the form of 0.005" foil was supplied by Materials Research Corporation, Orangeburg, NY 10962.
The molybdenum foil was rolled to size, chemically cleaned and packaged in inert atmosphere.

Annealed stainless steel foil was electrothinned in a 55% \( \text{H}_3\text{PO}_4 \)-25% \( \text{H}_2\text{SO}_4 \)-20% methanol solution at a potential of 10 volts. The resulting 0.1 mm foils were punched into 3 mm diameter discs and then jet-polished in a Struer's Tenupol unit to obtain electron-transparent thin areas. The electropolishing parameters are listed in Table 4.2.

For making miniature tensile samples, stainless steel foils with a thickness of 0.1 mm were prepared according to the above procedure. Molybdenum foils were annealed at 2000°C for 1 hour in dry hydrogen atmosphere [94]. The molybdenum foils were then mechanically ground to 800 grade using diamond sandpaper. The finished foil has a thickness of 0.1 mm. The thin foils of stainless steel and molybdenum obtained were subsequently photo-milled [95] to the specified size for tensile samples to be used in the double-tilt straining stage of KRATOS EM1500 high voltage electron microscope. A miniature tensile specimen obtained from photo-milling is shown in Figure 4.1.

The annealing of molybdenum and the solution treatment of stainless steel are aimed at obtaining samples with a grain size on the order of 30-50 \( \mu \text{m} \). This grain size range is desirable because it facilitates the crystallographic characterization by providing a large area of view in the same grain when the sample is studied in the electron
microscope.

The tensile specimens were jet-polished to obtain thin areas in Tenupol unit using a special masking technique developed by Hardiman et al [89]. The polishing solutions and parameters for both materials are listed in Table 4.2. The finished samples were checked in a JEOL 200CX TEM for small elliptical center hole with no cracks and uniform thin area zone. Figure 4.2 shows a tensile sample which is already electropolished to perforation to obtain the electron-transparent thin area.

Table 4.2. Electropolishing Conditions for Sample Preparations

<table>
<thead>
<tr>
<th>Material</th>
<th>Electrolyte</th>
<th>Voltage</th>
<th>Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stainless</td>
<td>25% nitric acid</td>
<td>8 Volt</td>
<td>-45°C</td>
</tr>
<tr>
<td>Steel 304</td>
<td>methanol solution</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pure</td>
<td>12% sulfuric acid</td>
<td>30 Volts</td>
<td>-40°C</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>methanol solution</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Figure 4.1. A Photo-Milled Miniature Tensile Sample

Figure 4.2. An Electro-polished Miniature Tensile Sample
4.2 Transmission electron microscopy procedures

Disc specimens were studied in a double-tilt goniometer specimen stage. First a high angle grain boundary with an interacting dislocation pileup is located. These grain boundary/dislocation pileup configurations arise from the deformation occurring during punching of the disc and subsequent flattening of the sample.

For several different tilts, Kikuchi patterns of both grains are recorded on micrographs. The Kikuchi line pattern is also used as a road map to tilt to different poles of each grain. Around each pole, two-beam diffraction conditions are established for each available diffraction vector.

Micrographs were taken from each grain with both bright and dark field illumination for the diffraction vector thus established. Corresponding diffraction vectors were also recorded on micrographs. Figure 4.3 shows a typical set of diffraction pattern, bright field and dark field micrographs.
Figure 4.3. A Typical Set of Micrographs Used to Identify the Dislocation Burgers Vector
Figure 4.4. Procedures for Misorientation Determination Using Kikuchi Patterns (Adapted from Ref. 13)
Kikuchi patterns obtained during the TEM experiment are used to determine the misorientation of the bicrystal using the computer programs developed by Heilman et al. [79], running in an IBM PC. These programs are: "Digit" which is used to digitize the Kikuchi lines; "Orient" which is used to index the Kikuchi lines and their intersecting poles from the digitized data; and "Mismat" which is used to determine the misorientation of the crystal pair from the information obtained from the "Orient" program. The procedure is outlined in Figure 4.4. The estimated accuracy is ±0.1° for the misorientation by this method [79].

The misorientation of the bicrystal can also be determined by plotting the orientations of each crystal on a stereographic projection. This method, which is less accurate (±1° [15]) than the Kikuchi pattern analysis, can be used to check the result obtained from the Kikuchi pattern analysis and control the tilting experiment.

Dislocation Burgers vectors are determined from the micrographs according to the standard image contrast procedure using the \( g \cdot b = 0 \) invisibility criterion [77,78]. The criterion states that the dislocation is invisible under two-beam imaging when \( g \cdot b = 0 \) for a screw and \( g \cdot (b \times \xi) = 0 \) for an edge. In the above \( g \) is the diffraction vector, \( b \) is the Burgers vector and \( \xi \) is the line direction. Although
this criterion relies on the material being elastically isotropic [78], it has been shown that when this criterion gives an extinct or weak image it was sufficient to identify dislocations of anisotropic materials [15], any ambiguity will be removed when image simulation described in section 2.5 is used to match computed and experimental dislocation micrographs.

Grain boundary normal, dislocation line directions and slip planes are found using stereographic trace analysis [78]. Any vector such as the dislocation line direction is projected to the micrograph as an apparent vector. The true vector must lie on a great circle passing through the apparent vector and the beam direction. Thus two projections using different beam directions can be used to locate the true vector direction. A third projection is normally used to check the correctness of the determination. Planes are determined the same way if two vectors lying on them can be identified.

Preliminary determination of the slip plane in fcc metals is accomplished by observing the profile of the trace from various beam directions and comparing it with the predicted behavior of the four fcc slip planes [15]. When a slip trace is present, the slip plane is determined from the cross product of the slip trace and the dislocation line direction [15]. In fcc metals, both optical microscopy [91] and electron microscopy [92] showed that \(\{111\}<110>\) is the
only slip system which is operative at room temperature. This is due to the fact that slip can occur much more easily on a plane of closest packing and in a direction of densest atomic distance [93]. As will be shown later in this thesis, this is the observed operative slip system in fcc austenitic stainless samples, which were analyzed quantitatively.

Finally, the dislocation spacings in a pileup were measured from the TEM negative with a Nikon Measurescope. The spacings measured in this way has an error smaller than the width of dislocation image on the negative, approximately ±10 nm.

The above crystallographic characterization procedure can be explained most clearly by an illustration using a particular boundary in static TEM experiments. The following procedure and micrographs refer to boundary number 4, as presented in Chapter V. The characterization process will be presented step by step in the following section. Dislocation parameters of the pileup will be obtained explicitly.
Figure 4.5 Effect of the relative angle between slip plane and beam direction on the dislocation pileup image.
1. Slip plane determination

By observing the dislocation images taken near the (011) pole, the two slip planes (111) and (111) can be ruled out. The reason is that if dislocations were on these two slip planes, the pileup would have the appearance as sketched in Figure 4.5(b) instead of the appearance shown in Figure 4.5(a), which agrees with the TEM observations. Moreover, when the crystal was tilted toward (111) pole, the image length of dislocations shortened and when the crystal was tilted toward the (111) pole, the image length of dislocation lengthened. This indicated that the pileup slip plane is (111).

2. Dislocation line direction and boundary plane determination

The dislocation nearest the grain boundary was first examined for line direction. For a chosen beam direction, the angle between the projection of the line to be indexed (line direction or one of the two vectors lying in the grain boundary plane) and the imaging diffraction vector is measured. Both the diffraction vector and this projection should lie on the great circle perpendicular to the beam direction. Thus the projection can be marked on the stereogram of the reference crystal (the crystal containing the dislocation pileup). Next a great circle is drawn through the projection and the beam direction. The true
direction is on this great circle. Let this great circle be called the solution great circle. This step is shown in Figure 4.6(a).

The above step is then repeated for two more beam directions. The intersection of the solution great circles is the true direction, as shown in Figure 4.6(b). By measuring the angles between the line direction and the known poles shown in Figures 4.6(a) and 4.6(b), the line direction is determined as [\bar{1}67]. In the same manner, two vectors lying on the grain boundary were indexed and their cross product is the boundary normal.

3. Burgers vector determination

Figure 4.7 shows the pileup dislocation image using several two-beam diffracting vectors. Table 4.3 lists predicted imaging condition using $g\cdot b$ criteria along with the observed imaging condition. The Burgers vector will be determined by this truth table first and then confirmed by the image simulation technique in the following paragraphs.
Figure 4.6(a) Determination of the Great Circle Containing True Line Direction

Figure 4.6(b) Determination of Line Direction
Figure 4.7 Dislocation imaging under two-beam diffraction conditions

(a) $g = 202$
(b) $g = \bar{2}20$
(c) $g = 002$
(d) $g = 11\bar{1}$
(e) $g = 200$
(f) $g = \bar{1}1\bar{1}$
Table 4.3 Truth Table for Identifying Pileup Dislocation Burgers Vector

<table>
<thead>
<tr>
<th>Burgers Vector</th>
<th>g=202</th>
<th>g=220</th>
<th>g=002</th>
<th>g=111</th>
<th>g=200</th>
<th>g=111</th>
</tr>
</thead>
<tbody>
<tr>
<td>a/2[110]</td>
<td>1</td>
<td>2</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>a/2[101]</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>a/2[011]</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>a/2[110]</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
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<tr>
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<td>1</td>
<td>1</td>
<td>1</td>
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<td>0</td>
</tr>
<tr>
<td>a/2[011]</td>
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<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

Observed Contrast

S: Strong Contrast  W: Weak Contrast

From the contrast analysis shown in Table 4.3, it was determined that the Burgers Vector is either [011] or [011], which have the same contrast behavior in this analysis.

Next, image simulations [78] were performed for these two cases. Table 4.4 lists the parameters used in the image simulation. The specimen thickness in units of the extinction distance \( f \) was estimated from the image [78] and adjusted so that the calculated and photographed images match each other. The calculated and TEM images of pileup dislocations are shown and compared in Figures 4.8 and 4.9.

It was determined from the image matching that the Burgers
vector of the pileup dislocations is \([0\bar{1}1]\).

Table 4.4 Parameters used in dislocation image simulation

Elastic constants \([45]\):

\[
\begin{align*}
c_{11} & = 2.42 \\
c_{12} & = 1.465 \\
c_{44} & = 1.12
\end{align*}
\]

Line Direction = \([\bar{1}67]\)

Beam direction = \([2\bar{1}1\bar{9}]\)

Foil Normal = \([57\ 20\ 77]\)

Specimen Thickness = 5.4 \(\xi_{g}^{111}\)

Dimensionless Parameter \(w = s\xi_{g} = 0.1\)

where \(s\) is the amount of deviation from Bragg diffraction.
Figure 4.8 Bright field dislocation image matching. \( g = [111] \)

\[ b = [0\bar{1}1] \text{ match} \quad b = [01\bar{1}] \text{ no match} \]

Figure 4.9 Dark field dislocation image matching. \( g = [\bar{1}1\bar{1}] \)

\[ b = [0\bar{1}1] \text{ match} \quad b = [01\bar{1}] \text{ no match} \]
4.3 High voltage electron microscopy procedures

Miniature tensile specimens were mounted in the double-tilt tensile straining stage. The final image is either shown on the fluorescent screen of the microscope or displayed on a television monitor which gets the signal from a video camera mounted at the bottom of the microscope column.

4.3.1 Dynamic in-situ straining in HVEM

The grain boundary-dislocation interactions are dynamic. Therefore, in order to understand the process it is essential to observe them continuously while the specimen is under stress. Moreover, the higher voltage employed enables dislocation and grain boundary structures in thicker areas to be studied. As the thickness increases, the structure of defects and their stress field becomes closer to those in the bulk materials. Since we are interested in relating electron microscope studies to the bulk properties of materials, this ability is particularly relevant. The mechanisms and models proposed based on the static observations can be tested by these experiments. Our knowledge of the yielding process is enhanced by such
Because of higher accelerating voltage, the electron wave length decreases, resulting in a Ewald sphere with a flatter surface. It becomes very easy to excite many beams at one time. On one hand, more excited beams means the grains with different orientations can be in contrast, which is advantageous when the goal is to observe dislocation-grain boundary interaction taking place in different grains simultaneously. On the other hand, it is more difficult to establish the two-beam diffraction condition essential for determination of dislocation Burgers vectors.

4.3.2 Detailed straining and monitoring procedures

In order to avoid excessive radiation damage to the sample area under observation, proper voltages are selected (500 kV for stainless steel, 800 kV for molybdenum). In the thin area surrounding the perforation, an area of interest with grain boundary and dislocations was sought. The ideal area is the grain boundary with dislocations on both sides and at least on one side a regular array of dislocations is apparent. Kikuchi line patterns were photographed from both sides of the grain boundary for the determination of relative orientations of the bicrystal. Micrographs of prominent features were also recorded for later comparisons.
For the selected area, a two-beam condition was set up for both crystals. Thus it was possible to monitor the behavior of the dislocation on both sides of the grain boundary during the straining experiment.

The straining operation was first performed by a mechanical tensile drive. The imaging conditions change as the stress is applied because of the non-uniform sample thickness and irregular geometry of the thin area, which cause changes in crystal orientation. It is therefore very important to maintain the original imaging condition by periodically checking the diffraction pattern. When the thin area began to experience the tensile strain, as was indicated by the movement of bend contours, the mechanical drive was stopped and a piezo-electric drive was used for further straining. The area of interest was shown on the television monitor and recorded on a video cassette tape. When the maximum allowed voltage on the piezo-electric drive was reached, the voltage was returned to zero and any slack resulted from this was taken up with the mechanical drive. Then the piezo-electric drive was used again. This procedure was repeated until noticeable movement occurred at or near the area being monitored. At that time, the interaction events taking place were recorded and straining operation was carried out slowly.

During straining, if there was a dislocation pile-up, it was periodically checked for any detectable dislocation
movement. Early indications of the straining of the observed area could come from the movement of dislocations away from the grain boundary. The resistance to flow from both the grain boundary and other dislocations is less farther away from the boundary due to lower dislocation densities away from the boundary.

Uniaxial tensile stress can be assumed for the area under observation which has a width much smaller than the size of the center hole [90]. In the miniature samples studied, thin area width to minor axis ratios are under one fifth. The center hole and thin area are shown schematically in Figure 4.10. The stress distribution is shown in Figure 4.11 for an elliptical hole with applied tensile stress $S$. The stress along the coordinate $\eta$ which spans the thin area is plotted. Another parameter $\xi$ which is a measure of the hole size is assumed to be constant, since the thin area is only a narrow strip. The center hole is assumed to be an ellipse with its major axis being twice of its minor axis. For this case, the stress component $\sigma_\eta$ which is plotted in Figure 4.11 can be expressed as follows [91]:

$$
(\sigma_\eta) = S \frac{7 - \frac{1}{3} \cos 2\eta}{\frac{5}{3} - \cos 2\eta} <4.1>
$$
Figure 4.10. Approximate Shape of the Center Hole and Thin Area of a Miniature Tensile Specimen

Figure 4.11. Calculated Stress Distribution for Thin Area
In this stage, any dislocation activities near the grain boundary are carefully observed and recorded. These fall mainly into two types. The first type is the direct dislocation movement toward the grain boundary and interaction with the boundary in various ways such as absorption, transmission, and reflection. The second type is the dislocation motion near the grain boundary which is influenced by the presence of the boundary.

Some guidelines from experience and experiment which tend to create favorable conditions for dislocation movement to be observed are listed as follows:

1. Smooth holes and a uniformly thin area are desirable. There should not be any harmful cracks, which will tend to break the sample if they develop further. The electron transparent region on the shores of the hole should be as uniform as possible both in terms of thickness and width to avoid premature tearing of the sample.

2. Samples are sought with a very long grain boundary running parallel to the long edge of the elliptical hole, which is also approximately the direction of tensile stress.

3. Existing pileups should make an angle close to 45 degrees with the tensile axis in order to maximize the Schmidt factor and consequently the activating stress.

When the above guidelines were followed and close attention was paid to the area of interest as the sample was strained, dislocation movement can often be observed.
However, patience and care are essential in these experiments to ensure success. The number of samples which broke before they could offer any result is several times the number of sample in which results were obtained.
CHAPTER V
RESULTS

5.1 Static observations of grain boundary-dislocation interaction configurations

Several types of pileup configurations were observed in static experiments carried out using JEOL 200CX transmission electron microscopy. These configurations all involve the dislocation pileups at the grain boundary and dislocation emission from the other side of the boundary.

In Figure 5.1, the pileup impinges on an advancing twin boundary step, and the transmission of each dislocation leaves a grain boundary dislocation (gbd) in the interface and extends the step by one gbd Burgers vector. In Figure 5.2(a) and (b), a pileup penetrates a boundary and nucleates a group of dislocations which remain attached to the grain boundary. In Figure 5.3, the pileup penetrates the boundary and generates another array of dislocations in the second crystal. In Figure 5.4, the dislocations emerging from the boundary are partial dislocation, which combine into lattice dislocations away from the boundary. The direction of dislocation motion in these figures was determined by the curvature of the dislocation lines and by the dislocation
spacings on the two sides of the grain boundary. This method of determining the dislocation movement direction was supported by the dynamic straining observations.

Figure 5.1. Grain Boundary 1, \( g = \bar{1}11 \)
(a) Pileup side, \( g = \overline{220} \)

(b) Emission Side, \( g = 0\overline{2}2 \)

Figure 5.2. Grain Boundary 2
Figure 5.3. Grain Boundary 3, $g = 11\overline{1}$

Figure 5.4. Grain Boundary 4, $g = 0\overline{2}2$
Crystallographic and numerical analyses were carried out for each of the four examples above. Table 5.1 lists the crystallographic parameters measured; the Miller indices for each parameter are expressed in their respective crystal coordinates.

Table 5.1. Crystallographic Parameters

<table>
<thead>
<tr>
<th>Bdy XI</th>
<th>Boundary Normal</th>
<th>Burgers Vector</th>
<th>Line Dir.</th>
<th>Slip Plane</th>
<th>Rotation Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(111)</td>
<td>(a/2)[101]</td>
<td>[110]</td>
<td>(111)</td>
<td>0.333 0.666 0.666</td>
</tr>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.666 0.666 0.333</td>
</tr>
<tr>
<td>2</td>
<td>(a/2)[101]</td>
<td>[231]</td>
<td>(111)</td>
<td>-0.66</td>
<td>0.333 0.666</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.666 0.666 0.333</td>
</tr>
<tr>
<td>1</td>
<td>(013)</td>
<td>(a/2)[110]</td>
<td>[421]</td>
<td>(111)</td>
<td>0.875 -0.17 0.452</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.127 0.983 0.131</td>
</tr>
<tr>
<td>2</td>
<td>(a/2)[110]</td>
<td>[615]</td>
<td>(111)</td>
<td>-0.47</td>
<td>-0.06 0.883</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>1</td>
<td>(214)</td>
<td>(a/2)[101]</td>
<td>[110]</td>
<td>(111)</td>
<td>0.333 0.666 -0.66</td>
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<td></td>
<td>-0.67 0.667 0.333</td>
</tr>
<tr>
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<td></td>
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<td>0.667 0.333 0.667</td>
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<tr>
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<td>(a/2)[011]</td>
<td>[155]</td>
<td>(111)</td>
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<td></td>
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<td></td>
<td>0.127 0.983 0.131</td>
</tr>
<tr>
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<td>(119)</td>
<td>(a/2)[011]</td>
<td>[670]</td>
<td>(111)</td>
<td>0.925 -0.38 -0.02</td>
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<td></td>
<td></td>
<td>0.372 0.918 -0.14</td>
</tr>
<tr>
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<td></td>
<td></td>
<td></td>
<td>0.372 0.918 -0.14</td>
</tr>
<tr>
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<td>[793]</td>
<td>(111)</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td>0.372 0.918 -0.14</td>
</tr>
</tbody>
</table>
In grain boundaries 1, 2 and 3, the (011) poles are within 10 degrees of the foil normal. Moreover, the number of $\Sigma=3$ twin (93) and non-twin boundaries (16) in the field of view of the microscope during the observations show clearly that the majority of the boundaries in the thin area are $\Sigma=3$ twin boundaries. Such boundaries are therefore expected to have a major influence on the initiation of the yielding process. Boundaries 1 and 3 are twin boundaries on (111) planes. Boundary 2 is about 3 degrees deviated away from the $\Sigma=45$ coincidence site boundary about [144]. Boundary 4 is a general high angle boundary, rotated 23 degrees about [319].

5.2. Slip Propagation Criteria

Dislocation transmission events observed in the TEM were fully characterized as described in the previous section. The parameters obtained were subsequently used in the computation of the stress field of the pileup and in the study of the detailed slip propagation process. The static experiments consists of four dislocation transmission events. In the following subsections, these events will be analyzed in the light of both geometric and stress calculations for the prediction of the activated slip systems.
The basic stress calculations used in the slip propagation criteria were based on the procedures outlined in Chapter III. The detailed applications of these calculations to the above dislocations propagation across grain boundary process are explained in the following:

1. The crystallographic parameters were obtained from the analysis procedures described in Chapter IV.

2. These parameters were used as input data for the stress calculation programs described in Chapter III. The anisotropic elastic stress fields of all the pileup dislocations were computed and summed.

3. The stress tensor at the position of the head dislocation (excluding its self stress field) was obtained.

4. This stress field was used to calculate the resolved shear stresses for each of the possible emission slip systems in the grain where the dislocations were emitted.

5.2.2. Proposed slip system selection criteria

It has been confirmed by previous studies by Bamford et al. [55] that the choice of the slip system for the emitted dislocation in the cases of dislocation transmission is predictable. The choice is not only affected by the grain boundary plane and the orientation relationships between two grains involved, it is also influenced by the resolved shear stress on the particular slip system. In the following.
several possible criteria for predicting the emitted slip system are compared for the observed transmission events.

1. Livingston and Chalmers' Criterion

Livingston and Chalmers [53] proposed that for a pure shear stress, the transmission parameter for a certain slip system can be expressed as:

\[ N = (e_1 \cdot e_1) \times (g_1 \cdot g_1) + (e_1 \cdot g_1) \times (e_1 \cdot g_1) \]  \( <5.1> \)

where the pileup dislocations lie in a slip plane with the normal \( e_1 \) and slip direction \( g_1 \), while \( e_1 \) and \( g_1 \) are the plane normal and slip direction in the emitted grain. All of the above are unit vectors. This formula is derived from the tensor transformation of the assumed pure shear stress on to a set of axes aligned with slip system \( i \). The operative slip system is predicted to be that for which \( N \) is a maximum.

In this criterion, only the crystal orientation is considered and the effect of the grain boundary plane is not taken into account.

2. Intersection Line and Slip Direction Criterion

The geometric criterion we propose here is based on minimizing the angles between the pileup Burgers vector and emission Burgers vector, and between the pileup intersection
line (with the boundary) and the emission intersection line (with the boundary). The intersection line is common to both the slip plane and the boundary plane, as shown in Figure 5.5. The slip which minimizes the angles between the intersection lines and the slip directions is chosen as the favored slip system. The maximizing factor M can be expressed as:

\[ M = (L_1 \cdot L_1)(g_1 \cdot g_1) \]  

where \( L_1 \) and \( L_1 \) are the intersection lines and \( g_1 \) and \( g_1 \) are slip directions in the pileup and emitted grains, respectively. Also, the dot product in each pair of parentheses can predict the favored slip plane and slip direction respectively.

Figure 5.5 Intersection lines and the angle between them
3. Stress Criterion

Since both the transmission and the nucleation processes are likely in slip propagation events, the forces exerted on a dislocation on either side of the boundary at the pileup tip are calculated. The forces on each slip system in the grain containing emitted dislocations are calculated using the Peach-Koehler equation [45] and the anisotropic elastic solution discussed in Chapter III., and used as a criterion for the most favorable slip system. In order to compare the effect of the boundary with that of the dislocation stress field, forces are calculated for three different cases:
A. On the pileup side, including the boundary term.
B. On the emission side, including the boundary term.
C. Without the boundary term (either side).

The chosen slip system in each case is that for which the force on the head dislocation is maximized.

4. Combined Geometric and Stress Criterion

The slip plane was first chosen, using criterion 2, and the slip direction is then chosen according to the above stress criterion.
All the possible operative slip systems in fcc metals at room temperature are listed in Table 5.2. Results for emission slip system analysis are shown in Table 5.3. Each criterion predicts the most likely slip system activated by the dislocation pileup in the neighboring grain for the boundary. The subsets of criteria three and four all predict the same results as the main criteria. Therefore, only one column is listed for each.

The entire crystallographic and stress analysis procedure is outlined in Figure 5.6. In the figure, $F$ is the resolved shear stress per unit length exerted on the head dislocation of the pileup by the pileup under the applied stress. $\sigma^\infty$ is the equivalent pileup tip stress which is $F/|b|$, a measure of the pileup strength. $\bar{\sigma}$ is the total stress $\sigma^\infty$ divided by the number of the "free" dislocations in the pileup.
Table 5.2. Numbering of Available FCC Slip Systems

<table>
<thead>
<tr>
<th>Slip System</th>
<th>Burgers Vector</th>
<th>Slip Plane</th>
<th>Slip System</th>
<th>Burgers Vector</th>
<th>Slip Plane</th>
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<td>7</td>
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<td>2</td>
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<td>-1 1 1</td>
<td>12</td>
<td>1 -1 0</td>
<td>1 1 -1</td>
</tr>
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</table>

Table 5.3. Summary of the Transmission Criteria

<table>
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<th>Criterion</th>
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<th>2</th>
<th>3</th>
<th>4</th>
<th>Observed</th>
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<td></td>
</tr>
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<tr>
<td>4</td>
<td>10</td>
<td>4</td>
<td>11</td>
<td>4</td>
<td>4</td>
</tr>
</tbody>
</table>
PILEUP SLIP SYSTEM (CRYSTAL A)

TEM
- MISORIENTATION (A/B)
- SLIP SYSTEM CHARACTERIZATION (A)

TEM OBSERVATION
- SLIP SYSTEM (B)

COMPARE

ANISOTROPIC ELASTIC STRESS CALCULATION

PREDICTED SLIP SYSTEM (B) (CRIT. 1,2,3,4)

\[ F \quad \sigma^* \]

\[ \sigma \]

FIGURE 5.6 Outline of the Slip Propagation Study
As can be seen from Table 5.2, both the geometrical and static stress field calculations are more satisfactory than the criterion proposed by Livingston and Chalmers [53]. However, neither can make correct predictions for all cases. Although the dislocation and grain boundary interaction forces at the time of the interaction can be successfully approximated by the above scheme, little information about the distribution of the external stress field can be obtained from the static observations, especially when the stress field might be modified by other local features, such as a nearby crack or precipitates. In boundary 4, the presence of partial dislocations introduce another dimension of complexity, which has not been considered here. The geometric criterion (thereafter this denotes the one proposed here), while not able to pinpoint the correct slip system for boundary 1, does give correct slip plane for all the boundaries. The failure to predict the correct Burgers vector for boundary 1 may be related to the energy minimization of the dislocation-boundary interactions. From these results, it is clear that the activated slip plane in slip propagation via dislocation transmission is controlled by the geometric factors, which include both the misorientation and the grain boundary plane. The criterion based on Livingston and Chalmers' work was not satisfactory because of its exclusion of the
boundary effect. However, the slip direction of activated dislocations is controlled by the resolved shear stress calculated from elastic anisotropic stress field of the dislocation pileup.

For the pileup configurations shown above, the head dislocations have forces acting on them in the direction of the pileup (i.e., toward the boundary) according to the stress field analysis. The values of the forces exerted on the head dislocation of the pileup by the stressed pileup are shown in Table 5.4, and represent a lower bound estimate of the obstacle strength. The tip force is converted to an "equivalent tip stress" by dividing the force by the magnitude of the Burgers vector. The equivalent stress represents the shear stress necessary at the location of the head dislocation to produce the same force as calculated above. When the total equivalent stress is divided by the number of free dislocations in the pileup the average applied stress on each free dislocation, at the time the pileup spacings were established, is obtained. The value of this average applied stress can range from a minimum (the lattice friction stress) to a maximum applied stress for slip propagation. It is interesting to note that the pileup tip stresses are comparable to the order of magnitude as the bulk yield stress of annealed 304 stainless steel (210 MPa [46]). However, it is only an indication that the stresses calculated are in a reasonable range. These stresses are
required for the slip propagation via dislocation transmission and represent obstacle strength of the individual grain boundaries in a polycrystalline metal.

Table 5.4. Pileup Tip Forces and Equivalent Stresses

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Total Tip Force (N/m)</th>
<th>Equivalent Tip Stress (MPa)</th>
<th>Average Stress (MPa)</th>
<th>Average Force (N/m)</th>
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</thead>
<tbody>
<tr>
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<td>0.096</td>
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<td>19</td>
<td>0.0048</td>
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<tr>
<td>2</td>
<td>0.072</td>
<td>280</td>
<td>19</td>
<td>0.0048</td>
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<td>3</td>
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<td>4</td>
<td>0.102</td>
<td>400</td>
<td>33</td>
<td>0.0085</td>
</tr>
</tbody>
</table>

5.4. Results from dynamic in-situ straining experiments

The first set of straining experiments was carried out on the KRATOS EM1500 high voltage electron microscope in Argonne National Laboratory. Seven miniature tensile specimens were studied. For each of these samples, one or more grain boundary orientations were characterized by taking Kikuchi patterns across the boundary and micrographs with two-beam condition established. The tensile load was then applied by mechanical and piezo-electric drives as outlined in the recommendations in section 4.3. 1.7 KV is
the maximum voltage applied on piezo-electric crystals to avoid sparking. However, when the piezo-electric drive was turned off to let the mechanical drive to take up the slack, the dislocation motion only slows down and does not reverse its direction as observed in molybdenum in video tapes recorded by Clark [61]. The field of view was carefully chosen according to the guidelines listed in section 4.3 to increase the probability of the interaction process being recorded on the video-tape. After the termination of the dynamic interaction process caused by specimen tearing, micrographs were again taken if possible. The three specific dislocation pileup/grain boundary interactions described were recorded in specimens number 2, 6 and 7.

The second set of dynamic experiments were carried out on the same type of microscope in Lawrence Berkeley National Laboratory. Out of six samples studied (three 304 stainless steel and three molybdenum), dislocation-grain boundary interactions were observed in one stainless steel sample and two molybdenum samples.

Since the pileup dislocations seem to be generated during the deformation process and the specimen upon completion of the dynamic observations were not amenable for crystallographic characterizations due to extensive thin area damages, quantitative results are extremely difficult to obtain. Therefore, out of seven dislocation-grain boundary interaction events observed in the HVEM experiments, only in
one event the characterization of grain boundary and dislocation parameters was successfully carried out. This interaction event consists of dislocation absorption into the grain boundary and dislocation emission from the other side of the boundary. Consequently, it is possible to analyze the stress fields and compare with the criteria established above during the static TEM experiments.

A multitude of dislocation-grain boundary interaction processes are observed in the dynamic experiments. The interaction events recorded are the ones which appear to be more common and take place most frequently under the experimental arrangement.

Because of rapid tearing of the specimens when the dislocations move and interact with grain boundaries, it is not always possible to record the post-deformation image on the micrograph. Because of the above-mentioned difficulties in the dynamic in-situ straining experiments, for many dislocation-grain boundary interaction events it was not possible to perform crystallographic characterization. In fact, in more than twenty-three samples strained, interaction events were recorded from six samples, and only in one dislocation transmission case was the crystallographic characterization successfully carried out. Although great efforts were applied to obtain these important results on clearer micrographs, in some cases video images are the only evidence on which the discussions will be based. Therefore,
only the dislocation transmission across the grain boundary will be presented and analyzed quantitatively in sub-section 5.4.1. Nevertheless, the qualitative results from these experiments offer useful insight into the initial stages of polycrystalline metal deformation and will be presented qualitatively in the remaining sub-sections.

5.4.1. Dislocation transmission across the grain boundary

As shown in Figure 5.7(a), a dislocation pileup forms in grain 1 and moves against the grain boundary. In grain 2, we can see a trace left by emitted dislocations. Figure 5.7(b) shows the transmission event in more detail. These micrographs were taken while the specimen was under the applied stresses and the dislocations involved were still moving. Moreover, the formation process of the dislocation pileup shown here was recorded on the video tape. This configuration is frequently observed in both the static TEM and dynamic HVEM experiments. Therefore, as in the case of static studies, both crystallographic and stress analyses are performed for this case.
(a) Dislocation Pileup of the Dynamic HVEM Experiment

(b) Details of transmission

Figure 5.7. Dynamic dislocation transmission event
For this dynamic dislocation transmission event, the crystallographic parameters are listed in Table 5.5. This is a $\Sigma = 3$ high angle grain boundary in a stainless steel sample. The results from stress field calculations using the same method which was described in 5.1 are shown in Table 5.6. It should be mentioned that these values are within the range of the values listed in Table 5.4 for the grain boundaries studied using static TEM technique. The same slip transmission criteria developed for the above-mentioned static experiments were used to check this event and the result is shown in Table 5.7. The same criterion number 4 which worked best for the static cases predicted the correct dislocation emission slip system that was activated.

Table 5.5. Crystallographic Parameters
For the Dynamic Dislocation Transmission

<table>
<thead>
<tr>
<th>Crystal Boundary</th>
<th>Burgers Line</th>
<th>Slip</th>
<th>Rotation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal Vector</td>
<td>Dir. Plane</td>
<td></td>
<td>Matrix</td>
</tr>
<tr>
<td>1 (01\bar{1})</td>
<td>(a/2)[10\bar{1}]</td>
<td>[011]</td>
<td>(111)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.667 -0.33 -0.66</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.666 0.666 0.333</td>
</tr>
<tr>
<td>2 (a/2)[101]</td>
<td>[\bar{1}10]</td>
<td>(\bar{1}11)</td>
<td>0.333 -0.67 0.666</td>
</tr>
</tbody>
</table>
Table 5.6. Results of Stress Calculations for the Dynamic Dislocation Transmission

<table>
<thead>
<tr>
<th>Total Tip Force (N/m)</th>
<th>Equivalent Tip Stress (MPa)</th>
<th>Average Stress (MPa)</th>
<th>Average Force (N/m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1605</td>
<td>629</td>
<td>33</td>
<td>0.0084</td>
</tr>
</tbody>
</table>

Table 5.7. Transmission Criteria Application to the Dynamic Case

<table>
<thead>
<tr>
<th>Criterion</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4*</th>
<th>Observed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slip System</td>
<td>10</td>
<td>6</td>
<td>5</td>
<td>5</td>
<td>5</td>
</tr>
</tbody>
</table>

5.4.2. Dislocation transmission and reflections at grain boundaries

One predominant process in stainless steel samples is the simultaneous transmission across and reflection from the grain boundary. This phenomena was observed in three out of a total of six dislocation-grain boundary interaction events recorded from dynamic in-situ straining experiments. Figure 5.8 shows a series of still pictures taken from the video recording of a dynamic experiment. The dislocations which seem to be reflected move much slower compared to the ones emitted on the other side of the grain boundary. It could
be dislocations with negative Burgers vectors which naturally would move in the opposite direction under the same applied stress. On the other hand, the extra slip system of these reflected dislocation might be involved to satisfy the compatibility criterion for polycrystalline materials. Unfortunately, these interactions could not be fully characterized crystallographically. The main reasons of the lack of information are the rapid tearing of the sample and dynamic formation of the dislocation pileups involved. However, since it seems to be a mode of dislocation-grain boundary interaction not mentioned hitherto in the literature, it is worthwhile to look into it more deeply. An attempt will be made to describe the detailed process and to discuss its implication in polycrystalline metal deformation.

While Figure 5.8 shows the sequence of events of this type of interaction, Figure 5.9 shows sketches of the same sequence. This sketch is based on actual video observations and will be discussed below.
Figure 5.8 Dislocation Pileup Reflection at Grain Boundary
Figure 5.9 Sketches of the dislocation emission and reflection activated by a stressed dislocation pileup
The following is a list of the facts established from the experimental result:

1. The reflected dislocations are in a different slip plane from that of the incoming pileup dislocations.

2. The advance of the pileup dislocations, the emission of dislocations from the other side of the grain boundary and the reflection of dislocations take place at the same time, i.e., those motions are coordinated.

3. The reflection process only lasts a short time at the beginning of the interaction, while the pileup advances and dislocation emission continues after the reflection terminates.

4. All three slip planes: pileup, emission and reflection are at relatively small angles to each other when they intersect the grain boundary plane.

Based on the above facts, the details of this type of dislocation-grain boundary interaction process can be proposed as follows. Figure 5.9 shows sketches of possible reaction mechanism. In Figure 5.9(a), the head dislocation labeled "h" with the Burgers vector \( b \) of an advancing pileup enters the grain boundary under the applied stress. Then in Figure 5.9 (b) the dislocation dissociates into several grain boundary dislocations, two of which are labeled "a" and "b" with Burgers vectors \( b_1 \) and \( b_2 \). This dissociation would be energetically favored if Frank's \( \Sigma b^2 \)
criterion [45] is satisfied. At this moment stress concentration can make these resulting dislocations rotate and glide on the grain boundary so as to conform to other available slip planes in both grains other than the pileup slip plane, as shown in Figure 5.9(c). Under the applied stress, the dislocation segment marked b is emitted into the neighboring grain, while the segment marked a is emitted into the grain which contains the original pileup.

Dislocations with different Burgers vectors from those of the pileup dislocations were previously observed by Wise [34] in static TEM experiments. This phenomena could not be explained in relation to the dislocation pileup. Therefore these dislocations were considered to be extraneous to the pileup-grain boundary interaction event. From the dynamic experiments, these extra dislocations may very well come from the dislocation reflection. Moreover, this would imply that this dislocation reflection phenomena is not due to some thin film effect.

5.4.3. Dislocation pileup absorbed into the grain boundary and induced grain boundary dislocation movement

As shown in Figure 5.10, a lattice dislocation pileup moves into the stainless steel grain boundary under the applied stress. In the recorded video-tape, it can be seen that when the head dislocations enter the grain boundary,
an array of dislocations move inside the grain boundary. The grain boundary is a $\Sigma = 3$ twin boundary. As was shown by Wise and Clark [43,54], it is possible for lattice dislocations entering the twin boundary to split into glissile grain boundary dislocations. Hence the stress concentration is relieved and slip propagation to the other grain is prohibited.
Figure 5.10(a) Dislocation Absorption into the Grain Boundary

Figure 5.10(b) Sketches of Figure 5.10(a)
5.4.4. Pole mechanism of dislocation generation near the grain boundary

In the dynamic straining experiments of molybdenum samples, dislocation-grain boundary interaction events were also observed. Molybdenum sample number two shows a pole dislocation generation mechanism, in which a dislocation segment pinned at one end were seen to rotate and emit dislocations. The sequence of events was shown in Figure 5.11. Figure 5.12 shows schematic drawings of this sequence.

As shown in Figures 5.11 and 5.12, two dislocation segments are lying close to the grain boundary. One segment is fixed and another segment moves under the applied stress. While one end of the moving segment near the boundary is anchored, the other end sweeps around and constantly generate dislocations.
Figure 5.11. Dislocation Pole Mechanism in Molybdenum
Figure 5.12 Sketches of the dislocation pole mechanism
5.4.5. Some general observations in dynamic in-situ straining experiments

In all of the observed cases of dislocation-grain boundary interactions, the existing dislocation arrays tend to remain stationary while nearby new pileups originate and move. This is most likely due to the greater pinning force experienced by the existing dislocations. This pinning effect might be caused by the solute atom atmosphere formed around the dislocation [45].

Sample tearing always takes place when the strain reaches a certain level. At a stress sufficient to activate dislocation movement into the grain boundary, the sample tears or cracks rapidly. When a crack forms near the thin area under observation, applied stress can no longer be transmitted to this area. Therefore the stress concentration needed for dislocation movement crossing grain boundaries is relieved and this in turn terminates the observed dislocation-boundary interactions. This indicates that the dislocation-boundary interaction events under observation are at a stress level corresponding to the magnitude of yield or flow stress. This fact is another evidence that the calculated stress level from the dislocation pileup configurations are in the right range.
There are other observations of dislocation-grain boundary interaction processes from dynamic in-situ straining experiments which were recorded on video tapes but not presented here because no clear picture could be obtained. These processes might still provide certain insight into the slip propagation mechanisms in polycrystalline metals. They will be mentioned briefly here.

1. In a stainless steel sample, a dislocation pileup was observed to form and move against a high angle grain boundary. Under the applied stress, a dislocation loop was seen to form on the other side of the boundary. With further straining the dislocations were seen to be emitted from that loop. The pileup dislocations disappeared rapidly as the emission was taking place.

2. Again in the stainless steel samples, dislocations emitted from one grain boundary due to a dislocation pileup were seen to pile up against another grain boundary and the same process was repeated. This could be one explanation of the fact that the sources of the observed dislocation pileups could not be found by tracing back along the pileup.

3. Dislocation density was still relatively low in the thin film when dislocation transmission across grain boundaries were observed. This was evidenced by the absence of other dislocations interfering with the pileup under observation.
4. In three cases of dislocation transmission through grain boundary it was observed that the number of dislocation accumulated before the transmission took place vary widely. A rough estimation shows that this number ranges from 10 to more than 50 for different grain boundaries in stainless steel.
CHAPTER VI
DISCUSSIONS

6.1 Preliminaries

Grain boundary strengthening is a method widely used to obtain desirable mechanical properties in polycrystalline metals. In the past, the effect of grain boundaries on mechanical properties of polycrystalline metals were studied at several levels. First, the relations between the grain size and such properties as the yield strength of the material were obtained from macroscopic experiments. Next, optical microscopes were used to study interactions between slip lines and grain boundaries. More recently, TEM techniques are used to study the grain boundary structure, dislocation configuration both in grain interiors and grain boundaries.

Deformation in polycrystalline metals propagates from one grain to another through the movement of slip across grain boundaries. In the magnification ranges available in optical microscopes, slip lines are the evidence and results which can offer quantitative data to the studies [26-28]. On the other hand, slip process can be studied at the individual dislocation level by using transmission electron
microscopy techniques [54,55].

The onset of deformation in polycrystalline metals consists of a number of microscopic processes both in the grain interior and in the grain boundary region. Slip propagation across grain boundaries is an important mode of interaction by which the deformation can be extended to the entire sample under an applied stress. This study reveals an important aspect of the slip propagation processes in polycrystalline metals: interactions between known dislocation pileups and fully characterized grain boundaries by static and dynamic electron microscopy experiments. In addition, anisotropic elastic stress calculations are used to calculate the stress field involved in such processes. These calculations are employed in this study to estimate stress levels of the dislocation-grain boundary interaction events and to calculate resolved shear stresses on the possible activated slip systems, thereby the selection of the observed activated slip systems can be explained quantitatively.

6.2. Comparison of dislocation pileup configurations

As described in the previous chapter, anisotropic elastic stress calculations were performed for dislocation pileup configurations obtained from static TEM and dynamic HVEM experiments for stainless steel samples. The validity
of this practice depends on the ability of the material to maintain the dislocation pileup configuration after the removal of the applied stress.

In order to compare the results of static and dynamic experiments, similar dislocation pileup configurations in both types of experiments are compared in the following. A calculated dislocation pileup which has the same crystallographic parameters as grain boundary number 3 shown in Figure 5.3 was also obtained. The equilibrated dislocation positions were obtained by calculating the force on each dislocation and moving each dislocation until the net force is zero. Furthermore, the same stress field at the pileup tip as that of the experimental pileup was obtained by the same calculation method. Therefore the calculated pileup would have experienced the same obstacle strength as the experimental one. The dislocation positions measured directly from the micrograph and those obtained from calculations for the same grain boundary are shown in Figure 6.1. In Figures 6.1 and 6.2, the reciprocal of the individual dislocation spacing, which is a measure of dislocation density, is plotted against the distance of the dislocation from the grain boundary. It can be seen that dislocation pileup configuration obtained from a static TEM experiment is very close to the configuration obtained from calculations.

Furthermore, dislocation spacings from both the static
(post-deformation state) TEM experiment and the dynamic (as stressed) HVEM experiment were compared. Measured dislocation positions of the pileup of grain boundary 3 shown in Figure 5.3 from static TEM experiments were used to compare with the measured dislocation positions of the dynamic grain boundary shown in Figure 5.7. As was described in Chapter V, both dislocation pileups meet a $\Sigma = 3$ grain boundary in stainless steel. Although the dynamic pileup has more dislocations, only the measured positions of nineteen dislocations (the number of dislocations in the static pileup) are plotted in Figure 6.2, the positions of the dynamic dislocation pileup being multiplied by a factor so that the dislocation positions farthest from the grain boundary in both cases coincide. As can be seen from Figure 6.2, the pileup configurations are similar for the static and dynamic case. It should be pointed out that the micrographs of the dynamic pileup were taken while the stress was still applied to the tensile sample and the slip propagation process was still going on. This might explain the slight "irregularities" shown in the figure for the dynamic dislocation pileup.
Figure 6.1 Comparison of Measured and Calculated Pileups

Figure 6.2 Comparison of Static and Dynamic Pileups
6.3 Stresses involved in slip propagation processes

The stress level involved in the slip propagation events was calculated, allowing slip propagation mechanisms to be quantified and compared. It was observed from both static and dynamic electron microscopy studies that dislocation pileups impinging at a grain boundary is the most dominant form of slip propagation process in the 304 stainless steel samples.

For several static cases, and one dynamic case, of dislocation transmission across high angle grain boundaries in stainless steel, detailed crystallographic characterization and stress field analysis were carried out. The analysis showed these interaction events follow certain rules which can only be studied at the individual dislocation level.

As was shown in Tables 5.4 and 5.6, values of the forces and stresses involved in the dislocation transmission processes were calculated using anisotropic elastic solutions. The total tip force is the force exerted by the stressed pileup at the head dislocation of the pileup in the direction of the pileup movement on its slip plane. The equivalent stress, which is the total tip force divided by the magnitude of the pileup dislocation Burgers vector, is thus a measure of the grain boundary obstacle strength to
the movement of the dislocation pileup.

In the static cases, the equivalent stress is a lower bound of the stress needed to overcome the grain boundary barrier during slip propagation. The values range from 280 to 870 MPa for four different boundaries. Although the number of grain boundaries involved is not large enough to yield a statistical correlation with the bulk material properties, such as the yield strength, its significance to the fundamental understanding of the slip propagation process can be presented.

All the values are greater than the bulk yield strength of the material: 210 MPa [46]. The yield strength can be considered as an average of the contributions from both the grain interior and the grain boundaries. This means that for grain boundary number 2, the grain boundary barrier to the dislocation pileup can be overcome with a stress (280 MPa) very close to the yield strength of the material, while in boundary number 3, a quadrupled stress value was necessary to overcome the barrier. In a previous study of pure screw dislocations passing through a 304 stainless steel \( \Sigma = 3 \) grain boundary, Clark and Wagoner [54] showed that a stress of 130 MPa was needed for the dislocation transmission. They pointed out that for that special case, colinear Burgers vectors are available on both sides of the boundary and the impediment might be the lowest possible a boundary can provide to dislocation transmission because no
residual dislocation was left at the boundary. For all the boundaries in this study, however, residual dislocations must be left at the boundary for the slip propagation to take place, thus the higher values of the equivalent stress.

The above discussion of the stress calculation results shows quantitatively that the grain boundaries are barriers to slip propagation. Moreover, the barrier strength is different for different grain boundaries. Therefore, not only is the grain size important to the polycrystalline metal strengthening, the types of grain boundaries present in the material also play a prominent role in such strengthening. This could be a significant point for studying grain boundary strengthening mechanisms in polycrystalline metals with nonuniformly distributed grain orientations. For example, in sheets or wires of metal with severe textures resulting from forming operations the majority of grain boundaries may have special characteristics. As an example, about 85% of the grain boundaries in the thin areas of the stainless steel samples used in this study are \( \Sigma = 3 \) twin boundaries. One such effect could be the dominance of grain boundaries of higher barrier strength causing more pileup formation. This could lead to more brittle behavior of the material by crack nucleation because of higher stress concentrations.

The average stress and force were obtained by dividing the tip force and the equivalent stress by the number of
free dislocations in the pileup. These estimates represent
the net elastic stresses (and forces) external to the pileup
felt by each free dislocation in the pileup. Since the
pileups are in a state of static equilibrium, the stresses
correspond to lattice friction stresses when the pileup is
far removed from other sources of internal stress [54].

In the analysis results for the dynamic dislocation
pileup listed in Table 5.6, it is notable that the
above-discussed quantities lie in the same range as those
obtained from static results. This is another indication
that dislocation pileup configurations in static TEM
experiments are useful in the study of bulk slip propagation
processes. Furthermore, the two-dimensional effect of the
miniature tensile specimen thin area is not prominent enough
to severely affect the outcome of the dynamic in-situ
experiments.

6.4 Slip propagation criteria

Both crystallographic characterization and the stress
field analysis were used to form criteria for slip system
selections in slip propagation processes. The stress
calculation was used to compare the resolved shear stresses
on all the possible slip systems in the dislocation emission
grain, thereby establishing slip propagation criteria
discussed in section 5.2. From the performance of different
criteria in predicting the activated emission slip systems, it is possible to make some inferences, discussed below.

The first criterion, which states that pileup imposed different resolved shear stresses to different emission slip systems in the adjacent grain and the slip system with the maximum shear stresses is most likely to be activated. The presence and the position of the grain boundary is not considered. Its failure to predict correct activated slip systems shows that the slip propagation process is not dependent solely on the slip systems involved. For instance, elastic anisotropy and grain boundaries are neglected in this criterion.

The second criterion takes the grain boundary into consideration. It requires that the rotation needed for the dislocation to transfer from the pileup slip plane to the emission slip planes at the grain boundary is a minimum. This criterion is successful in predicting all the activated emission slip planes. When the slip direction is predicted by the first criterion, it correctly identifies half of the emission slip systems. Therefore, this criterion represents a better understanding of the dislocation transmission processes.

The anisotropic stress field calculations were used in the third criterion. This criterion still failed to predict all the activated emission slip systems correctly. However, when it is used to predict the slip direction with the slip
plane already known, it worked well. The fourth criterion uses the geometric criterion (number 2) to predict the slip plane and the stress criterion (number 3) to predict the slip direction. This combined criterion succeeded in predicting the activated emission slip system for all four static and one dynamic dislocation transmission slip propagation events. It follows that for the dislocation emission, the slip plane is chosen to make it easiest for the pileup dislocation to rotate to the emission slip system. This is achieved when the two slip planes meet at the grain boundary at an angle as small as possible. On the other hand, the emission slip direction is chosen so that the activating force on the dislocation exerted by the pileup is maximized.

6.5 Qualitative results from dynamic in-situ HVEM straining experiments

In addition to the fully characterized dislocation pileup and grain boundary interaction event, many interaction events were observed during dynamic in-situ HVEM straining experiments. These qualitative results revealed various processes during polycrystalline metal deformation which can provide us with some insight into the details of the deformation mechanism.

The dislocation reflection mechanism observed in the
stainless steel samples might play an important role in its deformation process. It is likely that the reflected dislocations are produced to accommodate the plastic compatibility required at the grain boundary [26-28].

Dislocation absorption into the stainless steel Σ = 3 grain boundary is a confirmation of static TEM studies [43]. The dislocations absorbed into the grain boundary were seen to move rapidly on the boundary plane. Since at room temperature, climb is very difficult for the dislocation in stainless steel, it can be assumed that glissile grain boundary dislocations were involved in such a movement. These glissile dislocations could be produced as the lattice dislocations entered the boundary and underwent dislocation reactions.

In a molybdenum sample, it was observed that a dislocation pole source can operate near the grain boundary with the produced dislocations interacting with the grain boundary. Therefore, it can be inferred that in molybdenum samples slip can be initiated in different grains under the applied stress without direct dislocation transmission across grain boundaries as in stainless steel samples.

6.6 Summary

Several criteria for predicting the slip system activated ahead of a dislocation pileup at a grain boundary
have been compared. A criterion derived from considering the intersection of the slip plane with the grain boundary was successful in predicting the proper slip plane in each case. The proper choice of Burgers vector was found by maximizing the force on the dislocation ahead of the pileup. This combined criterion accurately predicted slip system for all four grain boundary-pileup configurations studied.

The pileups observed using TEM have an equivalent stress at the tip ranging from 280 to 870 MPa, according to calculations based on anisotropic elasticity. These numbers correspond approximately to the values representing barrier strength of the grain boundaries to the dislocation movement.

Several dislocation propagation events through a grain boundary were observed, including dislocation transmission, transmission with a residual gbd and adsorption of lattice dislocations with emission of partial dislocations.

In dynamic in-situ straining experiments, one dislocation pileup-grain boundary interaction is similar to those obtained from static experiments. This dynamic dislocation transmission across a grain boundary was analyzed using the same procedure. It was found that the slip propagation criterion developed for the static experiments predicted correct activated emission slip system for this dynamic event as well.

A new dislocation-grain boundary interaction process which was not evident in static studies was discovered.
This process is the simultaneous dislocation transmission and reflection at the intersection of an incoming dislocation pileup and the grain boundary. This three-way process was discussed in light of the experimental observations and in terms of micromechanisms of polycrystalline metal deformation.

Other dislocation-grain boundary interactions in stainless steel and molybdenum samples were also discussed qualitatively because of the lack of crystallographic information. These interaction processes provide evidence and confirmation of the micromechanism of polycrystalline slip propagation, as was demonstrated by dislocation absorption into a grain boundary to form a moving boundary dislocation array in stainless steel and pole mechanism of a dislocation source near a molybdenum grain boundary.
CHAPTER VII
CONCLUSIONS

7.1. Slip system selections for emitted dislocations

When dislocation transmission across grain boundaries take place, the slip system of the emitted dislocation can be predicted. The model which gives the best results is one based on a combination of stress field calculations and the geometry of the dislocation pileup and the grain boundary, i.e., the emitted slip plane is chosen by the geometric factors including the grain boundary plane and the emitted slip direction is chosen by the resolved shear stress. It applies to the results obtained both from static TEM experiments and dynamic HVEM experiments.

7.2. Grain boundary roles in strengthening polycrystalline metals

Grain boundaries impede slip propagation from one grain to another by several modes. Among them are absorption of dislocations into the grain boundary, absorption and emission, and absorption-emission-reflection. In all these cases, dislocation movement was observed to be obstructed by
the presence of the grain boundary. The stress calculations showed that the stresses needed for dislocation transmission are higher than the macroscopic yield stress. Moreover, the value of these stresses varies widely (280 to 870 MPa), implying that the grain boundary contribution to the material strengthening is a statistical average of individual barriers with varying degrees of strength. Dislocation sources in or near the grain boundaries also contribute to the material strengthening by increasing the dislocation density. These effects presumably contribute to the well-known but empirical Hall-Petch relationship between flow strength and grain size.

7.3. Dynamic in-situ HVEM straining experiments of slip propagation through grain boundaries

The most frequently observed mode of dynamic dislocation-grain boundary interaction in stainless steel is dislocation transmission through the grain boundary, often accompanied by dislocation reflection in the original grain. The three-fold mechanism (pileup with emission on both sides of the grain boundary) is difficult to observe in static experiments and is previously unreported. Quantitative results were obtained for the dynamic dislocation transmission across a stainless grain boundary and found to agree with those obtained from the static TEM experiments.
Qualitative results for dislocation reflection and other processes were also presented. These processes are important in understanding the slip propagation process because they show that certain events such as dislocation transmission across a grain boundary take place at a variety of local stresses and encounter a wide range of obstacle strengths.
APPENDIX A - PROGRAM LISTING FOR TUCKER’S METHOD

IMPLICIT REAL*8(A-H,O-Z)
character*80 TITLE
REAL*8 UD(3)
REAL*8 CONT(6),C(3,3,3,3),B(3,20,2),DC(3,3),CR(3,3,3,3),XD(20,2),
A YD(20,2),F(3,3,3),S(3,3),BP(3,20),norm(6,2),comp(6,2),bl(6,6),ps(3)
COMPLEX*16 Q(7),P(3,2),A(3,3,2),LA(3,3,2),MA(3,3,2),W(3,3,2),
A JA(3,3,2),GA(3,3,2),JAB(3,3,2),LAB(3,3,2),HOLD(3,3,2),
B HOLD1(3,3,2),HOLD2(3,3,2),R1(3,3,2),R1B(3,3,2),MG(3,3,2),
C MGB(3,3,2),R(3,3,2),RB(3,3,2),R2(3,3,20,2),R2B(3,3,20,2),FA(3),
D PB(3,2),PI(3),R2G(3,3,20,2),RG(3,3,2),Z,Z1
INTEGER ml(3),m2(3),L1(6),L2(6),IQ(2),NUM(2),ns(4,2)
COMMON B , XD, YD, S, COMP, P, LA, MG, MGB, R, RB, R2, R2B, FA, PB,
A R2G, RG, R1, R1B, IQ, NUM, C44P, X, Y, UD, A

data ml/2,3,1/,m2/3,1,2/,11/1,2,3,3,2/,12/1,2,3,3,2,1,1/,iq/2,1/
format(3(2x,f10.5,3H +I,fl0.5))
520 format(6H C11 =,f8.5,6H C12 =,f8.5,6H C44 =,f8.5)
read(10,*) TITLE ! Read in the title, grid
write(21 ,*)title
read(10,*)ylower,yupper,ystep ! configuration, isostresses.
C DO 20 IP=1,2 ! For crystal 1 and 2:
read(10,*)C11,C12,C44
WRITE(21,*)C11,C12,C44 ! read and print elastic consts.
C11=C11/C44 ! Normalize elastic constants.
C44P=C44 ! Save the proportionality.
C44=1.DO
CALL DEFINE(L1,L2,C11,C12,C44,C) ! Get elastic constant tensor.
WRITE(21,520)(ps(I),1=1,3),(NORM(I),1=1,3)
WRITE(21,410)(IP,(ps(I),1=1,3),(NORM(I),1=1,3)
410 FORMAT(6H IN XL,I1.3H U=,3f6.3,5H PN=,3F6.3)
read(10,*) NUM(IP) ! Read and print line direction,
IF (NUM(IP).EQ.0)GO TO 240 ! plane normal and number of
NUN=NUM(IP) ! dislocations
DO 30 N=1,NUN ! For each dislocation:
read(10,*) XD(N,IP),YD(N,IP),(B(I,N,IP),I=1,3),BMAG
WRITE(21,420)N,IP,XD(N,IP),YD(N,IP),(B(I,N,IP),I=1,3),BMAG
420 FORMAT(IX,' DISLOCATION*.12.' IN XL,'I2,' IN XL', ' X=','F15.5,' Y=','F15.5
1 ,/,' BURGERS VECTOR*.3F6.2,'/','F8.5) ! Read and print position
do 30 I=1,3 ! Burgers vectors
30 B(I,N,IP)=B(I,N,IP)*BMAG ! Scale the Burgers vector.
240 CALL DIRECT(m1,m2,ps,NORM,DC) ! Calculate direction cosines.
IF (NUM(IP).EQ.0)GO TO 180 ! Does this crystal have any
NUN=NUM(IP) ! dislocations? If not, skip.
do 40 N=1,NUN ! For each dislocation:
do 40 I=1,3 ! rotate to problem coordinates.
BP(I,N)=0.DO

114
do 40 J=1,3
BP(I,N)=BP(I,N)+DC(I,J)*B(J,N,IP)
WRITE(21,FMT='(6H IN XL,12,24H BURGERS VECTORS ROTATED,/)')IP
WRITE(21,FMT=('DISLOCAT',I3,3F8.5')K,(BP(J,K),J=1,3),K=1,NUN)
NUN=NUM(IP) ! Print rotated Burgers vectors.
180 CALL ROT9X9(IP,DC,C,CR,b1,COMP) ! Rotate elastic constants tensor
CALL GETF(CR,F) ! Get coefficients for the sextic
CALL GETQ(m1,m2,F,Q) ! equation.
CALL NEWTON(Q,PI) ! Solve the sextic equation.
ZR=CR(3,2,3,1)/CR(3,2,3,2) ! Order the roots so that root
ZI=DSQRT(DABS(CR(3,2,3,2)*CR(3,1,3,1)-CR(3,2,3,1)
A **2)/C(3,2,3,2)) ! 3 is closest being a root of
Z=DCMPLX(ZR,ZI) ! c(5,5)+2p*c(4,5)+p*p*c(4,4) to
do N=1,2 ! ensure a nondegenerate A.
IF(CDABS(Z-PI(N)).GT.CDABS(Z-PI(N+1)))GO TO 60
Z1=PI(N) ! Swop the roots if necessary.
PI(N)=PI(N+1)
PI(N+1)=Z1
60 end do
CALL GETAL(IP,m1,m2,PI,F,CR,A,LA)
CALL INVERT(IP,m1,m2,LA,MA) ! Get A, L, M = L inverse
CALL MULT33(IP,A,IP,MA,IP,W) ! Get W = A*M
WRITE(21,*)'F IN CRYSTAL*.IP ! Output Matrices.
WRITE(21,fmt='(9(2x,f6.2))')F
WRITE(21,*)'POLYNOMIAL COEFFICIENTS IN CRSTAL'.IP
WRITE(21,fmt='(4(1x,f8.3,3H +I,f8.3))')Q
WRITE(21,*)'ROOTS IN CRYSTAL*. IP
WRITE(21,fmt=*(3(lx,f10.5.3H +1.f10.5))*)PI
Do 20 1=1,3
P(I,IP)=PI(I) ! Store Roots.
20 PB(I,IP)=DOONJG(P1(I)) ! End crystal loop.
CALL GETJG(IQ,m1,m2,W,JA,GA) ! Get J and G.
CALL CONJ(JA,JAB) ! Get J conjugate.
CALL CONJ(LA,LAB) ! Get L conjugate.
WRITE(21,*)'LA IN CRYSTALS' ! Write out matrices.
WRITE(21,500)LA
WRITE(21,*)'MA IN CRYSTALS'
WRITE(21,500)MA
WRITE(21,*)'W IN CRYSTALS'
WRITE(21,500)W
WRITE(21,*)'JA IN CRYSTALS'
WRITE(21,500)JA
WRITE(21,*)'GA IN CRYSTALS'
WRITE(21,500)GA
WRITE(21,*)'JAB IN CRYSTALS'
WRITE(21,500)JAB
WRITE(21,*)'LAB IN CRYSTALS'
WRITE(21,500)LAB
do 70 IP=1,2 ! For crystal 1 and 2:
CALL MULT33(IP,GA,IP,JAB,IP,HOLD)! H = G*JB
H1=G*JB*LB
CALL MULT33(IP,HOLD,IP,LAB,IP,HOLD1)
do 80 I=1,3 ! H = delta(i,j) + G*JB
16
80 HOLD(I,1,IP)=HOLD(I,1,IP)+1.DO ! H2 = H+LB
70 CALL MULT33(IP,HOLD,IP,LAB,IP,HOLD2)
CALL conj(HOLD,HOLD) ! H = H2 conjugate.
do 90 IP=1,2 ! For crystal 1 and 2:
I=IQ(IP) ! Get mixed matrices.
call MULT33(IP,MA,IP,HOLD,IP,R1)
90 call MULT33(I,MA,IP,HOLD,IP,R1B)! R1 = M*H1 R1B = M(h)*H(g)
write(21,*)' R1 IN CRYSTALS' ! Output Matrices.
write(21,500)R1
write(21,*)' R1B IN CRYSTALS'
write(21,500)R1B
do 100 IP=1,2 ! For crystal 1 and 2:
do 110 I=1,3
  do 110 J=1,3
110 HOLD(I,J,IP)=-DIMAG(W(I,J,IP)) ! Get MG and MGB.
call INVERT(IP,m1,m2,HOLD,HOLD1)
100 call MULT33(IP,MA,IP,HOLD1,IP,MG)
call conj(MG,MGB)
write(21,*)'MG IN CRYSTALS'
write(21,500)MG
write(21,*)'MG IN CRYSTALS'
write(21,500)MGB
open(unit=8,file='tucker.dat',status='new')
x=0.0
iflag=0
do 120 i=ylower,yupper,ystep
  y=dfloat(i)
  if(i.eq.0) y=-0.0001
goto 6010
6000 if(i.eq.0) y=0.0001
  iflag=1
6010 continue
  call STRESS
  write(8,200)y,s(1,1),s(1,2),s(2,2),s(1,3),s(2,3),s(3,3)
  write(12,200)y,UD
  if((i.eq.0).and.(iflag.eq.0)) goto 6000
120 continue
200 format(1x,7f10.5)
close(unit=8)
end
subroutine define(L1,L2,C11,C12,C44,C)
integer L1(6),L2(6)
real*8 C(3,3,3,3),B,C11,C12,C44
do 1 I=1,6
  do 1 J=1,6
    B=C12
    if(I.EQ.J) B=C11
    if(I.GT.3.OR.J.GT.3) B=0.DO
    if(I.EQ.J.AND.J.GT.3)B=C44
    c(L1(I),L2(I),L1(J),L2(J))=B
    c(L1(I),L2(I),L2(J),L1(J))=B
    c(L2(I),L1(I),L1(J),L2(J))=B
    c(L2(I),L1(I),L2(J),L1(J))=B
    c(L1(I),L2(I),L1(J),L2(J))=B
1 continue
C
SUBROUTINE DIRECT(P1,P2,P,N,D)
INTEGER P1(3),P2(3)
REAL*8 D(3,3),P(3),N(3),R1,R2,R3
R1=DSQRT(P(1)*P(1)+P(2)*P(2)+P(3)*P(3))
R2=DSQRT(N(1)*N(1)+N(2)*N(2)+N(3)*N(3))
R3=R1*R2
DO 1 I=1,3
D(2,I)=N(I)/R2
D(3,I)=P(I)/R1
1 D(1,I)=(N(P1(I))*P(P2(I))-N(P2(I))*P(P1(I)))/R3
RETURN
END
C
SUBROUTINE ROT9X9(IP,D,A,B,b1,COO)
REAL*8 A1(6,6),B1(6,6),COM(6,2),Z(6),D(3,3),A(3,3,3,3),B(3,3,3,3)
INTEGER 0,P,F(3,3)
DATA F/1,6,5,6,2,4,5,4,3/
write(15,*)'Direction Cosines in Crystal',IP
write(15,fmt=*(5x,3f15.5)')d
DO 2 1=1,3
DO 2 J=1,I
DO 2 K=1,3
DO 2 L=1,K
B(I,J,K,L)=0.DO
DO 1  M=1,3
DO 1  N=1,3
DO 1  O=1,3
DO 1  P=1,3
B(I,J,L,K)=B(I,J,K,L)
B(J,I,K,L)=B(I,J,K,L)
1 B(J,I,L,K)=B(I,J,K,L)
2 A1(F(I,J),F(K,L))=B(I,J,K,L)
write(15,*)'Rotated elastic constants'
write(15,fmt=*(1x,6f12.6)')((A1(I,J),J=1,6),I=1,6)
12 FORMAT(9F8.4)
write(15,*)'Elastic Constants Tensor'
write(15,12) ((((A(I,J,K,L),L=1,3),K=1,3),J=1,3),I=1,3)
write(15,*)'Rotated Elastic Constants Tensor'
write(15,12) ((((B(I,J,K,L),L=1,3),K=1,3),J=1,3),I=1,3)
do 3 ii=1,6
do 3 jj=1,6
3 bl(ii,jj)=al(ii,jj)
call invers(bl,6)
write(15,*)'Compliance Coefficients'
write(15,fmt=*(1x,6f12.6)')((B1(I,J),J=1,6),I=1,6)
DO 4 I=1,6
4 COM(I,IP)=B1(3,I)
SUBROUTINE GETF(CR,F)
REAL*8 CR(3,3,3,3),F(3,3,3)
DO 1 I=1,3
DO 1 J=1,3
F(I,J,1)=CR(I,1,J,1)
F(I,J,2)=CR(I,2,J,1)+CR(I,1,J,2)
1 F(I,J,3)=CR(I,2,J,2)
RETURN
END

SUBROUTINE GETQ(P1,P2,F,Q)
INTEGER P1(3),P2(3)
REAL*8 F(3,3,3)
COMPLEX*16 Q(7)
DO 1 M=1,7
1 Q(M)=(0.DO,0.DO)
DO 2 I=1,3
DO 2 J=1,3
DO 2 K=1,3
DO 2 L=1,3
2 Q(J+K+L-2)=Q(J+K+L-2)+F(1,1,J)*(F(2,P1(I),K)*F(3,P2(I),L)-
+ F(2,P2(I),K)*F(3,P1(I),L))
RETURN
END

SUBROUTINE NEWTON(Q,P)
IMPLICIT REAL*8(A-H,O-Z)
COMPLEX*16 Q(7),P(3),X,Y,T,Z
Z=(.1DO,1.0DO)
DO 156 N=1,6
N=8-NA
K=0
DO 152 KA=1,70
X=(0.0DO,0.0DO)
Y=(0.0DO,0.0DO)
DO 151 J=1,N
Y=Z*Y+X
M=M+1-J
T=Z*X+Q(M)
IF(K.EQ.0)GO TO 150
Q(M)=X
150 X=T
151 CONTINUE
IF(K.NE.0)GO TO 153
T=X/Y
Z=Z-T
IF(CDABS(T)/CDABS(Z).GT.1.0D-6)GO TO 152
K=1
152 CONTINUE
WRITE(*,*)'POLY DOESNT CONVERGE ON ',NA,'TH ROOT' STOP
153 IF(DABS(DIMAG(Z)).GT.1.0D-5)GO TO 154
WRITE(*,*)NA,'TH ROOT IS REAL. = ',DREAL(Z)
154 LA=NA/2
R=DFLOAT(NA)/2.0DO
DLA=LA
IF(R-DLA.LT.0.1D0)GO TO 155
Z=DOONJG(Z)
GO TO 156
155 P(LA)=DCOMPLEX(DREAL(Z),DABS(DIMAG(Z)))
IF(LA.EQ.1)Z=(.5D0,.9D0)
IF(LA.EQ.2)Z=-DOONJG(Z)
156 CONTINUE
RETURN
END
 C
SUBROUTINE GETAL(IP,P1,P2,P,B,C,A,LA)
COMPLEX*16 P(3),A(3,3,2),LA(3,3,2),F(3,3,3)
REAL*8 B(3,3,3),C(3,3,3,3)
INTEGER P1(3),P2(3)
DO 1 I=1,3
DO 1 J=1,3
DO 1 K=1,3
 1 F(I,J,K)=B(I,J,1)+B(I,J,2)*P(K)+B(I,J,3)*P(K)*P(K)
DO 2 I=1,3
DO 2 J=1,3
 2 A(J,I,IP)=F(P1(I),P1(J),I)*F(P2(I),P2(J),I)-
     F(P1(I),P2(J),I)*F(P2(I),P1(J),I)
DO 3 I=1,3
DO 3 J=1,3
LA(I,J,IP)=(0.DO,0.DO)
DO 3 K=1,3
 3 LA(I,J,IP)=LA(I,J,IP)+(C(I,2,K,1)+P(J)*C(I,2,K,2))*A(K,J,IP)
RETURN
END
C
SUBROUTINE INVERT(IP,P1,P2,A,B)
INTEGER P1(3),P2(3)
COMPLEX*16 A(3,3,2),B(3,3,2),DET
DET=(0.DO,0.DO)
DO 1 I=1,3
 1 DET=DET+A(1,I,IP)*A(2,P1(I),IP)*A(3,P2(I),IP)-
     A(2,P1(I),IP)*A(3,P2(I),IP)*A(3,P1(I),IP))
DO 2 I=1,3
DO 2 J=1,3
 2 B(J,I,IP)=(A(P1(I),P1(J),IP)*A(P2(I),P2(J),IP)-
     A(P1(I),P2(J),IP)*A(P2(I),P1(J),IP))/DET
RETURN
END
C
SUBROUTINE MULT33(IA,A,IB,B,IC,C)
COMPLEX*16 A(3,3,2),B(3,3,2),C(3,3,2)
DO 1 I=1,3
DO 1 J=1,3
C(I,J,IC)=(0.0D0,0.0D0)
DO 1 K=1,3
1 C(I,J,IC)=C(I,J,IC)+A(I,K,IA)*B(K,J,IB)
RETURN
END

SUBROUTINE GETJG(IQ,P1,P2,A,B,C)
INTEGER IQ(2),P1(3),P2(3)
COMPLEX*16 A(3,3,2),B(3,3,2),C(3,3,2),Z,D(3,3,2)
Z=(0.0D0,0.5D0)
DO 2 IP=1,2
DO 1 I=1,3
DO 1 J=1,3
B(I,J,IP)=Z*(A(I,J,IP)-A(I,J,IQ(IP)))
1 D(I,J,IP)=Z*(A(I,J,IP)-DOCONJG(A(I,J,IQ(IP))))
2 CALL INVERT(IP,P1,P2,D,C)
RETURN
END

SUBROUTINE DOCONJG(A,B)
COMPLEX*16 A(3,3,2),B(3,3,2)
DO 1 IP=1,2
DO 1 I=1,3
DO 1 J=1,3
B(I,J,IP)=DOCONJG(A(I,J,IP))
RETURN
END

SUBROUTINE GETR2(X,Y,P,PB,XD,YD,NUM,R2,R2B,R2G)
INTEGER NUM(2),IQ(2)
DATA IQ/2,1/
DO 3 IP=1,2
IF(NUM(IP).EQ.0)GO TO 3
DO 2 I=1,3
DO 2 J=1,3
NUN=NUM(IP)
DO 2 N=1,nun
R2G(I,J,N,IP)=X+P(I,IP)*Y-XD(N,IP)-P(J,IP)*YD(N,IP)
R2B(I,J,N,IP)=X+P(I,IP)*Y-XD(N,IP)-PB(J,IP)*YD(N,IP)
R2(I,J,N,IP)=X+P(I,IQ(IP))*Y-XD(N,IP)-P(J,IP)*YD(N,IP)
2 CONTINUE
3 CONTINUE
RETURN
END

SUBROUTINE FOALPH(NUM,B,R2,R2B,R2G,MG,MGB,R,RB,UG,UMB,URG)
IMPLIED REAL=8(A-H.O-Z)
COMPLEX*16 R(3,3), RB(3,3), HOLD2(3,3,3)
COMPLEX*16 UR(3,3), FOLD2(3,3,3)
COMPLEX*16 R2(3,3,20,3), R2B(3,3,20,2), MG(3,3,2), MGB(3,3,2)
INTEGER NUM(2)
REAL*8 B(3,20,2)
COMPLEX*16 HOLD1(3,3,3), R2G(3,3,20,2), RG(3,3,2)
COMPLEX*16 FOLD1(3,3,3), FOLD(3,3,3), URB(3,3,2), URG(3,3,2)
DO 4 IP=1,2
IF (NUM(IP).EQ.0) GO TO 4
DO 1 I=1,3
DO 1 J=1,3
DO 1 K=1,3

HOLD2(I,J,K)=(0.D0,0.D0)
HOLD(I,J,K)=(0.D0,0.D0)
HOLD1(I,J,K)=(0.D0,0.D0)
FOLD2(I,J,K)=(0.D0,0.D0)
FOLD(I,J,K)=(0.D0,0.D0)
FOLD1(I,J,K)=(0.D0,0.D0)

NUM=NUM(IP)
DO 2 L=1,NUM
HOLD2(I,J,K)=HOLD2(I,J,K)+B(I,L,IP)/R2G(J,K,L,IP)
HOLD(I,J,K)=HOLD(I,J,K)+B(I,L,IP)/R2(J,K,L,IP)
HOLD1(I,J,K)=HOLD1(I,J,K)+B(I,L,IP)/R2B(J,K,L,IP)
FOLD2(I,J,K)=FOLD2(I,J,K)+B(I,L,IP)*CDLOG(R2G(J,K,L,IP))
FOLD(I,J,K)=FOLD(I,J,K)+B(I,L,IP)*CDLOG(R2(J,K,L,IP))
FOLD1(I,J,K)=FOLD1(I,J,K)+B(I,L,IP)*CDLOG(R2B(J,K,L,IP))

2 CONTINUE
HOLD1(I,J,K)=HOLD1(I,J,K)+B(I,L,IP)/R2B(J,K,1,IP)
FOLD1(I,J,K)=FOLD1(I,J,K)+B(I,L,IP)*CDLOG(R2B(J,K,1,IP))

1 CONTINUE
DO 3 I=1,3
DO 3 J=1,3

RG(I,J,IP)=(0.D0,0.D0)
R(I,J,IP)=(0.D0,0.D0)
RB(I,J,IP)=(0.D0,0.D0)
URG(I,J,IP)=(0.D0,0.D0)
UR(I,J,IP)=(0.D0,0.D0)
URB(I,J,IP)=(0.D0,0.D0)

DO 3 K=1,3
RG(I,J,IP)=RG(I,J,IP)+RG(J,K,IP)*FOLD2(K,I,J)
RB(I,J,IP)=RB(I,J,IP)+MGB(J,K,IP)*FOLD1(K,I,J)
URG(I,J,IP)=URG(I,J,IP)+MG(J,K,IP)*FOLD2(K,I,J)
UR(I,J,IP)=UR(I,J,IP)+MG(J,K,IP)*FOLD1(K,I,J)
URB(I,J,IP)=URB(I,J,IP)+MGB(J,K,IP)*FOLD1(K,I,J)

3 CONTINUE
4 CONTINUE
RETURN
END

subroutine invers(a,n)
real*8 a(n,n), big, ab, temp
integer inter(20,2)
do k=1,n  ! Calculate elements of reduced
  jj=k
  if (k.eq.n) go to 70
  big=abs(a(k,k))
  ab=abs(a(i,k))  ! element
  if(big.lt.ab) then
    big=ab
    jj=i
  end if
  end do
70
  inter(k,1)=k
  inter(k,2)=jj
  if(jj.ne.k) then  ! Check if the row change is
    do j=1,n  ! necessary. If so, simply
      temp=a(jj,j)
      a(jj,j)=a(k,j)
      a(k,j)=temp  ! swap the values of the
    end do
  end if  ! position vector components
  do j=1,n  ! matrix
    if(j.ne.k) a(k,j)=a(k,j)/a(k,k)
  end do  ! New pivot row elements
  a(k,k)=1./a(k,k)  ! element replacing pivot
  do i=1,n  ! New elements not in pivot
    if(i.ne.k) then  ! row or pivot column
      do j=1,n
        if(j.ne.k) a(i,j)=a(i,j)-a(k,j)*a(i,k)
      end do
    end if
  end do  ! New elements for pivot
  do i=1,n
    if(i.ne.k) a(i,k)=-a(i,k)*a(k,k)
  end do  ! column - except pivot element
  end do
  l=1,n
  k=n-l+1
  kr=inter(k,1)
  ir=inter(k,2)
  if(kr.ne.ir) then
    do i=1,n
      temp=a(i,kr)
      a(i,kr)=a(i,ir)
      a(i,ir)=temp
    end do
  end if
  end do
end do
SUBROUTINE STRESS
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 B(3,20,2),XD(20,2),YD(20,2),S(3,3),COMP(6,2),UD(3)
COMPLEX*16 P(3,2), LA(3,3,2), MG(3,3,2), MGB(3,3,2), R(3,3,2), & R2(3,3,20,2), R2B(3,3,20,2), FA(3), PB(3,2), & R2G(3,3,20,2), RG(3,3,20,2), R1(3,3,2), R1B(3,3,2), & URG(3,3,2), UR(3,3,2), URB(3,3,2), F0(3), A(3,3,2)
INTEGER IQ(2), NUM(2)
COMMON B, XD, YD, S, COMP, P, LA, MG, MGB, R, RB, R2, R2B, FA, PB, & R2G, RG, R1, R1B, IQ, NUM, C44P, X, Y, UD, A
LOGICAL L1, L2
CALL GETR2(X, Y, P, PB, XD, YD, NUM, R2, R2B, R2G)
CALL F0ALPH(NUM, B, R2, R2B, R2G, MG, MGB, R, RB, RG, UR, URB, URG)
IP=2
IF(Y.GE.0.0)IP=1
L1=NUM(IP).EQ.0
L2=NUM(IQ(IP)).EQ.0
DO 1=1,3
FA(I)=RG(I,1,IP)
FO(I)=URG(I,1,IP)
IF(L1) THEN
FA(I)=(0.0,0.0)
FO(I)=(0.0,0.0)
END IF
DO J=1,3
IF(L1) THEN
FA(I)=FA(I)+R1B(I,J,IP)*R(I,J,IP)
FO(I)=FO(I)+R1B(I,J,IP)*UR(I,J,IP)
ELSE IF(L2) THEN
FA(I)=FA(I)+R1(I,J,IP)*RB(I,J,IP)
FO(I)=FO(I)+R1(I,J,IP)*URB(I,J,IP)
ELSE
FA(I)=FA(I)+R1(I,J,IP)*RB(I,J,IP)+R1B(I,J,IP)*R(I,J,IP)
FO(I)=FO(I)+R1(I,J,IP)*URB(I,J,IP)
END IF
ENDO
ENDO
DO I=1,3
FA(I)=C44P*FA(I)/6.28318D0
FO(I)=C44P*FO(I)/6.28318D0
ENDO
DO I=1,3
UD(I)=.0.D0
S(I,1)=.0.D0
S(I,2)=.0.D0
DO J=1,3
UD(I)=UD(I)+DREAL(A(I,J,IP)*FO(J))
S(I,1)=S(I,1)+DREAL(P(J,IP)*LA(I,J,IP)*FA(J))
S(I,2)=S(I,2)+DREAL(LA(I,J,IP)*FA(J))
ENDO
ENDO
S(1,3)=S(3,1)
S(2,3)=S(3,2)
S(3,3)=-(1/COMP(3,IP))*(COMP(1,IP)*S(1,1)+COMP(2,IP)*
& S(2,2) + COMP(4,IP)*S(3,2) + COMP(5,IP)*S(3,1) + COMP(6,IP)*S(2,1))
RETURN
END
APPENDIX B - PROGRAM LISTING FOR TEWARY'S METHOD

C
C PROGRAM TO CALCULATE V. K. TEWARY'S GREEN FUNCTION FOR
C A COMPOSITE SOLID WITH A PLANAR INTERFACE, DIFFERENT MATERIALS
C
C Zhiyong Shen
C
C August 14, 1986
C
C IMPLICIT REAL*8(A-H, O-Z)
CHARACTER*80 TITLE
REAL*8 C(3,3,3,3),B(3,20,2),DC(3,3),CR(3,3,3,3),XD(20,2),bb(3),
A YD(20,2),F(3,3,3),S(3,3),BP(3,20),NORM(3),COMP(6,2),B1(6,6),PS(3)
C
C GAMMA(I,J,ALFA,IP), SIGMA(I,J,ALFA,IP)
C
C GAMMASUM(I,J,IP), SIGMASUM(I,J,IP)
C
C COMPLEX*16 Q(7),P(3,2),PB(3,2),PI(3),UPLOW(3,3,2),QA,Z,Z1,
A GAM(3,3,3,2),GAMSUM(3,3,2),SIG(3,3,3,2),SIGSUM(3,3,2),MN(3,3,2).
C
C TEMPORARY STORAGE MATRICES
C
B LUMP(3,3,3,4),TEMP(3,3,2),TEMPI(3,3,2),TEMP2(3,3,2).
D MNEX(3,3,3,4).
C
C CONJUGATE MATRICES
C
E GAM(3,3,3,2),GAMSUB(3,3,2),SIG(3,3,3,2),SIGSUB(3,3,2).
C
C INVERSE MATRICES
C
F GAMSUV(3,3,2),SIGSUV(3,3,2),GAMSUV(3,3,2),SIGSBV(3,3,2).
C
C SUMMATION MATRICES FOR GREEN FUNCTION
C SUM(I,J,BETA,ALPHA,CASE)
C
G SUM(3,3,3,3,4).
C
C MATRICES FOR STRESS CALCULATIONS
C
H LA(3,2,3,3),LB(3,2,3,3),LAB(3,2,3,3),LBB(3,2,3,3).
I GUM(3,3,3,3,4)
C
INTEGER IQ(2),NUM(2),NS(4,2),ALFA,BETA
REAL*8 U(3),green(3,3)
common GAM,GAMB,P,PB,LA,LAB,LB,LBB,SUM,XD,YD,NUM,BB,COMP,U,S,
A green
DATA IQ/2.1/,VPI/0.3183098862DO/
C FOR CRYSTALS 1 AND 2

DO 520 IP=1,2
   READ(10,*) C11,C12,C44
   CALL DEFINE(C11,C12,C44,C)
   WRITE(16,510)C11,C12,C44
C
   READ(10,*) (PS(I),I=1,3), (NORM(I),I=1,3)
   WRITE(16,410)IP,(PS(I),I=1,3),(NORM(I),I=1,3)
410 FORMAT(6H IN XL,I1.3H U=.3f10.6./.5H PN=.3F10.6)

READ(10,*) NUM(IP) ! Read and print line direction,  
   IF (NUM(IP).EQ.O)GO TO 240 ! plane normal and number of  
      NUM=NUM(IP) ! dislocations
C
C FOR EACH DISLOCATION

DO 550 N=1,NUN
   READ(10,*) XD(N,IP),YD(N,IP),(B(I,N,IP),I=1,3),BMAG
   WRITE(16,420)N,IP,XD(N,IP), YD(N,IP),(B(I,N,IP),I=1,3),BMAG
420 FORMAT(IX.' DISLOCATION1.12.* IN XL'.I2.1  X='.F15.5,'  Y='.F15.5  
   1  ./.'  BURGERS VECTOR',3F6.2.' / ',F8.5)
   DO 550 1=1,3
      550 B(I,N,IP)=B(I,N,IP)*BMAG ! Scale the Burgers vector.
C
C Calculate direction cosines.

240 CALL DIRECT(PS,NORM,DC)
C
C ROTATION MATRIX FROM PROBLEM TO CRYSTAL 2 COORDINATES
C
180 CALL ROT9X9(IP,DC,C,CR,B1,COMP) ! Rotate elastic constants tensor     
   IF(IP.EQ.1) THEN
      DO I=1,3
         BB(I)=0.0
         DO J=1,3
            BB(I)=BB(I)+DC(I,J)*B(J,1,1)
         END DO
      END DO
   END IF
C
C COEFFICIENTS OF THE LAMBDA MATRIX
C
   CALL GETF(CR,F)
   WRITE(16,*)' F IN CRYSTAL',IP
   WRITE(16,910)(((F(I,J,K),I=1,3),J=1,3),K=1,3)
910 FORMAT(3(' F(',I1.',',I1.' ,'I1.',',I1.' ') ',F6.2))
C POLYNOMIAL COEFFICIENTS

CALL GETQ(F, Q)
WRITE(16, *) 'POLYNOMIAL COEFFICIENTS IN CRSTAL', IP
WRITE(16, 920)(I, Q(I), I=1, 7)
920 FORMAT(3(' Q(' , I1, ',') ', F8.3, ' + I ', F8.3))
QA = Q(7)

C SOLVE THE SEXTIC EQUATION

CALL NEWTON(Q, PI)

ZR = -CR(3, 2, 3, 1) / CR(3, 2, 3, 2) ! Order the roots so that root
ZI = DSQRT(DABS(CR(3, 2, 3, 2) * CR(3, 1, 3.1) - C(3, 2, 3, 1)
A ** 2) / C(3, 2, 3, 2)) ! 3 is closest being a root of
Z = DCMPLX(ZR, ZI) ! c(5.5) + 2p*c(4.5) + p*p*c(4.4)

C REARRANGE ROOTS

DO 60 N = 1, 2
IF(CDABS(Z - PI(N)).GT.CDABS(Z - PI(N+1))) GO TO 60
Z1 = PI(N)
PI(N) = PI(N+1)
PI(N+1) = Z1
60 CONTINUE

C WRITE(16, *) 'ROOTS IN CRYSTAL', IP
WRITE(16, 930)(I, PI(I), I=1, 3)
930 FORMAT(3(' P(' , I1, ',') ', F8.3, ' + I ', F8.3))

Do 80 I = 1, 3
P(I, IP) = PI(I)
PB(I, IP) = DCONJG(PI(I))
80 CONTINUE

C GET LA AND LBB MATRICES

IF(IP.EQ.1) THEN
DO 54 J = 1, 2
DO 51 ALFA = 1, 3
DO 52 I = 1, 3
DO 53 K = 1, 3
LAB(I, J, K, ALFA) = CR(I, J, K, 1) + CR(I, J, K, 2) * PB(ALFA, 1)
53 CONTINUE
52 CONTINUE
51 CONTINUE
54 CONTINUE
ENDIF

C IF(IP.EQ.2) THEN
DO 64 J = 1, 2
DO 61 ALFA = 1, 3
61 CONTINUE
64 CONTINUE
DO 62 I=1,3
   DO 63 K=1,3
      LB(I,J,K,ALFA)=CR(I,J,K,1)+CR(I,J,K,2)*P(ALFA,2)
      LBB(I,J,K,ALFA)=CR(I,J,K,1)+CR(I,J,K,2)*PB(ALFA,2)
   CONTINUE
   63 CONTINUE
   62 CONTINUE
   61 CONTINUE
   64 CONTINUE
ENDIF

C
C GET GAMMA AND SIGMA MATRICES
C
CALL GETGAM(IP,PI,F,CR,GAM,GAMSUM,QA,SIG,SIGSUM)

C END OF BICRYSTAL LOOP
C
520 CONTINUE

C WRITE(16,*) 'GAMMA(I,J,ALPHA) IN CRYSTAL A'
WRITE(16,1)(((I,J,K,GAM(I,J,K,1),J=1,3),I=1,3),K=1,3)
WRITE(16,1) 'GAMMA(I . J,ALPHA) IN CRYSTAL B '
WRITE(16.1)(((I.J.K.GAM(I.J.K.2).J=1,3).I=1.3).K=1.3)
1 FORMAT(3('  GAM('Il.'.'.Il.'.P'.Il,')  '.F8.3, '+ I '.F8.3))

C WRITE(16,*) 'GAMMA SUM IN CRYSTAL A'
WRITE(16,2)((I,J,GAMSUM(I,J,1),J=1,3),I=1,3)
WRITE(16.*) 'GAMMA SUM IN CRYSTAL B'
WRITE(16,2)((I,J.GAMSUM(I,J,2),J=1,3).I=1.3)
2 FORMAT(3( '  GAMSUM( '.  Il.' *.  * .  Ill.'  )  ',F8.3.'  + I  ',F8.3))

C WRITE(16,*) 'SIGMA(I,J,ALPHA) IN CRYSTAL A'
WRITE(16,3)(((I,J,K,SIG(I,J,K,1),J=1,3),I=1,3),K=1,3)
WRITE(16,3) 'SIGMA(I . J,ALPHA) IN CRYSTAL B'
WRITE(16,3)(((I,J,K,SIG(I,J,K,2),J=1,3),I=1,3),K=1,3)
3 FORMAT(3('  SIG('Il.'.'.Il.'.P*.Il.')  ',F8.3.'  + I ',F8.3))

C WRITE(16,*) 'SIGMA SUM IN CRYSTAL A'
WRITE(16,4)((I,J,SIGSUM(I,J,1),J=1,3),I=1,3)
WRITE(16.*) 'SIGMA SUM IN CRYSTAL B'
WRITE(16,4)((I,J.SIGSUM(I,J,2).J=1.3).I=1.3)
4 FORMAT(3('  SIGSUM( ',Il.' *.  * .  * .  Ill.'  )  ',F8.3.'  + I ',F8.3))

C CONJUGATE MATRICES
C
CALL CONJX(GAM,GAMB)
CALL CONJX(SIG,SIGB)
CALL CONJX(GAMSUM,GAMSUB)
CALL CONJX(SIGS SUM,SIGSUB)

C WRITE(16,*) 'GAMMA CONJ(I,J,ALPHA) IN CRYSTAL A'
WRITE(16,5)(((I,J,K,GAMB(I,J,K,1),J=1,3),I=1,3),K=1,3)
WRITE(16,*) 'GAMMA CONJ(I, J,ALPHA) IN CRYSTAL B'
WRITE(16,5)(((I,J,K,GAMB(I,J,K,2),J=1,3),I=1,3),K=1,3)
FORMAT(3(' GAMB(',I1,','' ,I1,'',P',I1,' ') ',F8.3,' + I ','F8.3))
C
WRITE(16,6)' GAMMA CONCATURATE SUM IN CRYSTAL A'
WRITE(16,6)((I,J,GAMSUB(I,J,1),J=1,3),I=1,3)
WRITE(16,6)' GAMMA CONCATURATE SUM IN CRYSTAL B'
WRITE(16,6)((I,J,GAMSUB(I,J,2),J=1,3),I=1,3)
FORMAT(3(' GAMSUB(',I1,','' ,I1,) ',F8.3,' + I ','F8.3))
C
WRITE(16,7)' SIGMA CONCAT(I,J,ALPHA) IN CRYSTAL A'
WRITE(16,7)(((I,J,K,SIGB(I,J,K,1),J=1,3),I=1,3),K=1,3)
WRITE(16,7)' SIGMA CONCAT(I,J,ALPHA) IN CRYSTAL B'
WRITE(16,7)(((I,J,K,SIGB(I,J,K,2),J=1,3),I=1,3),K=1,3)
FORMAT(3(' SIGB(',I1,','' ,I1,'',P',I1,' ') ',F8.3,' + I ','F8.3))
C
GET INVERSE MATRICES
CALL INVERT(GAMSUM,GAMSUV)
CALL INVERT(SIGSUM,SIGSUV)

WRITE(16,8)((I,J,GAMSUV(I,J,1),J=1,3),I=1,3)
WRITE(16,8)' GAMMA SUM INVERSE IN CRYSTAL A'
WRITE(16,8)((I,J,GAMSUV(I,J,2),J=1,3),I=1,3)
WRITE(16,8)' GAMMA SUM INVERSE IN CRYSTAL B'
FORMAT(3(' GAMSUV(',I1,','' ,I1,) ',F8.3,' + I ','F8.3))
C
WRITE(16,9)((I,J,SIGSUV(I,J,1),J=1,3),I=1,3)
WRITE(16,9)' SIGMA SUM INVERSE IN CRYSTAL A'
WRITE(16,9)((I,J,SIGSUV(I,J,2),J=1,3),I=1,3)
WRITE(16,9)' SIGMA SUM INVERSE IN CRYSTAL B'
FORMAT(3(' SIGSUV(',I1,','' ,I1,) ',F8.3,' + I ','F8.3))
C
WRITE(16,10)((I,J,GAMSBV(I,J,1),J=1,3),I=1,3)
WRITE(16,10)' GAMMA CONCATURATE SUM INVERSE IN CRYSTAL A'
WRITE(16,10)((I,J,GAMSBV(I,J,2),J=1,3),I=1,3)
WRITE(16,10)' GAMMA CONCATURATE SUM INVERSE IN CRYSTAL B'
FORMAT(3(' GAMSBV(',I1,','' ,I1,) ',F8.3,' + I ','F8.3))
C
WRITE(16,11)((I,J,SIGSBV(I,J,1),J=1,3),I=1,3)
WRITE(16,11)' SIGMA CONCATURATE SUM INVERSE IN CRYSTAL A'
WRITE(16,11)((I,J,SIGSBV(I,J,2),J=1,3),I=1,3)
WRITE(16,11)' SIGMA CONCATURATE SUM INVERSE IN CRYSTAL B'
FORMAT(3(' SIGSBV(',I1,','' ,I1,) ',F8.3,' + I ','F8.3))
C T(B) = SIGSUB(B) * GAMSBV(B)
C T(A) = SIGSUM(A) * GAMSUV(A)
C T1(A) = T(B) - T(A)
C T2(A) = INVERSE(T1(A))
C MN(A) = GAMSUV(A) * T2(A) = M
C MN(B) = GAMSBV(B) * T2(A) = N
C UPLOW(A) = SIGSUB(B) * GAMSBV(B) = UP
C UPLOW(B) = SIGSUM(A) * GAMSUV(A) = LOW
C
CALL MULT33(2, SIGSUB, 2, GAMSBV, 2, TEMP)
CALL MULT33(1, SIGSUM, 1, GAMSUV, 1, TEMP)
CALL SUBT33(2, TEMP, 1, TEMP, 1, TEMP1)
CALL SUBT33(2, TEMP, 1, TEMP, 2, TEMP1)
CALL INVERT(TEMP1, TEMP2)
CALL MULT33(1, GAMSUV, 1, TEMP2, 1, MN)
CALL MULT33(2, GAMSBV, 1, TEMP2, 2, MN)
C
WRITE(16, *) 'M MATRIX'
WRITE(16, 13)((I, J, MN(I, J, 1), J=1,3), I=1,3)
  13 FORMAT(3(' M(', I1, ',', I1, '),', F8.3, ', + I ', F8.3))
C
WRITE(16, *) 'N MATRIX'
WRITE(16, 14)((I, J, MN(I, J, 2), J=1,3), I=1,3)
  14 FORMAT(3(' N(', I1, ',', I1, '),', F8.3, ', + I ', F8.3))
WRITE(16, *) 'TEMP(A) MATRIX'
WRITE(16, 15)((I, J, TEMP(I, J, 1), J=1,3), I=1,3)
  15 FORMAT(3(' TA(', I1, ',', I1, '),', F8.3, ', + I ', F8.3))
C
WRITE(16, *) 'TEMPB MATRIX'
WRITE(16, 16)((I, J, TEMP(I, J, 2), J=1,3), I=1,3)
  16 FORMAT(3(' TB(', I1, ',', I1, '),', F8.3, ', + I ', F8.3))
C
WRITE(16, *) 'TEMP1 MATRIX'
WRITE(16, 17)((I, J, TEMP1(I, J, 1), J=1,3), I=1,3)
  17 FORMAT(3(' TM1(', I1, ',', I1, '),', F8.3, ', + I ', F8.3))
C
WRITE(16, *) 'TEMP2 MATRIX'
WRITE(16, 18)((I, J, TEMP2(I, J, 1), J=1,3), I=1,3)
  18 FORMAT(3(' TM2(', I1, ',', I1, '),', F8.3, ', + I ', F8.3))
CALL MULT33(2, SIGSUB, 2, GAMSBV, 1, UPLow)
CALL MULT33(1, SIGSUM, 1, GAMSUV, 2, UPLow)
C
C GET LUMP MATRICES INVOLVING ONLY BETA
C
DO 605 M=1,4
DO 610 BETA=1,3
  620 I=1,3
    DO 630 J=1,3
      IF(M .LE. 2) LUMP(I, J, BETA, M) = SIGB(I, J, BETA, 1)
      IF(M .GT. 2) LUMP(I, J, BETA, M) = SIG(I, J, BETA, 2)
  640 K=1,3
C
IF(M.LE.2) LUMP(I,J,BETA,M) = LUMP(I,J,BETA,M) - 
  A UPL0W(I,K,M)*GAMB(K,J,BETA,1) 
  IF(M.GT.2) LUMP(I,J,BETA,M) = LUMP(I,J,BETA,M) - 
  A UPL0W(I,K,M-2)*GAM(K,J,BETA,2) 

640 CONTINUE 
630 CONTINUE 
620 CONTINUE 
610 CONTINUE 
605 CONTINUE 
C 
C Multiply M, N Matrices by Lump Tensors 
C 
DO 655 M=1,4 
MM=M-(M-1)/2*2 
DO 660 BETA=1,3 
  DO 670 I=1,3 
  DO 680 J=1,3 
  MNEX(I,J,BETA,M)=(0.0DO,0.0DO) 
  DO 690 K=1,3 
    MNEX(I,J,BETA,M)=MNEX(I,J,BETA,M) + A MN(I,K,MM)*LUMP(K,J,BETA,M) 
 690 CONTINUE 
680 CONTINUE 
670 CONTINUE 
660 CONTINUE 
655 CONTINUE 
C 
C Get Tensors in i, j, beta, alpha 
C 
DO 985 M=1,4 
DO 950 ALFA=1,3 
  DO 960 BETA=1,3 
  DO 970 I=1,3 
  DO 980 J=1,3 
  SUM(I,J,BETA,ALFA,M)=(0.0DO,0.0DO) 
  DO 990 K=1,3 
    IF(M.EQ.1.OR.M.EQ.3) SUM(I,J,BETA,ALFA,M)= 
      A SUM(I,J,BETA,ALFA,M)+GAM(I,K,ALFA,1)*MNEX(K,J,BETA,M) 
    IF(M.EQ.2.OR.M.EQ.4) SUM(I,J,BETA,ALFA,M)= 
      A SUM(I,J,BETA,ALFA,M)+GAMB(I,K,ALFA,2)*MNEX(K,J,BETA,M) 
990 CONTINUE 
980 CONTINUE 
970 CONTINUE 
960 CONTINUE 
950 CONTINUE 
985 CONTINUE 
C 
C DISPLACEMENT AND STRESS 
C 
WRITE(28,*') X2 U1 U2 U3 
C 
X=0.0DO
flag = 0
DO 310 II = YLOWER, YUPPER, YSTEP
  Y = DFLOAT(II)
  IF (II .EQ. 0) Y = -0.0001
  goto 6010
6000 IF (II .EQ. 0) Y = 0.0001
  IFLAG = 1
6010 CONTINUE
C
CALL GETSTRESS(X, Y)
S11 = S(1, 1) * 0.0001
S12 = S(1, 2) * 0.0001
S13 = S(3, 1) * 0.0001
S22 = S(2, 2) * 0.0001
S23 = S(3, 2) * 0.0001
S33 = S(3, 3) * 0.0001
WRITE(29, 300) Y, S11, S12, S22, S13, S23, S33
WRITE(13, 300) Y, GREEN(1, 1), GREEN(1, 2), GREEN(2, 1), GREEN(2, 2)
300 FORMAT(1X, 7F10.5)
IF ((II .EQ. 0) .AND. (IFLAG .EQ. 0)) goto 6000
310 CONTINUE
END
SUBROUTINE DEFINE(C11, C12, C44, C)
INTEGER L1(6), L2(6)
REAL C(3, 3, 3, 3), B, C11, C12, C44
DATA L1/1, 2, 3, 3, 2, 1/, L2/1, 2, 3, 2, 1, 1/
DO 1 I = 1, 6
DO 1 J = 1, 6
  B = C12
  IF (I .EQ. J) B = C11
  IF (I .GT. 3 .OR. J .GT. 3) B = 0.0
  IF (I .EQ. J .AND. J .GT. 3) B = C44
  C(L1(I), L2(I), L1(J), L2(J)) = B
  C(L1(I), L2(I), L2(J), L1(J)) = B
  C(L2(I), L1(I), L1(J), L2(J)) = B
  C(L2(I), L1(I), L2(J), L1(J)) = B
1 C(L2(I), L1(I), L2(J), L1(J)) = B
RETURN
END
C
SUBROUTINE DIRECT(P, N, D)
INTEGER P1(3), P2(3)
REAL D(3, 3), P(3), N(3), R1, R2, R3
DATA P1/2, 3, 1/, P2/3, 1, 2/
R1 = DSQRT(P(1) * P(1) + P(2) * P(2) + P(3) * P(3))
R2 = DSQRT(N(1) * N(1) + N(2) * N(2) + N(3) * N(3))
R3 = R1 * R2
DO 1 I = 1, 3
  D(2, I) = N(I) / R2
  D(3, I) = P(I) / R1
1 D(1, I) = (N(P1(I)) * P(P2(I)) - N(P2(I)) * P(P1(I))) / R3
RETURN
END
SUBROUTINE ROT9X9(IP,D,A,B,bl,OOM)

RETURN

4 C

COMPLEX(CR(I,6))(I,16)

CALL INVERSE(D)

DO 1 J=1,6

(2X(I,J),(F(K,L)=B(I,J,K,L))

B(I,J,L)=B(I,J,K,L)

B(I,J,K,L)=B(I,J,L)

B(I,J,K,L)=B(I,J,L)

DO I=1,6

DO I=0,1,3

DO I=N,1,3

DO I=M,1,3

B(I,J,K,L)=0.0

DO 2 J=1,6

DO 2 K=1,3

DO 2 I=1,3

DATA PI/2,3.1415926/7

DATA PI/2,3.1415926/7

COMPLEX(CR(I,6))(I,16)

REAL(CR(I,6))(I,16)

INTEGER PI(3),P2(3)

SUBROUTINE GEFF(CR(6))

END

RETURN

END

DO 4 I=1,6

CALL INVERSE(D)

4 DO I=1,6

2X(I,J),(F(K,L)=B(I,J,K,L))

B(I,J,L)=B(I,J,K,L)

B(I,J,K,L)=B(I,J,L)

B(I,J,K,L)=B(I,J,L)

DO I=1,6

DO I=0,1,3

DO I=N,1,3

DO I=M,1,3

B(I,J,K,L)=0.0

DO 2 J=1,6

DO 2 K=1,3

DO 2 I=1,3

DATA PI/2,3.1415926/7

DATA PI/2,3.1415926/7

COMPLEX(CR(I,6))(I,16)

REAL(CR(I,6))(I,16)

INTEGER PI(3),P2(3)

SUBROUTINE GEFF(CR(6))
SUBROUTINE NEWTON (Q,P)
IMPLICIT REAL*8(A-H,O-Z)
COMPLEX*16 Q(7),P(3),X,Y,T,Z
Z=(.1D0,.1D0)
DO 156 NA=1,6
N=8-NA
K=0
DO 152 KA=1,70
X=(0.0D0,0.0D0)
Y=(0.0D0,0.0D0)
DO 151 J=1,N
Y=Z*Y+X
M=N+1-J
T=Z*X+Q(M)
IF(K.EQ.0)GO TO 150
Q(M)=X
150 X=T
151 CONTINUE
IF(K.NE.0)GO TO 153
T=X/Y
Z=Z-T
IF(CDABS(T)/CDABS(Z).GT.1.0D-6)GO TO 152
K=1
152 CONTINUE
WRITE(1,*) ' POLY DOESN'T CONVERGE ON * ',NA,' TH ROOT '
STOP
153 IF(DABS(DIMAG(Z)).GT.1.0D-5)GO TO 154
WRITE(1,*)NA,' TH ROOT IS REAL, = ',DREAL(Z)
154 LA=NA/2
R=DFLOAT(NA)/2.0DO
DLA=LA
IF(R-DLA.LT.0.1D0)GO TO 155
Z=DCONJG(Z)
GO TO 156
155 P(LA)=DCMPLX(DREAL(Z),DABS(DIMAG(Z)))
IF(LA.EQ.1)Z=(.5D0,.9D0)
IF(LA.EQ.2)Z=-DCONJG(Z)
156 CONTINUE
RETURN
END

SUBROUTINE GETGAM(IP,P,B,C,GAM,GAMSUM,Q,SIG,SIGSUM)
COMPLEX*16 P(3),A(3,3,3),F(3,3,3),DENOM(3)
COMPLEX*16 L(3,3,3),QA
COMPLEX*16 GAM(3,3,3),GAMSUM(3,3,2)
COMPLEX*16 SIG(3,3,3),SIGSUM(3,3,2)
REAL*8 B(3,3,3),C(3,3,3,3)
INTEGER P1(3),P2(3),ALFA
DATA P1/2,3,1/,P2/3,1,2/
QA=Q*(2.0D0,0.0D0)
C LAMBDA(I, J, ALFA)
C DO 10 I=1,3
   DO 20 J=1,3
      DO 30 K=1,3
         F(I,J,K)=B(I,J,1)+B(I,J,2)*P(K)+B(I,J,3)*P(K)*P(K)
30 CONTINUE
20 CONTINUE
10 CONTINUE
C WRITE(16,*)' LAMBDA MATRICES'
WRITE(16,500)F
C CAPGAMMA(I, J, ALFA), COFACTOR MATRIX OF LAMBDA
C DO 50 I=1,3
   DO 60 J=1,3
      DO 70 K=1,3
         A(I,J,K)=F(P1(I),P1(J),K)*F(P2(I),P2(J),K)-
            F(P1(I),P2(J),K)*F(P2(I),P1(J),K)
70 CONTINUE
60 CONTINUE
50 CONTINUE
C WRITE(16,*)' COFACTOR(CAPITAL GAMMA) MATRICES'
WRITE(16,500)A
C DENOMINATORS OF THE GAMMA MATRIX
C DENOM(1)=QA*DIMAG(P(1))*(P(1)-P(2))*(P(1)-DOONJG(P(2)))*
A (P(1)-P(3))*(P(1)-DOONJG(P(3)))
DENOM(2)=QA*DIMAG(P(2))*(P(2)-P(1))*(P(2)-DOONJG(P(1)))*
A (P(2)-P(3))*(P(2)-DOONJG(P(3)))
DENOM(3)=QA*DIMAG(P(3))*(P(3)-P(2))*(P(3)-DOONJG(P(2)))*
A (P(3)-P(1))*(P(3)-DOONJG(P(1)))
C GAMMA MATRICES
C DO 100 I=1,3
   DO 110 J=1,3
      GAMSUM(I,J,IP)=(0.0D0,0.0D0)
      DO 120 K=1,3
         GAM(I,J,K,IP)=A(I,J,K)/DENOM(K)
         GAMSUM(I,J,IP)=GAMSUM(I,J,IP)+GAM(I,J,K,IP)
120 CONTINUE
110 CONTINUE
100 CONTINUE
C
C SIGMA MATRICES

DO 150 I=1,3
  DO 160 J=1,3
    DO 170 K=1,3
      L(I,J,K)=C(I,2,J,1)+C(I,2,J,2)*P(K)
  170 CONTINUE
  160 CONTINUE
  150 CONTINUE

DO 200 I=1,3
  DO 210 J=1,3
    SIGSUM(I,J,IP)=(0.0DO,0.0DO)
    DO 220 ALFA=1,3
      SIG(I,J,ALFA,IP)=(0.0DO,0.0DO)
      DO 230 K=1,3
        SIG(I,J,ALFA,IP)=SIG(I,J,ALFA,IP)+A(I,K,ALFA)*GAM(K,J,ALFA,IP)
      230 CONTINUE
    SIGSUM(I,J,IP)=SIGSUM(I,J,IP)+SIG(I,J,ALFA,IP)
  220 CONTINUE
  210 CONTINUE
  200 CONTINUE
RETURN
END

C INVERT 3x3 MATRICES IN BOTH CRYSTALS

SUBROUTINE INVERT(A,B)
  INTEGER P1(3), P2(3)
  COMPLEX*16 A(3,3,2),B(3,3,2),DET(2)
  DATA P1/2,3,1/,P2/3,1,2/
  DET(1)=(0.DO,0.DO)
  DET(2)=(0.DO,0.DO)
  DO 10 IP=1,2
    DO 1  I=1,3
      DET(IP)=DET(IP)+A(I,1,IP)*(A(2,P1(I),IP)*A(3,P2(I),IP) -
      A(2,P2(I),IP)*A(3,P1(I),IP))
    1 CONTINUE
  10 CONTINUE
  DO 20 IP=1,2
    DO 2  I=1,3
      DO 3 J=1,3
        B(J,I,IP)=(A(P1(I),P1(J),IP)*A(P2(I),P2(J),IP) -
        A(P1(I),P2(J),IP)*A(P2(I),P1(J),IP))/DET(IP)
    3 CONTINUE
  2 CONTINUE
  20 CONTINUE
RETURN
END

C CONJUGATE FOR EACH ALFA
SUBROUTINE CONJX(A,B)
COMPLEX*16 A(3,3,3,2),B(3,3,3,2)
DO 10 IP=1,2
   DO 20 ALFA=1,3
      DO 30 J=1,3
         DO 40 I=1,3
            B(I,J,ALFA,IP)=DOONJG(A(I,J,ALFA,IP))
   40 CONTINUE
30 CONTINUE
20 CONTINUE
10 CONTINUE
RETURN
END

C MULLPLY 3x3 MATRICES
C
SUBROUTINE MULT33(IA,A,IB,B,IC,C)
COMPLEX*16 A(3,3,2),B(3,3,2),C(3,3,2)
DO 1 I=1,3
   DO 1 J=1,3
      C(I,J,IC)=(0,D0,0.D0)
   1 CONTINUE
   DO 1 K=1,3
      C(I,J,IC)=C(I,J,IC)+A(I,K,IA)*B(K,J,IB)
   RETURN
END

SUBROUTINE SUBT33(IA,A,IB,B,IC,C)
COMPLEX*16 A(3,3,2),B(3,3,2),C(3,3,2)
DO 1 I=1,3
   DO 1 J=1,3
      C(I,J,IC)=A(I,J,IA)-B(I,J,IB)
   RETURN
END

SUBROUTINE CONJ(A,B)
COMPLEX*16 A(3,3,2),B(3,3,2)
DO 1 IP=1,2
   DO 1 I=1,3
      DO 1 J=1,3
         B(I,J,IP)=DOONJG(A(I,J,IP))
   RETURN
END

C INVERT AN NxN REAL MATRIX
C
SUBROUTINE invers(a,n)
REAL*8 a(n,n),big,ab,temp
INTEGER inter(20,2)
DO k=1,n ! Calculate elements of reduced
   jj=k
   IF (k.EQ.N) GO TO 70

big = abs(a(k,k))
do i = k+1, n ! Search for largest pivot
    ab = abs(a(i,k)) ! element
    if(big lt ab) then
        big = ab
        jj = i
    end if
end do
inter(k,1) = k
inter(k,2) = jj
if(jj ne k) then ! Check if the row change is necessary. If so, simply
    do j = 1, n
        temp = a(jj,j)
        a(jj,j) = a(k,j)
        a(k,j) = temp ! swap the values of the
    end do
end if ! position vector components
70 inter(k,1) = k
inter(k,2) = jj
if(jj ne k) then ! Check if the row change is necessary. If so, simply
    do j = 1, n
        if(j ne k) a(k,j) = a(k,j)/a(k,k)
    end do ! New pivot row elements
    a(k,k) = 1/a(k,k) ! element replacing pivot
    do i = 1, n ! New elements not in pivot
        if(i ne k) then ! row or pivot column
            if(j ne k) a(i,j) = a(i,j) - a(k,j)*a(i,k)
        end do
        end if
    end do ! New elements for pivot
end do ! column - except pivot element
end do
70 do 1 = 1, n
    k = n - l + 1
    kr = inter(k,1)
    ir = inter(k,2)
    if(kr ne ir) then
        do i = 1, n
            temp = a(i,kr)
            a(i,kr) = a(i,ir)
            a(i,ir) = temp
        end do
    end if
    end do
end do
end subroutine GETSTRESS(X,Y)

C GLOBAL VARIABLES
C
REAL*8 XD(20,2), YD(20,2), S(3,3), BB(3), COMP(6,2), U(3), g(3,3)
COMPLEX*16 GAM(3,3,3,2), P(3,2), PB(3,2), Gamb(3,3,3,2),
A LA(3,2,3,3), LAB(3,2,3,3), LB(3,2,3,3), LBB(3,2,3,3),
B SUM(3,3,3,3,4), gc(3,3)
C
C LOCAL VARIABLE
C
INTEGER ALFA, BETA, NUM(2)
COMPLEX*16 UP(3,3), FALFA(3,3), FBETA(3,3), GREEN(3,3,3),
A DERIV(3,3,3), GALBE(3,3,3,3), DALBE(3,3,3,3), SS(3,3)
COMPLEX*16 z(3,2), zb(3,2), zp(3,2), zpb(3,2)
COMMON GAM, GAMB, P, PB, LA, LAB, LB, LBB, SUM, XD, YD, NUM, BB, COMP, U, S,
A g
C
DATA VPI/0.3183098862D3/, ia/1/, ib/2/, VP/0.3183098862D0/
C
DO 10 I=1,3
U(I)=0.0D0
DO 20 J=1,3
 gc(I, J)=(0.0D0, 0.0D0)
 SS(I, J)=(0.0D0, 0.0D0)
20 CONTINUE
10 CONTINUE
C
do 50 alfa=1,3
do 60 ip=1,2
 z(alfa, ip)=x+p(alfa, ip)*y
 zb(alfa, ip)=x+pb(alfa, ip)*y
60 continue
50 continue
C
DO 1810 JJ=1, NUM(1)
XP=XD(JJ,1)
YP=YD(JJ,1)
do 100 alfa=1,3
do 110 ip=1,2
 zp(alfa, ip)=xp+p(alfa, ip)*yp
 zpb(alfa, ip)=xp+pb(alfa, ip)*yp
110 continue
100 continue
DO 1300 I=1,3
 DO 1310 J=1,3
 UP(I, J)=(0.0D0, 0.0D0)
 FALFA(I, J)=(0.0D0, 0.0D0)
 FBETA(I, J)=(0.0D0, 0.0D0)
 DO 1320 ALFA=1,3
 GREEN(I, J, ALFA)=(0.0D0, 0.0D0)
 DERIV(I, J, ALFA)=(0.0D0, 0.0D0)
 DO 1330 BETA=1,3
 GALBE(I, J, BETA, ALFA)=(0.0D0, 0.0D0)
 DALBE(I, J, BETA, ALFA)=(0.0D0, 0.0D0)
1330 CONTINUE
1320 CONTINUE
1310 CONTINUE
1300 CONTINUE
C
C GET GREEN FUNCTION TENSOR AND ITS DERIVATIVES
C
DO 700 1=1,3
   DO 710  J=1,3
      DO 720 ALFA=1,3
C
C CASE 1. X AND XP IN UHP (Y>0, YP>0)
C
   IF ((Y.GT.0.0).AND.(YP.GT.0.0)) THEN
      FALFA(I,J)=FALFA(I,J)+BB(ALFA)*LA(ALFA,2,I,J)
      FBETA(I,J)=FBETA(I,J)+BB(ALFA)*LAB(ALFA,2,I,J)
      GREEN(I,J,ALFA)=-GAM(I,J,ALFA,1)*
         A CDLOG(z(alfa,ia)-zp(alfa,ia))
      gc(i,j)=gc(i,j)+green(i,j,alfa)
      DERIV(I,J,ALFA)=-GAM(I,J,ALFA,1)/
         A (z(alfa,ia)-zp(alfa,ia))
   DO 730 BETA=1,3
      GALBE(I,J,BETA,ALFA)=-SUM(I,J,BETA,ALFA,1)*
         A CDLOG(z(alfa,ia)-zp(alfa,ia))
      gc(i,j)=gc(i,j)+galbe(i,j,alfa)
      DALBE(I,J,BETA,ALFA)=-SUM(I,J,BETA,ALFA,1)/
         A (z(alfa,ia)-zp(alfa,ia))
   CONTINUE
C
C CASE 2. X IN LHP, XP IN UHP (Y=<0, YP>0)
C
   ELSE IF ((Y.LE.0.0).AND.(YP.GT.0.0)) THEN
      FBETA(I,J)=FBETA(I,J)+BB(ALFA)*LAB(ALFA,2,I,J)
      DO 780 BETA=1,3
         GALBE(I,J,BETA,ALFA)=-SUM(I,J,BETA,ALFA,2)*
            A CDLOG(z(alfa,ia)-zp(alfa,ia))
         gc(i,j)=gc(i,j)+galbe(i,j,alfa)
         DALBE(I,J,BETA,ALFA)=-SUM(I,J,BETA,ALFA,2)/
            A (z(alfa,ia)-zp(alfa,ia))
   CONTINUE
C
C CASE 3. X IN UHP, XP IN LHP (Y>0, YP=<0)
C
   ELSE IF ((Y.GT.0.0).AND.(YP.LE.0.0)) THEN
      FBETA(I,J)=FBETA(I,J)+BB(ALFA)*LB(ALFA,2,I,J)
      DO 830 BETA=1,3
         GALBE(I,J,BETA,ALFA)=SUM(I,J,BETA,ALFA,3)*
            A CDLOG(z(alfa,ia)-zp(alfa,ia))
         gc(i,j)=gc(i,j)+galbe(i,j,alfa)
         DALBE(I,J,BETA,ALFA)=SUM(I,J,BETA,ALFA,3)/
            A (z(alfa,ia)-zp(alfa,ia))
   CONTINUE
C
C CASE 4. X AND XP IN LHP (Y=<0, YP=<0)
C
   ELSE
      FALFA(I,J)=FALFA(I,J)+BB(ALFA)*LBB(ALFA,2,I,J)
FBETA(I,J)=FBETA(I,J)+BB(ALFA)*LB(ALFA,2,I,J)
GREEN(I,J,ALFA)=-GAMB(I,J,ALFA,2)\*A CDLOG(zb(alfa,ib)-zpb(alfa,ib))
gc(i,j)=gc(i,j)+green(i,j,alfa)
 DERIV(I,J,ALFA)=-GAMB(I,J,ALFA,2)/A (zb(alfa,ib)-zpb(alfa,ib))
DO 880 BETA=1,3
 GALBE(I,J,BETA,ALFA)=SUM(I,J,BETA,ALFA,4)\*A CDLOG(zb(alfa,ib)-zp(beta,ib))
gc(i,j)=gc(i,j)+galbe(i,j,beta,alfa)
 DALBE(I,J,BETA,ALFA)=SUM(I,J,BETA,ALFA,4)/A (zb(alfa,ib)-zp(beta,ib))
 880 CONTINUE
  END IF
 720 CONTINUE
 710 CONTINUE
 700 CONTINUE
C
C GET DISPLACEMENT AND STRESS
C
C FIRST TERM OF DISPLACEMENT
C
IF((Y*YP).GE.0.0) THEN
  DO 2000 J=1,3
    DO 2010 ALFA=1,3
      DO 2020 I=1,3
        U(J)=U(J)+FALFA(I, ALFA)*GREEN(J,I,ALFA)
      2020 CONTINUE
    2010 CONTINUE
  2000 CONTINUE
END IF
C
C DISPLACEMENT
C
  DO 2100 J=1,3
    DO 2110 BETA=1,3
      DO 2120 ALFA=1,3
        DO 2130 I=1,3
          U(J)=U(J)+DREAL(FBETA(I, BETA)*GALBE(J,I, BETA, ALFA))
        2130 CONTINUE
      2120 CONTINUE
    2110 CONTINUE
  2100 CONTINUE
C
C FIRST TERM OF DISPLACEMENT GRADIENT
C
IF((Y*YP).GE.0.0) THEN
  DO 2200 J=1,3
    DO 2210 ALFA=1,3
      DO 2220 I=1,3
        UP(J,ALFA)=UP(J,ALFA)+FALFA(I,ALFA)*DERIV(J,I,ALFA)
      2220 CONTINUE
    2210 CONTINUE
  2200 CONTINUE
CONTINUE

END IF

C DISPLACEMENT GRADIENT

C

DO 2300 J=1,3
  DO 2310 ALFA=1,3
    DO 2320 BETA=1,3
      DO 2330 I=1,3
        UP(J,ALFA)=UP(J,ALFA)+
          A FBETA(I,BETA)*DALBE(J,I,BETA,ALFA)
      2330 CONTINUE
  2320 CONTINUE
  2310 CONTINUE
  2300 CONTINUE
C
C Calculate Stress
C

DO 2400 I=1,3
  DO 2410 J=1,2
    DO 2420 ALFA=1,3
      DO 2430 K=1,3
        IF(Y.GT.O) THEN
          SS(I,J)=SS(I,J)+
            A LA(I,J,K,ALFA)*UP(K,ALFA)
        ELSE
          SS(I,J)=SS(I,J)+
            A LBB(I,J,K,ALFA)*UP(K,ALFA)
        END IF
      2430 CONTINUE
    2420 CONTINUE
  2410 CONTINUE
  2400 CONTINUE
C
1810 CONTINUE
C
IP=2
IF(Y.GE.O) IP=1
SS(3,3)=-(1/COMP(3,IP))*((COMP(1,IP)*SS(1,1)+COMP(2,IP)*
  A SS(2,2)+COMP(4,IP)*SS(2,2)+COMP(5,IP)*SS(3,1))
B +COMP(6,IP)*SS(2,1))
C
DO 1200 I=1,3
  U(I)=U(I)*VPI
  DO 1210 J=1,3
    g(J,I)=dreal(gc(j,i))*vp
    S(J,I)=DREAL(SS(J,I))*VPI
  1210 CONTINUE
1200 CONTINUE
RETURN
END
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