Dislocations and Plane Boundaries
in Elastic Continua

A thesis submitted to the University of Surrey in partial
fulfilment of the requirements for the degree of
Doctor of Philosophy

by

Michael Owen Tucker
Department of Physics
University of Surrey
Guildford, Surrey

October, 1969
Summary

The principal objective has been to develop realistic elastic models of slip bands in polycrystalline materials to enable a more complete study to be made of the suggested mechanisms of yield propagation across grain boundaries. Existing models are reviewed in Chapter 1, special emphasis being given to those in which the slip band is represented by a continuous distribution of infinitesimal dislocations, an approximation used throughout the present work.

A detailed description of the Wiener-Hopf technique for solving singular integral equations is given in Chapter 2, and is used in Chapter 3 to obtain the equilibrium distribution function of an array of screw dislocations inclined at certain angles to the plane interface between two different isotropic elastic half-spaces, and piled-up against this boundary under the influence of a uniform applied stress. Special attention is given in Chapter 4 to the case when the undislocated half-space is rigid, and to an infinitely thin notch in antiplane strain inclined at an arbitrary angle to a free surface.

Solutions to certain boundary-value problems associated with elastically anisotropic half-spaces deformed in generalised plane strain are derived in Chapter 5, and used to investigate the interaction of dislocations with free surfaces and welded and freely-slipping interfaces between two such half-spaces. With the use of these results the analysis of Chapter 3 is generalised in Chapter 6 for cases when the half-spaces are elastically anisotropic, provided
that they possess certain symmetry elements.

The significance of the results is discussed in Chapter 7, where their application to the Hall-Petch relation for yield is considered in detail.
Acknowledgements

The Author wishes to thank most sincerely Dr. A.G. Crocker, both for his supervision of the research reported in this thesis and for his friendship and practical assistance given so readily during the last three years. The many useful discussions with Dr. M.C. Jones and Dr. P.T. Heald, and the assistance of Mrs. G. Smith with computations were also much appreciated. Thanks are also due to the Ministry of Technology for their financial support of this work.

Finally the Author wishes to express his deep sense of gratitude to his family, to his wife Sandra for her infinite patience and understanding, and to his children, Mark, Susan, Sarah, Rachel and Kirstie for "leaving Daddy to get on with his work".
Contents

Chapter 1  Introduction  Page 1
1.1 Theoretical Problems in Polycrystalline Deformation.  1
1.2 Linear Arrays of Dislocations.  3
1.3 Stresses in Inhomogeneous Solids.  7
1.4 Dislocation Pile-Ups.  10
1.5 Dislocation Pile-Ups and the Hall-Petch Equation.  15

Chapter 2  The Wiener-Hopf Technique with Mellin Transforms  20
2.1 Basic Properties of the Mellin Transform.  20
2.2 The Wiener-Hopf Procedure.  22
2.3 Formulation of the Wiener-Hopf Problem for Linear Screw Dislocation Arrays Inclined to Plane Boundaries.  24

Chapter 3  Screw Dislocation Pile-Ups in Two Phase Materials of Finite Rigidity  32
3.1 Solution of the Integral Equation.  32
3.2 The Number of Dislocations in the Pile-Up.  38
3.3 Stresses Near to the Tip of the Pile-Up.  39
Appendix 3.1  43
Appendix 3.2  46

Chapter 4  Two Special Cases of Screw Dislocation Pile-Ups Near to Plane Boundaries  47
4.1 Screw Dislocation Pile-Ups Against a Rigid Second Phase.  48
4.2 The Infinitely-Sharp Notch in Antiplane Strain  52
  4.2.1 The Wiener-Hopf Approach.  53
  4.2.2 The Conformal Mapping Approach.  57
  4.2.3 The Crack Growth Condition.  59
4.3 Summary.  60
Chapter 5  Plane Boundaries and Straight Dislocations in Elastically Anisotropic Materials  Page 66

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1 Introduction</td>
<td>66</td>
</tr>
<tr>
<td>5.2 Generalised Plane Strain in an Infinite Homogeneous Anisotropic Material.</td>
<td>68</td>
</tr>
<tr>
<td>5.3 The Classical Boundary-Value Problems for a Half-Space.</td>
<td>70</td>
</tr>
<tr>
<td>5.4 The Interface between Two Elastically Different Half-Spaces.</td>
<td>73</td>
</tr>
<tr>
<td>5.4.1 Introduction</td>
<td>73</td>
</tr>
<tr>
<td>5.4.2 The Welded Interface</td>
<td>75</td>
</tr>
<tr>
<td>5.4.3 The Freely Slipping Interface</td>
<td>77</td>
</tr>
<tr>
<td>5.4.4 Discussion</td>
<td>78</td>
</tr>
<tr>
<td>5.5 The Interaction between Straight Dislocations and Plane Boundaries.</td>
<td>80</td>
</tr>
<tr>
<td>5.5.1 Introduction</td>
<td>80</td>
</tr>
<tr>
<td>5.5.2 Two Dislocations in One Half-Space.</td>
<td>81</td>
</tr>
<tr>
<td>5.5.3 Two Dislocations Separated by a Plane Boundary.</td>
<td>85</td>
</tr>
<tr>
<td>5.6 Related Groups of Interfaces.</td>
<td>87</td>
</tr>
<tr>
<td>5.6.1 Extension of the General Theory.</td>
<td>87</td>
</tr>
<tr>
<td>5.6.2 A Simple Application.</td>
<td>91</td>
</tr>
<tr>
<td>5.7 Discussion</td>
<td>92</td>
</tr>
<tr>
<td>Appendix 5.1</td>
<td>98</td>
</tr>
</tbody>
</table>

Chapter 6  Screw Dislocation Pile-Ups in Elastically Anisotropic Two-Phase Materials  Page 101

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.1 Introduction</td>
<td>101</td>
</tr>
<tr>
<td>6.2 Screw Dislocation Pile-Ups in Bicrystals of Two-Fold Symmetry.</td>
<td>104</td>
</tr>
<tr>
<td>6.3 Screw Dislocation Pile-Ups Against a Second Phase of General Anisotropy.</td>
<td>109</td>
</tr>
<tr>
<td>6.4 Summary</td>
<td>114</td>
</tr>
</tbody>
</table>
Chapter 7 Conclusion

7.1 Results of the Present Work.

7.2 Application to the Hall-Petch Yield Stress Relationship.
   7.2.1 The Hall Mechanism.
   7.2.2 The Petch Mechanism.

7.3 Outstanding Problems Associated with the Present Work.

References.
1.1 Theoretical Problems in Polycrystalline Deformation

In his May Lecture to the Institute of Metals in 1938, Professor G.I. Taylor outlined the major problems in the theoretical treatment of polycrystalline metals. "The essential difficulty in connecting experimental results obtained with single crystals with those obtained in aggregates is to imagine how it is possible for slipping to go on inside crystals so that the boundaries of neighbouring crystal grains shall still be in contact after slipping has taken place. All attempts made so far to correlate the mechanical properties of crystalline aggregates with those of single crystals rest on the same fallacy, namely that each crystal grain can be treated as though its neighbours did not exist." Because of the misorientation between neighbouring grains in a polycrystal, the grain boundaries are ideally surfaces of discontinuity in the structure and hence the mechanical properties of the material. When a grain deforms by slip, twinning or fracture the deformation can only proceed in an unchanged way as far as this boundary, further deformation occurring when the stress intensification is sufficient to trigger off one or more of these processes in the surrounding material so as to reduce the total energy of the system. It is not possible to predict in a given situation which processes will occur without a knowledge of the initiation mechanisms, but because of the difficulties in observing these effects directly few such mechanisms have been
proposed with any degree of certainty.

As Taylor points out, in the absence of intergranular fracture neighbouring grains must remain in contact during this stress relaxation process. In macroscopic treatments of the elastic and plastic deformation of polycrystals which take into account the granular structure this requirement may be expressed in the form of compatibility conditions. Since a vast majority of crystalline materials are elastically anisotropic adjacent grains will in general undergo different elastic deformations under the influence of a given applied stress. Thus an elastic incompatibility will exist between them necessitating additional elastic strains in the boundary region if the grains are to remain in contact. Although mathematical treatment of this condition is intractable in all but the simplest geometries, there is no reason to suppose that in principle the condition cannot always be satisfied for boundaries of finite extent. Attempts to formulate a macroscopic theory of polycrystalline plasticity have been less successful. If the plastic deformation of a crystal is considered to be homogeneous, von Mises\(^2\) has pointed out that the material must possess five independent slip systems if it is to be able to undergo an arbitrary plastic strain without a change in volume. This criterion has been used extensively as a condition for the plastic compatibility of polycrystalline aggregates, based on the observed slip modes of single crystals, but is apparently not obeyed by a number of non-cubic materials which are in practice ductile\(^3\).

The most likely reason for the breakdown of the von Mises criterion is the assumption of homogeneous deformation.
In the grains of deformed polycrystals dislocations in high densities and twin lamellae are observed, whilst the homogeneous theory presupposes their absence. It appears necessary therefore to invoke the dislocation theory of plasticity to achieve a better understanding of polycrystalline ductility. Moreover, because of the analogies between dislocation arrays and cracks\(^{(4,5)}\) the elastic properties of these arrays may be used to assess the effects of fracture, a phenomenon which must by nature be excluded from a homogeneous deformation theory.

1.2 Linear Arrays of Dislocations

Eshelby, Frank and Nabarro\(^{(6)}\) proposed a single planar array of infinite, straight and parallel dislocations in an infinite homogeneous solid as an idealised model of a slip band in a real crystal. Assuming that each dislocation was free to move in the plane of the array under the combined influence of applied and internal stresses they developed a method of determining the static equilibrium configuration of the array. The mathematical complexities involved in treating the dislocations as discrete entities are prohibitive however in all but the simplest problems, and the need arises to use an approximate but more versatile model. In his calculation of the equilibrium width of a single dislocation Eshelby\(^{(7)}\) introduced the concept of an infinitesimal dislocation, and Leibfried\(^{(8)}\) was first to apply this concept to linear dislocation arrays. Although a continuous distribution of infinitesimal dislocations is an inexact representation of an array of discrete dislocations Head and Louat\(^{(4)}\) have demonstrated the validity of the approximation when the number of discrete
dislocations is large.

In terms of the rectangular Cartesian axes $Ox_1$ ($i = 1, 2, 3$) consider a set of $N$ dislocations parallel to $Ox_3$ and contained in the plane $x_2 = 0$, in an elastically isotropic medium of shear modulus $G$ and Poisson's ratio $\nu$. In the plane of the array a dislocation at $x_1 = X$ of Burgers vector $b$ gives rise to a shear stress

$$\sigma_j(x) = A_j(x - X)^{-1}$$

at $x_1 = x$, where $j = 1$, $A_1 = Gb/2\pi(1-\nu)$ for a pure edge dislocation and $j = 3$, $A_3 = Gb/2\pi$ for a pure screw dislocation. Assuming the dislocations in the array to be all of the same character, and if the $\ell$th dislocation of Burgers vector $b_{\ell}$ is situated at $x_1 = x_{\ell}^\ell$, the shear stress at $x_1 = x$ due to the entire array may be written in the form

$$\sigma_j(x) = A_j \sum_{\ell=1}^{N} F_{\ell}(x - x_{\ell}^\ell)^{-1}$$  \hspace{1cm} (1.1)$$

where $F_{\ell} = b_{\ell} b_{\ell}^{-1}$. Letting $N \to \infty$ as $F_{\ell} \to 0$ so that the products $NF_{\ell}$ remain finite, a continuous distribution of infinitesimal dislocations is obtained. Equation (1.1) may now be written as the integral

$$\sigma_j(x) = A_j \int_{L} F(x') (x - x')^{-1} \, dx'$$ \hspace{1cm} (1.2)$$

where $F(x)$ describes the dislocation distribution along the dislocated segments $L$ of the $x_1$-axis. The notation $\int$ indicates that the Cauchy principal value of the integral is to be taken to exclude the self-stress of the dislocation at $x$. The continuous distribution may thus be thought to
represent an array of identical discrete dislocations of strength \( b \), there being \( F(x)dx \) in the interval \( x_1 = x \) to \( x_1 + dx \) and a total of \( \int_L F(x)dx \) such dislocations distributed over the regions \( L \).

In problems involving dislocation arrays of this type it is necessary to assume that the solid containing the dislocations is in a state of generalised plane strain, that is that all stresses and displacements are invariant in the \( x_3 \)-direction. This assumption clearly presupposes that the structure of the solid is also invariant in this direction and that all boundaries are infinite cylindrical surfaces parallel to the \( Ox_3 \) axis. Thus in the case discussed above the most general form of the total stress \( \sigma_{j2}^T \) acting at \( x_1 = x \) in the plane \( x_2 = 0 \) may be written

\[
\sigma_{j2}^T = A_3 \int_L F(x') (x-x')^{-1} dx' + \int_L F(x') \sigma_{j2}^1 (x, x') dx' + \sigma_{j2}^n (x), \quad (1.3)
\]

The term \( \sigma_{j2}^1 (x, x') \) includes both the "image" stresses of dislocations in the array due to the presence of boundaries, as discussed in the next section, and the stresses due to dislocation arrays identical to that in the region \( L \) but situated elsewhere in the solid. Stresses which are independent of the dislocation distribution in the array, such as those due to the applied load and to any other dislocations in the solid, are included in the term \( \sigma_{j2}^n (x) \).

The arrayed dislocations will be in static equilibrium under the influence of the stresses \( \sigma_{j2}^T \) given by (1.3) if
\[ A_j \int_L F(x') (x-x')^{-1} dx' + \int_L F(x') \sigma_{j2}(x,x') dx' \]
\[ + \sigma''_{j2}(x) = 0, \quad x \in L \]
\[ = \sigma''_{j2}, \quad x \notin L. \quad (1.4) \]

It has been pointed out by Head and Louat\(^{(4)}\) that if (1.4) can be written in the form

\[ \int_A \varphi(\xi')(\xi-\xi')^{-1} d\xi' + \psi''(\xi) = 0, \quad \xi \in \Lambda \]
\[ = \psi(\xi), \quad \xi \notin \Lambda, \quad (1.5) \]

where \( \Lambda \) consists of a finite number of segments, its solution may be obtained using the inversion theorem of Muskhelishvili\(^{(9)}\). Clearly for dislocations arrayed over finite regions of a single plane in an infinite homogeneous solid equation (1.4) is of the appropriate form since \( \sigma_{j2} = 0 \). In such cases solutions have been obtained by this method when \( \sigma_{j2} \) is both an algebraic function of \( x \) [e.g. Head and Louat\(^{(4)}\) and Smith\(^{(10)}\)] and a step function [e.g. Bilby, Cottrell and Swinden\(^{(11)}\) and Smith\(^{(12)}\)]. In certain other problems, when either the segments \( L \) are infinite in number\(^{(8,13)}\) or \( \sigma_{j2} \) is non-zero\(^{(14,15)}\) equation (1.4) may still, after some manipulation, be written in the form of (1.5) and solved exactly using the Muskhelishvili theorem.

In many important problems, however, the singular integral equation (1.4) cannot be solved by the direct application of this theorem, and an alternative approach is necessary. Iterative solutions have been obtained in some cases\(^{(16,17)}\) by writing \( F(x) \) as a Neumann series, each coefficient of which is the solution of an equation of
the form of (1.5). Recently Smith(18) has used a generalisation of the Muskhelishvili theorem due to Bueckner(19) for inversion of equation (1.4) when

\[ \sigma_{j2}(x,x') = \sum_{k=1}^{n} a_k x^{k-1}(x+x')^{-k}, \]

where \( a_k \) are real constants, whilst for more complicated kernels methods based on the Wiener-Hopf technique have been employed(20,21). The last approach is discussed in Chapter 2 of the present work.

Since the stresses and displacements in systems deformed in antiplane strain may be expressed in terms of a single harmonic function, problems involving screw dislocation arrays exclusively may also be treated by standard potential theory methods. Conformal mapping techniques may thus be employed to simplify the geometry of the system (22) and in many cases the need to solve integral equations is avoided(23,24,25). An example of the latter type is considered in Chapter 4.

1.3 Stresses in Inhomogeneous Solids

In the mathematical model of a linear dislocation array developed in the last section the effect of inhomogeneities on the dislocation distribution function \( F(x) \) is reflected in the forms of the functions \( \sigma_{j2}^{1} \) and \( \sigma_{j2}^{n} \) in equation (1.4). The stress fields of dislocations in the presence of boundaries contain the so-called image terms which are absent in infinite homogeneous solids, and these appear in \( \sigma_{j2}^{1} \) due to the dislocation array (and any identical arrays) and in \( \sigma_{j2}^{n} \) due to all other disloca-
tions present. Moreover, because of the elastic compatibility stresses the contribution of the applied load to $\sigma_{j2}^{\prime\prime}$ will also be dependent upon the structure of the solid. Discussion in this section is limited to elastically isotropic media, whilst the extension to solids composed of elastically anisotropic half-spaces is treated in Chapter 5.

Dundurs (26) and Smith (24) have evaluated the stress field of an isolated screw dislocation parallel to the axis of an infinite circular cylindrical inclusion of material (II) embedded in an elastically different material (I) when the dislocation is either within or outside the inclusion. Referred to axes $Ox_1$, suppose that the cylinder radius is $\rho$ and that its axis is coincident with $Ox_2$.

The non-zero stress components $\sigma_{k3}^{(I)}$ and $\sigma_{k3}^{(II)}$ ($k=1,2$) at points $(x_1,x_2)$ in media (I) and (II) respectively due to a screw dislocation at $(X_1,0)$ of Burgers vector $b$ may be written in the form

$$\begin{align*}
\sigma_{k3}^{(I)} &= \sigma_{k3}^{D(I)}(x_1,0) + \gamma \sigma_{k3}^{D(I)}(\rho^2/x_1,0) - \gamma \sigma_{k3}^{D(I)}(0,0), \\
\sigma_{k3}^{(II)} &= (1+\gamma)\sigma_{k3}^{D(I)}(x_1,0)
\end{align*}$$

when the dislocation is outside the inclusion, and

$$\begin{align*}
\sigma_{k3}^{(I)} &= (1-\gamma)\sigma_{k3}^{D(II)}(x_1,0) - \gamma \sigma_{k3}^{D(II)}(0,0) \\
\sigma_{k3}^{(II)} &= \sigma_{k3}^{D(II)}(x_1,0) - \gamma \sigma_{k3}^{D(II)}(\rho^2/x_1,0)
\end{align*}$$

when it is inside. The functions

$$\sigma_{k3}^{D(g)}(a_1,a_2) = \frac{G(g)}{2\pi} \rho (x_k-a_k)[(x_1-a_1)^2+(x_2-a_2)^2]^{-1} \quad (g=I,II)$$

are identical in form to the stress components at $(x_1,x_2)$.
due to an isolated screw dislocation at \((a_1, a_2)\) in an
infinite homogeneous medium of shear modulus \(G(g)\), and by
using this notation the interpretation of (1.6) and (1.7)
in terms of image dislocations, analogous to image charges
in electrostatics, is apparent. The Burgers vectors of
the image dislocations of both \(b\) and the constant
\[
\gamma = \frac{[G(II) - G(I)] [G(II) + G(I)]^{-1}}{}
\]  
(1.8)
From Smith's\(^{(24)}\) analysis it may also be shown that a
uniform load \(\sigma^A_{k3}\) applied at infinity gives rise to stresses
\[
\sigma_{13}^{(I)} = \sigma_{13}^A + \gamma \rho^2 \left[ \sigma_{13}^A (x_1^2 - x_2^2) + 2 \sigma_{13}^A x_1 x_2 \right] (x_1^2 + x_2^2)^{-2}\]
\[
\sigma_{23}^{(I)} = \sigma_{23}^A + \gamma \rho^2 \left[ \sigma_{23}^A (x_2^2 - x_1^2) + 2 \sigma_{23}^A x_1 x_2 \right] (x_1^2 + x_2^2)^{-2}\]
and
\[
\sigma_{k3}^{(II)} = (1+\gamma) \sigma_{k3}^A\]
(1.10)
at the point \((x_1, x_2)\).

By replacing \(x_1\) by \(x_1 + \rho\) and taking limiting values of
either equations (1.6) or (1.7) as \(\rho \to \infty\) the results of
Head\(^{(27)}\) for a screw dislocation near to the plane inter­
face \(x_1 = 0\) between two half-spaces are obtained, as given
in equation (2.11) and (2.12). Adopting the same procedure
with equations (1.9)
\[
\sigma_{13}^{(I)} = (1+\gamma) \sigma_{13}^A, \quad \sigma_{23}^{(I)} = (1-\gamma) \sigma_{23}^A\]
(1.11)
for finite \(x_1, x_2\), although as Smith\(^{(24)}\) has pointed out
this implies the necessity of subjecting the half-spaces to
different applied stresses at infinity. However this
objection is overcome if the plane interface results are
considered as approximations to those for inclusions of
large but finite radius, and on this basis the stresses
(1.10) and (1.11) will be used where appropriate in the present work.

Corresponding analyses\(^{(28,29)}\) have been presented for edge dislocation interactions with circular inclusions which reduce in a similar manner to Head's\(^{(30)}\) original results for the edge dislocation/plane interface problem. Dislocation interactions with inhomogeneities in the form of elliptical cylindrical inclusions and holes\(^{(31)}\), surface layers\(^{(32,33)}\) and lamellar inclusions\(^{(32,34)}\) have also been considered. Problems of screw dislocation arrays in half-spaces with irregular surface features such as steps\(^{(35)}\) and notches\(^{(22,36)}\) have been directly treated using potential theory, and analysis of the single dislocation interactions has been unnecessary in these cases.

1.4 Dislocation Pile-Ups

It is assumed in the following discussion that, unless otherwise stated, all dislocation pile-ups occupy regions \(0 \leq x_1 \leq \ell\) of planes \(x_2 = \text{constant}\) in an infinite solid. A uniform stress \(\sigma_{23} = -\sigma\) acts on the slip plane causing \(n-1\) freely-slipping dislocations to pile-up against an immobile dislocation at \(x_1 = 0\). The notation \(\sigma_{j2}^P(r)\) \((j=1,3)\) is used for components \(\sigma_{j2}\) of the stress due to the piled-up dislocations at points \(x_1 = -r\) on the slip plane beyond the fixed dislocation.

Using their discrete model Eshelby et al.\(^{(6)}\) deduced that, when all the dislocations are identical, their positions in the array coincide with the zeros of the first derivative of the \(n^{th}\) Laguerre polynomial \(L_n(2\sigma A x_1/A_3)\), and confirmed Cottrell's\(^{(37)}\) result that the stress \(\sigma_{j2}^P\)
on the leading dislocation was

\[ \sigma_{j2}^L = -n\sigma. \tag{1.12} \]

Moreover, for large \( n \), they derived the approximate results

\[ n = \frac{\sigma \ell}{2A_j} \tag{1.13} \]

and

\[ D = 1.84A_j/n\sigma \tag{1.14} \]

where \( D \) is the separation of the fixed and nearest free dislocations. In the continuous distribution approximation of a single pile-up Head and Louat\(^{(4)}\) have obtained the result (1.13) and shown that

\[ \sigma_{23}^P(r) = -\sigma(1+\ell/r)^{1/2} + \sigma \tag{1.15} \]

which, for \( r<\ell \), is in agreement with the approximate form given by Eshelby et al.\(^{(6)}\).

By means of the virtual work principle Smith\(^{(38)}\) has presented a useful generalisation of equation (1.12) which is applicable to continuously distributed dislocation pile-ups subject to non-uniform shear stress \( \sigma_{j2} = \sigma_{j2}^s(x) \) on the slip plane. In the notation of equation (1.3), by writing

\[ \sigma_{j2}^s(x) = \int_0^\ell f(x')\sigma_{j2}'(x,x')dx' + \sigma_{j2}''(x) \]

for \( 0<x<\ell \), the stress on the stationary dislocation is given by

\[ \sigma_{j2}^L = \int_0^\ell \sigma_{j2}^s(x)f(x)dx. \tag{1.16} \]

It is clearly not possible to derive relationships of the
type (1.14) using a continuous distribution model, although Smith has introduced semi-discrete models, which permit entirely algebraic treatment, suitable for calculating $D$. By replacing the $n-1$ freely-sliping dislocations in the discrete model by a continuous distribution in the region $e \leq x_1 \leq \ell$, whose distribution function $F(x_1)$ is bounded at each end-point, the result

$$e = \frac{0.54}{\mu} \frac{A}{n}$$

is obtained, where $e$ is regarded by Smith as a first approximation to $D$. When the leading glissile dislocation is also discrete, whilst the $n-2$ other dislocations are smeared into a continuous distribution, $D$ is given by the expression

$$D = 1.79 \frac{A}{n\sigma}$$

which is in very good agreement with (1.14). It is clear therefore that provided a dislocation pile-up contains a large number of dislocations the continuous distribution model may be used to determine the stress both in regions external to the pile-up and on the leading dislocation, together with the number of dislocations present as a function of its length, whilst a semi-discrete model can be employed to study the configuration of dislocations at the tip.

It was pointed out in Section 1.2 that a single array of coplanar dislocations is in itself only an approximation to a slip band, which in a real crystal will be composed of several parallel arrays. In the limiting case of an infinite sequence of identical stacked screw dislocation pile-ups (13) on planes $x_2 = \pm nh$ (n=1,2,... $\infty$)
\[ \sigma^P_{23}(r) = -\sigma[1+\tanh^2(\ell\pi/2h)]^{1/2} \left[1+\frac{\tanh(h\pi/h)}{\tanh(r\pi/h)}\right]^{1/2} + \sigma. \]

When there are two such pile-ups of pure screw dislocations, Smith (16, 38) has shown that, when \( r \ll \ell \) and for all values of \( h \), \( \sigma^P_{23}(r) \) exhibits the same \( r^{-1/2} \) dependence as in the case of a single dislocation pile-up although the constant of proportionality is a complicated function of \( \ell \) and \( h \). An iterative solution to the corresponding problem for edge dislocations has been obtained for \( \ell/h < 1 \) (16) demonstrating again an \( r^{-1/2} \) dependence for \( \sigma^P_{12}(r) \).

In each of these problems it has been simply assumed that the leading dislocation is identical to the other dislocations in the array and is fixed, without considering the nature of the obstacle preventing its movement. Chou (39) has generalised the discrete model of Eshelby et al. (6) for the case when the leading dislocation has a different Burgers vector \( (m\mathbf{b}) \) to that of the glissile dislocations \( (\mathbf{b}) \), and could represent either a sessile grown-in dislocation or a dislocation ledge on a grain boundary. The significant result arising from his analysis, which is valid for \( m \) real and positive, is that

\[ \sigma^L_{3i2} = [1+(\ell-1)/m]\sigma \]

which is strongly dependent on \( m \), whilst for \( r \ll \ell \) \( \sigma^P_{3i2}(r) \) is independent of this parameter.

If the leading dislocation is held up at a grain boundary or at the surface of an inclusion account must be taken of the effect of the difference in elastic properties of the materials on either side of the interface.
The piled-up dislocations must be in equilibrium under the combined influence of not only the applied stress and their mutual interactions but also the image stresses discussed in Section 1.3 due to the presence of the boundary. Using a continuous distribution model Barnett\(^{(17)}\) has considered the problem of a screw dislocation pile-up normal to a plane interface between two different isotropic elastic half-spaces (I), containing the dislocations, and (II). Defining the constant \(Y\) as in Section 1.3, for \(r < \ell\)

\[
\sigma_{23}^P(r) \sim -\sigma(1+Y)(2\text{sinc}\pi\text{sinc}\pi/2)^{-1}(2\ell/r)^c
\]  

where \(c=\pi^{-1}\cos^{-1}Y\). The case of an infinite sequence of such arrays has been considered by Chou and Barnett\(^{(49)}\) and their results are discussed in Section 6.1. Kuang and Mura\(^{(20)}\) have treated the problem of a single edge dislocation pile-up normal to a plane interface, although no attempt was made to calculate the stress \(\sigma_{23}^P(r)\). For the more general situation when screw dislocations are piled-up on the plane \(x_2=0\) against a circular cylindrical inclusion of radius \(\rho\) whose axis coincides with \(Ox_3\) Barnett and Tetelman\(^{(40)}\) have shown that the stress component \(\sigma_{23}^{(II)P}(r)\) within the inclusion has the approximate form

\[
\sigma_{23}^{(II)P}(r) \sim -\sigma B(2\ell/r)^c
\]

where \(B\) is a function of \(\rho\), \(\ell\) and \(Y\), and \(c\) is defined as in (1.17). Thus the nature of the singularity at the pile-up tip is a function only of the shear moduli of materials (I) and (II) and is independent of the inclusion radius. Although this result was originally derived assuming that the stress on the slip plane was uniform, it
has since been shown\(^{14,15,24}\) that, using the exact expression (1.9) for this stress due to a uniform loading at infinity, only the form of \(B\) in (1.18) is changed.

It has been demonstrated\(^{14,15,24}\) that for a screw dislocation pile-up against a rigid second phase \(\sigma_{23}^{(II)}(r)\) exhibits a logarithmic singularity at the tip. Since the assumption that the leading dislocation will reach the interface is doubtful, limiting the usefulness of the result, Smith\(^{31}\) has considered the problem of a screw dislocation array held up at a distance \(s\) from the boundary of an elliptical cylindrical inclusion. For \(r \ll s\), \(a_{23}^{(I)}(r)\) is proportional to \(r^{-1/2}\), the constant of proportionality being dependent upon the geometry of the system.

1.5 Dislocation Pile-Ups and the Hall-Petch Equation

Because of the practical difficulties involved in investigating on a microscopic scale the propagation of plastic deformation through grain boundaries it has not been possible to formulate a theoretical model of this process based on direct observations. However Hall\(^{42}\) and Petch\(^{43}\) have shown that, when samples of polycrystalline iron are tested in tension, the yield stress \(\sigma^Y\) was related to the average grain diameter \(d\) by an equation of the form

\[
\sigma^Y = \sigma^0 + k d^{-1/2}
\]

(1.19)

where \(\sigma^0\) and \(k\) are constants for given testing conditions and purity of specimens. On the assumption that the observed yield is due to a developed slip band in one grain initiating fresh slip in an adjacent grain two theories
have been proposed to explain the relationship (1.19), both of which utilise an isolated dislocation pile-up in a homogeneous medium as a model of the developed slip band held up at a grain boundary. Also both treatments assume that the dislocations move under the combined influence of a constant applied stress $-\sigma_{j2}^A$ and opposing internal stresses which may be represented by a constant stress $\sigma_{j2}^F<\sigma_{j2}^A$.

The first theory, proposed originally by Hall\(^{(42)}\) supposes that yield in the second grain occurs by means of dislocations generated by pre-existing sources which are activated by the stress intensification ahead of the pile-up. If the nearest source is a distance $r^S<\ell$ from the pile-up tip, and requires a critical activation stress $\sigma_{j2}^S$, from (1.15) the yield stress $\sigma_{j2}^Y=\sigma_{j2}^F$ is given by the relation

$$\sigma_{j2}^Y = \sigma_{j2}^F + r^S\sigma_{j2}^S \ell^{-1/2} \quad (j=1 \text{ or } 3).$$

(1.20)

By identifying $2\ell$ as the average grain diameter this theory predicts that, in equation (1.19), the Hall-Petch slope $k=(2r^S)^{1/2}\sigma_{j2}^S$, whilst $\sigma^0$ is just the average shear stress opposing dislocation motion. For materials exhibiting an upper yield stress $\sigma_{j2}^U$ Stroh\(^{(44)}\) has suggested that $\sigma_{j2}^S$ can be equated with $\sigma_{j2}^U$ and that $r^S$ has the form $\alpha Gb_{j2}/\sigma_{j2}^U$, where $\alpha$ is a constant of the order of, but greater than, unity, thus giving $k=(2\alpha Gb_{j2}/\sigma_{j2}^U)^{1/2}$. Whereas this model assumes that yield in the second grain occurs by activation of dislocation sources, the second theory due to Petch\(^{(45)}\) supposes that dislocations are nucleated at the boundary when the stress immediately ahead of the pile-up reaches a critical value $\sigma_{j2}^C$. Assuming that this stress is given
by an expression of the form of (1.12), and using the value of \( n \) in (1.13), the yield stress in this case is given by the expression

\[
\sigma_{Yj2} = \sigma_{j2}^p + (2\sigma_{j2}^C A_j)^{1/2} \varepsilon - 1/2.
\]

By taking \( d = 2\varepsilon \) the theory thus predicts that \( k = (4\sigma_{j2}^C A_j)^{1/2} \)

in equation (1.19).

Since the original experiments of Hall(42) and Petch(43) the observed functional dependence of \( \sigma_Y \) on \( d \) given by (1.17) has been confirmed by numerous investigators testing a variety of materials under different working conditions, as discussed for example by Armstrong, Codd, Douthwaite and Petch(45). In their simplest form, as shown above, the separate mechanisms proposed by Hall and Petch both give rise to relationships of the required type, differing only in the structure of the constant \( k \). Because of the difficulty in ascribing accurate values to parameters such as \( \sigma_{j2}^C, \sigma_{j2}^U \) and \( \alpha \) it is not at present possible to conclude by comparing the predicted and observed values of \( k \) which, if either, of the mechanisms is operative in a given experiment. This shortcoming is all the more significant in the light of Li's(46) alternative theory of the Hall-Petch relationship based on dislocation nucleation at grain boundary ledges. The need arises therefore to use physically more realistic models if the relative validity of the theories is to be assessed.

Cottrell(47) has discussed the inclusion of the dependency of \( \sigma^0 \) and \( k \) in (1.19) on strain-rate, temperature and impurity concentration, whilst Armstrong et al. (45) have treated the influence of the orientation relationship between
the basic elastic problem and therefore the functional dependence of yield stress on grain size. If the elastic anisotropy of the material is taken into account, however, the medium containing the dislocations can no longer be considered homogeneous, and dislocation image forces somewhat similar to those discussed in Section 1.3 for inhomogeneous isotropic materials must be taken into account.

Using the model, discussed in detail in Chapter 6, of a screw dislocation pile-up against the plane interface between two elastically anisotropic half-spaces of particularly high symmetry Chou and Barnett have confirmed the predictions of Armstrong and Head that the tip stresses have the general form of equation (1.17) obtained by Barnett when the two phases are isotropic but have different shear moduli. If Hall's mechanism is assumed to be operative the yield stress equation derived from these results contains a grain size dependency of \( d^{-c} \), where \( c \) is a function of the relative orientation of the two grains and of the elastic constants of the material, and lies in the range \( 0 \leq c < 1 \). Chou has proposed that the Pitch mechanism on the other hand still gives rise to an equation of the form of (1.19), although his calculations are based on the assumption that the stress \( \sigma_{23} \) on the leading dislocation is given by (1.12), the validity of which is discussed in Section 7.2.2.

Clearly the introduction of elastic anisotropy into the theories could play an important role in interpreting the Hall-Petch relationship, and therefore in formulating a satisfactory theory of polycrystalline ductility. How-
ever the model of Chou and Barnett\textsuperscript{(49)} lacks generality, being limited to screw dislocation pile-ups normal to plane boundaries between grains of high symmetry in special relative orientations. The purpose of the present work is therefore to develop more general models of screw dislocation arrays held-up at grain boundaries in which there are less restrictions on the slip band orientation relative to the boundary and on the symmetry of the neighbouring grains.
2.1 Basic Properties of the Mellin Transform

The theorems associated with the Mellin transformation are not well-documented, but may be derived by a suitable change of variable from the well-known results for the standard and bilateral Laplace transforms. For convenience therefore those theorems relevant to the subsequent application of the Wiener-Hopf technique will be summarised in this section.

A function \( f(t) \) is related to its Mellin transform \( F(s) \), \( s = \xi + i\zeta \), by the reciprocal formulae

\[
F(s) = \int_{0}^{\infty} f(t) t^{s-1} dt \quad (2.1)
\]

and

\[
f(t) = (2\pi i)^{-1} \int_{\gamma-i\infty}^{\gamma+i\infty} F(s) t^{-s} ds. \quad (2.2)
\]

Moreover if \( F_+(s) \) is a function regular in the half-plane \( \xi > \xi_- \), and \( s^{-1} F_+(s) \to 0 \) as the limit \( r \to \infty \) (where \( re^{i\theta} = s - \xi_+ - \zeta \), for arbitrary \( \varepsilon > 0 \)) is approached uniformly in the region \( -\pi/2 < \theta < \pi/2 \), then it may be shown that equation (2.2), with \( F(s) = F_+(s) \), is a solution of the integral equation

\[
F_+(s) = \int_{0}^{1} f(t) t^{s-1} dt \quad (2.3)
\]

provided \( \xi > \xi_- \). Similarly, if \( F_-(s) \) is a function regular in \( \xi < \xi_+ \), equation (2.2) with \( F(s) = F_-(s) \) is also the solution
of the equation

\[ F_-(s) = \int_{1}^{\infty} f(t) t^{s-1} dt \quad (2.4) \]

for \( \xi < \xi_+ \).

In certain instances in the following analysis unknown functions \( F_+(s) \) and \( F_-(s) \) are defined in terms of known functions \( f(t) \) by means of equations of the form (2.3) and (2.4). Then provided that \( f(t) \) has a finite number of maxima, minima and finite discontinuities along the path of integration and is bounded except at a finite number of points along this path,

(a) \( F_+(s) \) is regular in the half-plane \( \xi > \xi_- \) if
   \[ |f(t)| < At^{-\xi_-} \quad \text{as} \ t \to 0, \text{ and} \]
(b) \( F_-(s) \) is regular in \( \xi < \xi_+ \) if \( |f(t)| < Bt^{-\xi_+} \)
   \[ \text{as} \ t \to \infty, \]

where \( A \) and \( B \) are arbitrary constants.

The Abelian theorems for the finite transforms defined by equations (2.2) and (2.3) can be derived directly from the corresponding results for the standard Laplace transform (53)

\[ \mathcal{F}(s) = \int_{0}^{\infty} f(x) e^{-sx} dx \]

by making the substitution \( t = e^{-x} \) and may be stated thus:

If, for \( \beta > 0 \), \( f(t) \sim C(1-t)^{\beta-1}/\Gamma(\beta+1) \) \[ \begin{cases} \quad t \to 0_+ \\ t \to 1_- \end{cases} \]

then \( F_+(s) \sim Cs^{-\beta-1} \) \[ \begin{cases} \quad s \to 0_+ \\ s \to \infty \end{cases} \]
where $C$ is a constant. Here the notation $0^+$ and $1^-$ denotes the limits taken from the right and left respectively.

### 2.2 The Wiener-Hopf Procedure

To avoid unnecessary repetition the following notation will be used throughout the present work to describe three regions of the complex $s=\xi+i\eta$ plane:

- Region (i) $\xi<\xi_+$
- Region (ii) $\xi_-<\xi<\xi_+$, $-\infty<\eta<\infty$,
- Region (iii) $\xi_-<\xi$

where values of $\xi_+$ and $\xi_-$ will be specified for given problems. This division of the $s$-plane is shown schematically in Figure 2.1. By applying Mellin transforms to integral or partial differential equations a typical form of the resulting problem is to find unknown functions $X_-(s)$ regular in (i) and $Y_+(s)$ regular in (iii) which satisfy the equation

$$P(s)X_-(s) + Q(s)Y_+(s) + R(s) = 0 \quad (2.5)$$

in region (ii), where $P(s)$, $Q(s)$ and $R(s)$ are known functions regular in (ii), and where for simplicity it is assumed that $P(s)$ and $Q(s)$ are also non-zero in that region. In the following analyses (2.5) will be referred to as "the Wiener-Hopf equation". (If Fourier or Laplace transforms are used the resulting problem will be stated in an identical form except that the regions will be bounded by lines $\eta=\xi_+$ and $\eta=\xi_-$.)

Since the function $Q(s)/P(s)$ is regular and non-zero in (ii) it is always possible to write

$$Q(s)/P(s) = Q_-(s)Q_+(s) \quad (2.6)$$
where \( Q(s) \) and \( Q_+(s) \) are regular and non-zero in regions (i) and (iii) respectively. The factorisation (2.6) is the fundamental step in the Wiener-Hopf approach. In terms of these functions (2.5) may now be written in the form

\[
\frac{X(s)}{Q(s)} + \frac{Y(s)Q_+(s)}{P(s)Q(s)} + \frac{R(s)}{P(s)Q(s)} = 0, \quad (2.7)
\]

where \( \frac{X(s)}{Q(s)} \) is regular in (i) and \( Y_+(s)Q_+(s) \) is regular in (iii). If it is possible to decompose the third term so that

\[
\frac{R(s)}{P(s)Q(s)} = \frac{R_-(s)}{P(s)Q(s)} + \frac{R_+(s)}{P(s)Q(s)}, \quad (2.8)
\]

where \( R_-(s) \) and \( R_+(s) \) are regular in regions (i) and (iii) respectively, equation (2.7) may be written

\[
\frac{X(s)}{Q(s)} + \frac{R_-(s)}{P(s)Q(s)} = - \frac{Y_+(s)Q_+(s)}{P(s)Q(s)} - \frac{R_+(s)}{P(s)Q(s)}. \quad (2.9)
\]

Whilst the functions on either side of (2.9) are equal in (ii), \( \frac{X(s)}{Q(s)} + R_-(s) \) is analytic in (i) and \( -Y_+(s)Q_+(s) - R_+(s) \) is analytic in (iii). Thus by analytic continuation they represent the entire function \( J(s) \) defined throughout the \( s \)-plane. Finally if

\[
|\frac{X(s)}{Q(s)} + R_-(s)| < |s|^\ell \quad \text{as } s \to \infty \quad \text{in region (i)}
\]

\[
|Y_+(s)Q_+(s) + R_+(s)| < |s|^m \quad \text{as } s \to \infty \quad \text{in region (iii)}
\]

then by Liouville's theorem \( J(s) \) is a polynomial in \( s \) of degree less than or equal to the integral part of \( \min(\ell,m) \). Thus \( X_-(s) \) and \( Y_+(s) \) may be determined by this method to within a finite number of arbitrary constants.

The decomposition (2.8) may be effected using Cauchy's theorem provided that in region (ii), for \( n > 0 \),

\[
|\frac{R(s)}{P(s)Q(s)}| < D|\zeta|^{-n} \quad \text{as } |\zeta| \to \infty.
\]
For $\xi < c < \xi +$,

$$R_-(s) = (2\pi i)^{-1} \int_{c-i\infty}^{c+i\infty} R(u) \{P(u)Q(u)(u-s)\}^{-1} du$$

and

$$R_+(s) = -(2\pi i)^{-1} \int_{d-i\infty}^{d+i\infty} R(u) \{P(u)Q(u)(u-s)\}^{-1} du.$$

### 2.3 Formulation of the Wiener-Hopf Problem for Linear Screw Dislocation Arrays Inclined to Plane Boundaries

Consider a linear array of $n$ infinite straight right-hand screw dislocations, each of Burgers vector $b$, inclined to the welded boundary between two elastically isotropic half-spaces (I) and (II) of shear moduli $G(I)$ and $G(II)$ respectively. It is convenient to use the sets of rectangular Cartesian axes $Ox_i$ and $Oy_i$ related by a rotation of $\pi/2$ about $Ox_3$, and the cylindrical polar coordinates $(r, \theta, z=x_3)$ as shown in Figure 2.2. Unless otherwise stated all components of stress will be referred to axes $Ox_i$.

The dislocations, parallel to $Ox_3$, are arrayed on and can move in the plane $x_2=0$ under the influence of a stress component $\sigma_{23}=\sigma(x_1)$ which is invariant in the $x_3$-direction.

If the plane of the interface is $y_1=0$, the stresses at points $(r,\theta)$ in each half-crystal due to a single screw dislocation at $(x_1,0)$ may be derived either as a limiting case of equations (1.4) or directly from the results of Head (27), and may be written in the form

$$\sigma_{13}^{(1)} = -\frac{G(I)b}{2\pi} \left[ \frac{\sin\theta}{x_1^2 - 2x_1rcos\theta + r^2} + \frac{\gamma}{x_1^2 + 2x_1rcos(\pi + \theta) + r^2} \right].$$
\[ \sigma_{23} = \frac{G(\ell)b}{2\pi} \left[ \frac{r \cos \theta - x_1}{x_1^2 - 2x_1 r \cos \theta + r^2} + \frac{r \cos \theta + x_1 \cos \alpha}{x_1^2 + 2x_1 r \cos (\alpha + \theta) + r^2} \right] \]

\( (y_1>0) \) \hspace{1cm} (2.11)

and

\[ \sigma_{13} = -\frac{G(\ell)b(1+\gamma)}{2\pi} \frac{r \sin \theta}{x_1^2 - 2x_1 r \cos \theta + r^2}, \]

\[ \sigma_{23} = \frac{G(\ell)b(1+\gamma)}{2\pi} \frac{r \cos \theta - x_1}{x_1^2 - 2x_1 r \cos \theta + r^2} \]

\( (y_1<0) \) \hspace{1cm} (2.12)

where \( \gamma = [G(\ell) - G(\ell)] [G(\ell) + G(\ell)]^{-1} \). Following an identical argument to that described in Section 1.2 the conditions that each dislocation in the array is in equilibrium under the combined influence of \( \sigma(x_1) \) and the mutual repulsion of the \( n-1 \) other dislocations may be written, in the continuous distribution approximation, as the singular integral equation

\[ \frac{G(\ell)b}{2\pi} \int F(x) \left[ (x_1-x)^{-1} + \frac{\gamma}{2}(x_1+xe^{	ext{i}\alpha})^{-1} + \frac{\gamma}{2}(x_1+xe^{-\text{i}\alpha})^{-1} \right] dx \]

\[ + \sigma(x_1) = 0, \] \hspace{1cm} (2.13)

where the integral is taken over the dislocated segments of the \( x_1 \)-axis. In the following analysis attention will be devoted entirely to problems in which the dislocations are continuously distributed over the single segment \( 0<r<\ell \), in which case, by making the substitutions \( t=x_1/\ell, \eta=x/\ell, \Omega(\eta)=F(x) \) and \( \varphi(t)=2\pi[G(\ell)b]^{-1}\sigma(x_1) \) equation (2.13) may be rewritten in the form

\[ \varphi(t) = \int_0^1 k(t/\eta)\eta^{-1} d\eta \quad (0<t<1) \] \hspace{1cm} (2.14)
where
\[ k(t/\eta) = (1-t/\eta)^{-1/2} e^{i\eta t/\eta} (e^{i\eta t/\eta})^{-1/2} (e^{-i\eta t/\eta})^{-1}. \]

Equation (2.14) may be extended to the whole half-plane \( t>0 \) by defining the unknown function
\[ h(t) = \int_0^1 k(t/\eta) \eta^{-1} \eta d\eta \quad (1<t<\infty). \]  

(2.15)

Taking the Mellin transform of the sum of functions \( c(t) \) and \( h(t) \) the equation
\[ G(s) + H(s) = B_1(s) K(s) \]  

(2.16)

is obtained, in which the functions
\[ G(s) = \int_0^1 c(t) t^{s-1} dt, \]  

(2.17)

\[ K(s) = \int_0^\infty k(u) u^{s-1} du \]  

(2.18)

are known, and
\[ H(s) = \int_1^\infty h(t) t^{s-1} dt \]  

(2.19)

\[ B_1(s) = \int_0^1 \Omega(\eta) \eta^{s-1} d\eta \]  

(2.20)

are to be found.

From equations (2.14) and (2.18)
\[ K(s) = \pi [\cos\pi(s-1) + \gamma \cos\pi(s-1)] / \sin\pi(s-1) \]  

(2.21)

with zeros at \( s = \lambda + i\alpha \_i \) (\( i=1, 2, \ldots \infty \)), where \( \alpha \_i \) are the positive roots of the equation
\[ \cos \alpha_1 + Y \cos \alpha_1 = 0, \quad (2.22) \]

and are all real for \(-1 < Y < 1\). If \(\alpha_1\) is the smallest of these roots, \(0 < \alpha_1 < 1\), and by inspection \(K(s)\) is regular and non-zero within the infinite strip \(1 - \alpha_1 < \xi < 1, -\infty < \xi < \infty\).

Furthermore, from Section 2.1 \(G(s)\) is regular within the same strip provided that \(\tau(t)\) has a finite number of maxima, minima and finite discontinuities along the path of integration in equation (2.17), and is bounded at all but a finite number of points along this path. These conditions are satisfied for all realistic forms of \(\tau(t)\).

Thus, using the nomenclature of Section 2.2 with \(\xi_+ = 1 - \alpha_1\) and \(\xi_- = 1\), equation (2.16) is of the form of the Wiener-Hopf equation (2.5), with \(P(s) = 1, Q(s) = -K(s), R(s) = G(s), X_-(s) = H_-(s)\) and \(Y_+(s) = B_+(s)\), where functions \(H_-(s)\) and \(B_+(s)\), regular in regions (i) and (iii) respectively, must be found which satisfy the equation in region (ii).

Once the function \(B_+(s)\) has been determined following the procedure outlined in the previous section the distribution function \(\Omega(\eta) = F(x)\) may be obtained by inversion of equation (2.20) as in Section 2.1, that is

\[
\Omega(\eta) = (2\pi i)^{-1} \int_{\xi_- i\infty}^{\xi_+ i\infty} B_+(s) \eta^{-s} ds \quad [0 < \eta < 1, s \text{ in (iii)}] \\
= 0 \quad [\eta < 0, 1 < \eta] \quad (2.23)
\]

The number of dislocations in the pile-up is given by

\[
n = \ell \int_0^1 \Omega(\eta) d\eta \quad (2.24)
\]

and the stresses \(\sigma_{(P)}^{(g)}\) due to the piled-up dislocations
are determined by the integrals

\[ \sigma^{(g)}_{ji}(r, \theta) = \int_0^1 \sigma^{(g)}_{ji}(x_1, r, \theta) F(x_1) dx_1 \quad (g=I,II) \]  

(2.25)

where the forms of \( \sigma^{(g)}_{ji} \) are given in equations (2.11) and (2.12).

It is not always necessary, however, to evaluate the distribution function as an intermediate step in determining quantities such as \( n \) and \( \sigma^{(g)}_{ji} \). For instance it has been pointed out by Kuang and Mura\(^{(20)}\) that, by comparing equations (2.20) and (2.24) the number of piled-up dislocations is always given by

\[ n/\ell = \lim_{s \to 1} B_+(s). \quad (2.26) \]

Also the stress component \( \sigma^{(I)}_{23}(r>\ell,0) \), which is of interest in problems where \( F(x_1) \) is unbounded at \( x_1=\ell \), may be obtained by consideration of \( H_-(s) \) instead of \( B_+(s) \). It may be seen by inspection of equation (2.15) that

\[ \sigma^{(I)}_{23}(r>\ell,0) = G^{(I)}b(2\pi)^{-1}h(t). \quad (2.27) \]

Thus, if \( H_-(s) \) is determined as in the last section, it remains to invert the integral (2.19) as discussed in Section 2.1, to give

\[ h(t) = (2\pi)^{-1} \int_{\xi-i\infty}^{\xi+i\infty} H_-(s)t^{s-1} ds \quad (\xi<1). \quad (2.28) \]

Consequently these two important physical quantities can be obtained avoiding much lengthy manipulation.

In the present problem the factorisation of \( K(s) \) in
the manner of (2.6), that is

$$K(s) = K_-(s)K_+(s)$$

(2.29)

where $K_-(s)$ and $K_+(s)$ are regular and non-zero in regions (i) and (iii) respectively, may be carried out by inspection once values of $\alpha_1$ from equation (2.22) have been obtained. Although in general these must be determined numerically, analytic treatment is possible (1) for all values of $\gamma$ when $a$ is a rational number, and for all values of $a$ when (2) $\gamma = 1$ or (3) $\gamma = -1$.

Case (1) corresponds to a linear array of screw dislocations adjacent to the welded interface between two half-spaces with arbitrary elastic properties, at an angle $\pi/2q$ to the boundary normal, where $p$ and $q$ are integers. The solution of this problem, when the dislocations are piled-up at the boundary under the influence of the applied stress, is discussed in Chapter 3, whilst the limiting cases (2) and (3) are considered in Chapter 4.
The regions of the $s=\xi+i\zeta$ plane defined in Section 2.2 and extending to $s=\xi i\omega$. Functions marked in each diagram are regular in that region, and are also non-zero where indicated.
Figure 2.2  Schematic illustration of the linear array of right-hand screw dislocations discussed in Section 2.2, showing the relationship between the rectangular Cartesian axes Ox₁, Oy₁ and the cylindrical polar coordinates (r,θ,z=x₂=y₂). The materials (I) and (II) are welded together along the plane interface y₁=0.
CHAPTER 5

Screw Dislocation Pile-Ups in Two-Phase Materials of Finite Rigidity

In this chapter attention is devoted entirely to the problem of solving the integral equation (2.14) for arbitrary values of $\gamma$ in the range $-1<\gamma<1$, and for all rational values of $\alpha$ in the range $0<\alpha<1$. Moreover it is assumed that the stress $\sigma(x_1)$ acting on the slip plane is of such a form that the dislocations are piled-up against the plane interface, so that the solution for $\Omega(\eta)$ is unbounded at $\eta=0$ and bounded at $\eta=1$. The solution is obtained explicitly for the important case when $\sigma$ is constant.

3.1 Solution of the Integral Equation

As pointed out in Section 2.3, before the factorisation of $K(s)$ as in equation (2.29) can be carried out, it is necessary to find the roots $\alpha_1$ of (2.22). Since $\alpha$ is rational in the present case it may be replaced in (2.22) by $pq^{-1}$ where $p$ and $q$ are integers ($q>p$) to give

$$\cos q(\alpha_1/q) + \gamma \cos p(\alpha_1/q) = 0. \quad (3.1)$$

This equation may be expanded as a polynomial in $\cos(\alpha_1/q)$ of order $q$, and may be solved analytically in the thirteen distinct cases listed in Appendix 3.1, apart from the two limiting cases when $p=0$ and $p=q$. In all other instances the values of $\alpha_1$ must be obtained numerically, although the following analysis is equally valid for all rational values of $\alpha$. 
In terms of the $q$ values of $\alpha_i$ in the range $0 < \alpha_i < q$ the function $K(s)$ may be written in the form

$$K(s) = \prod_{i=1}^{q} \sin[\pi (s-l+\alpha_i)/2q] \sin[\pi (s-l-\alpha_i)/2q]$$

$$\times \sin^{-1}(s-l)$$

each sine term of which may now be expanded as an infinite product [for instance see Abramowitz and Stegun(54)] to give $K(s)$ in a suitable form for carrying out the factorisation (2.29) by inspection. In this way the functions $K_+(s)$ and $K_-(s)$ may be written

$$K_+(s) = 2^{-1/2} (\pi/q) e^{-\chi(s)} \prod_{i=1}^{q} \prod_{n=1}^{\infty} \left\{ (s-l+\alpha_i)[1+(s-l+\alpha_i)/2qn] \right\} \times [1+(s-l-\alpha_i)/2qn][1+(s-l)/n]^{-1}$$

(3.2)

and

$$K_-(s) = 2^{-1/2} (-\pi/q) e^{\chi(s)} \prod_{i=1}^{q} \prod_{n=1}^{\infty} \left\{ (s-l-\alpha_i)[1-(s-l+\alpha_i)/2qn] \right\} \times [1-(s-l-\alpha_i)/2qn](s-l)^{-1}[1-(s-l)/n]^{-1}$$

(3.3)

which satisfy the regularity requirements. The exponential factors $e^{-\chi(s)}$ and $e^{\chi(s)}$ have been included to ensure both the convergence of the infinite products and the algebraic behaviour of $K_+(s)$ and $K_-(s)$ as $s \to \infty$ so that Liouville's theorem may be applied at a later stage, as discussed in Section 2.2.

Making use of Euler's Infinite product formula for the gamma function equations (3.2) and (3.3) may be expressed more conveniently as
\[
K_+(s) = 2^{2q-1/2}q_e \chi'(s) \Gamma(s) \\
\times \left\{ \prod_{i=1}^{q} (s-1-\alpha_i) \Gamma \left[ (s-1+\alpha_i)/2q \right] \Gamma \left[ (s-1-\alpha_i)/2q \right] \right\}^{-1},
\]

\[
K_-(s) = -2^{2q-1/2}q_e \chi'(s) \Gamma(1-s) \\
\times \left\{ \prod_{i=1}^{q} (1-s-\alpha_i) \Gamma \left[ (1-s+\alpha_i)/2q \right] \Gamma \left[ (1-s-\alpha_i)/2q \right] \right\}^{-1}.
\]

The function \( \chi'(s) \) can now be chosen so that \( K_+(s) \) and \( K_-(s) \) behave algebraically as \( s \to \infty \) by employing Stirling's asymptotic formula for gamma functions. By placing

\[
\chi'(s) = (s-1) \ln(2q)
\]

then apart from a constant factor

\[
\text{Lt}_{s \to \infty} K_+(s) \to s^{1/2} \quad \text{and} \quad \text{Lt}_{s \to \infty} K_-(s) \to s^{-1/2}
\]

and the necessary behaviour is established.

The stage has now been reached when the Wiener-Hopf equation (2.16) may now be written in the form of (2.7), that is

\[
B_+(s)K_+(s) = G(s)/K_-(s) + H_-(s)/K_-(s).
\]

It is not possible to proceed with the decomposition

\[
G(s)/K_-(s) = G_-(s) + G_+(s)
\]

analogous to (2.8) without specifying the form of the stress component \( \sigma(x_1) \). Only the case when this component is constant will be considered in the present work, although the method of solution is valid for any form of \( \sigma(x_1) \) provided that it satisfies the conditions equivalent to those
for $\sigma(t)$ discussed in Section 2.3. If a constant stress $-\sigma_{23}^A$ is applied at infinity then by treating the problem as the limiting case of a pile-up external to a circular cylindrical inclusion of large radius as discussed in Section 1.3, the effective applied stresses in materials (I) and (II) are

$$\sigma_{23}^{(I)} = -(1-\gamma\cos\alpha)\sigma_{23}^A \quad \text{and} \quad \sigma_{23}^{(II)} = -(1+\gamma)\sigma_{23}^A$$

(3.8)

from (1.6) and (1.7). By assuming that the frictional stress $\sigma_{23}^F$ opposing the motion of the dislocations may be treated as being constant, the total stress $\sigma(x_1) = -\sigma$ acting on the slip plane is

$$\sigma = [(1-\gamma\cos\alpha)\sigma_{23}^A - \sigma_{23}^F] = G(I)b(2\pi)^{-1}\sigma. \quad (3.9)$$

Under these conditions $G(s) = -\omega s^{-1}$ from (2.17), and consequently the decomposition of the function $G(s)/K(s)$ as in equation (3.7) may be achieved by means of equations (2.10), giving

$$G_+(s) = (2\pi)^{-1}\omega s^{-1}\int_{d-i\infty}^{d+i\infty} [K(u)(u-s)]^{-1}du \quad (\xi<d<1)$$

$$= -\omega [sK_-(0)]^{-1}. \quad (3.10)$$

The evaluation of $G_-(s)$ is superfluous to the present problem.

The Wiener-Hopf equation (2.16) may now be used as in Section 2.2 to define the entire function $J(s)$ by the expressions
\[ J(s) = \frac{H(s)}{K(s)} + G(s) \text{ in region (i)} \]
\[ = K_+(s)B_+(s) - G_+(s) \text{ in region (iii)} \] (3.11)

and it remains to determine the form of \( J(s) \). From the end condition that \( \Omega(1) = 0 \) it is reasonable to assume that \( |\Omega(\eta)| \sim (1-\eta)^T \) where \( T > 0 \) as \( \eta \to 1 \). Using the Abelian theorem given in Section 2.1 this implies that \( |B_+(s)| \sim s^{-T-1} \), and consequently that

\[ |K_+(s)B_+(s) - G_+(s)| \sim s^{-T-1/2} \text{ as } s \to \infty \]

by taking into account the asymptotic behaviour of \( K_+(s) \) given in (3.6). Therefore, from Liouville's theorem \( J(s) = 0 \) and \( B_+(s) \) is given uniquely by the equation

\[ B_+(s) = G_+(s)/K_+(s). \] (3.12)

Because this function is analytic in region (iii) then by its definition (2.20) \( \Omega(\eta) \) must obey the relationship

\[ |\Omega(\eta)| < A\eta^{\alpha_1-1} \text{ as } \eta \to 0 \]

from the Mellin transform theorem of Section 2.1. Thus the second end condition, that \( \Omega(\eta) \) is unbounded at \( \eta=0 \), is also satisfied.

From equations (3.4), (3.5), (3.10) and (3.12)

\[ B_+(s) = 2\pi N(2q)^s \prod_{i=1}^{q} \left\{ \Gamma[(1+s-1-\alpha_i)/2q] \Gamma[(1+s-1-2q+\alpha_i)/2q] \right\} x \left\{ \Gamma[(s+1)]^{-1} \right\} \] (3.13)

where \( N = (2\pi)^{-2q} \prod_{i=1}^{q} \left\{ \Gamma[(1+\alpha_i)/2q] \Gamma[(1+2q-\alpha_i)/2q] \right\} \). (3.14)
The fact that this function is symmetric in \( \alpha_i \) and \( 2q-\alpha_i \) considerably simplifies the integration (2.23) to obtain the distribution function \( \Omega(\eta) = \mathcal{F}(x_1) \). By expanding the gamma functions in equation (3.13) as infinite products, this integral may be taken around the infinite semi-circle in the right-hand half-plane, when residue theory may be used to give

\[
\mathcal{F}(x_1) = 2\pi \sum_{j=1}^{q} \left\{ 2q^T_{2q-1}(\alpha_j;\alpha_i;x_1/\ell) + 2q^T_{2q-1}(2q-\alpha_j;\alpha_i;x_1/\ell) \right\} (3.15)
\]

where

\[
2q^T_{2q-1}(a_j;b_i;x) = \frac{a_j-1}{t_q(a_j;b_i)}
\]

\[
= \frac{2q}{2q^T_{2q-1}} \left[ \frac{(a_j+2i-3)/2q,(a_j+2i-2)/2q}{(a_j+2q-b_i)/2q,(a_j+b_i)/2q,a_j/q} \right]^x^{2q}
\]

and

\[
t_q(a_j;b_i) = (2q)^{2-a_j} \prod_{i=1}^{q} \left\{ \Gamma \left[ \frac{(b_i-a_j)/2q}{(2q-b_i-a_j)/2q} \right] x \Gamma \left[ \frac{(1-a_j/q)}{\Gamma (2-a_j)} \right] \right\}
\]

The function \( 2q^T_{2q-1} \) is the generalised hypergeometric function (55) defined as

\[
\begin{align*}
_{A}F_{B} \left[ \begin{array}{c}
a_1, a_2, \ldots, a_A; \\
b_1, b_2, \ldots, b_B;
\end{array} \right] = \sum_{n=0}^{\infty} \frac{(a_1)_n(a_2)_n \cdots (a_A)_n}{(b_1)_n(b_2)_n \cdots (b_B)_n} \frac{z^n}{n!}
\end{align*}
\]

where the Pochhammer's symbol

\[
(a)_n = \frac{\Gamma (a+n)}{\Gamma (a)}
\]

has been used. Expressions such as \( (a_j+2i-3)/2q \) appearing in this function represent a sequence of \( q \) terms obtained by placing \( i=1,2,\ldots,q \), and the dash indicates that the term
for which \(i=j\) is omitted. In the limiting case when \(a=0\), for a pile-up perpendicular to the boundary, the result previously derived by Barnett\(^{17}\) for the distribution function \(F(x_1)\) is obtained, namely

\[
F(x_1) = c(\pi \sin c_0/2)^{-1} \sinh[c \cosh^{-1}(\ell/x_1)] \quad (3.17)
\]

where \(c = n^{-1} \cos^{-1} \gamma\). The other limiting case, when \(a=1\) and the dislocations are distributed in the interface, gives rise to a distribution function similar to that for a pile-up in a homogeneous solid\(^4\), and has the form

\[
F(x_1) = c[\pi(1+\gamma)]^{-1}(\ell/x_1-1)^{1/2}.
\]

3.2 The Number of Dislocations in the Pile-Up

With the aid of the relation (2.26) the number of dislocations, \(n\), in the pile-up may be readily obtained from equation (3.13) and is given by

\[
n/\ell = 4cNq\prod_{i=1}^{q} \sin(\pi \alpha_i/2q)^{-1} \quad (3.18)
\]

When the pile-up is perpendicular to the interface \((a=0)\) this expression reduces to

\[
n/\ell = cc(1-\gamma^2)^{-1/2}
\]

where \(c\) is defined as in equation (3.17), whilst for the pile-up in the interface \((a=0)\)

\[
n/\ell = c/2(1+\gamma).
\]
Although the distribution function $\mathcal{P}(x_1)$ given by (3.15) appears in a rather complicated form, it has the advantage of being a power series in $(x_1/c)$ and therefore the integral (2.25) giving the components of stress $\sigma^P_{j3}$ due to the pile-up may be carried out term by term. Since the stresses in the immediate vicinity of the pile-up tip are of primary interest approximate expressions for these may be obtained fairly simply by neglecting terms involving powers of $r$ greater than zero.

It is convenient in this calculation to employ the alternative set of polar coordinates $(r,\phi,z)$ defined as in Figure 3.1. Inspection of the form of both the distribution function given in (3.15) and the stress components (2.11) and (2.12) indicates that the integral (2.25) may be expanded as the sum of an infinite number of integrals of the general form

$$\int_0^1 \eta^m (\eta^2 - 2r\eta \cos \psi + r^2)^{-1} d\eta$$

where $m$ can have any value greater than -1. The evaluation of such integrals is considered in Appendix 3.2, where a recurrence procedure is developed enabling in principle solution of all integrals of this form.

From these results the stress components $\sigma^P_{j3}$ due to the entire dislocation array, at the point $(r,\phi)$ near to the tip may be calculated using equations (2.11), (2.12), (2.25) and (3.15), giving
\[ \sigma_{13}^{(I)P} \sim 2\sigma \left\{ C_1 (l/r)^{1-\alpha_1} \sin[(1-\alpha_1)\phi] + Y \sin[(1-\alpha_1)\phi - \alpha_1(a+1)\pi] \right\} - C_2(\sin\phi), \]

\[ \sigma_{23}^{(I)P} \sim -2\sigma \left\{ C_1 (l/r)^{1-\alpha_1} \cos[(1-\alpha_1)\phi] + Y \cos[(1-\alpha_1)\phi - \alpha_1(a+1)\pi] \right\} - C_2(1-\cos\phi), \] (3.19)
in medium (I), where positive and negative signs are to be taken in regions 
\(-\pi<\phi<-(1+a)\pi/2\) and 
\((1-a)\pi/2<\phi<\pi\) respectively, and

\[ \sigma_{13}^{(II)P} \sim 2\sigma (1+Y) C_1 (l/r)^{1-\alpha_1} \sin(1-\alpha_1)\phi, \]

\[ \sigma_{23}^{(II)P} \sim -2\sigma (1+Y) \left[ C_1 (l/r)^{1-\alpha_1} \cos(1-\alpha_1)\phi - C_2 \right] \]

\[ \left[ -(1+a)/2<\phi<(1-a)/2 \right] \] (3.20)
in medium (II). The constants \(C_1\) and \(C_2\) are defined as

\[ C_1 = nt_q (\alpha_1 ; \alpha_1) [\sin\alpha_1]^{-1} \] (3.21)

and

\[ C_2 = \sum_{j=1}^{q} \left\{ 2q+1 \frac{T^*_q (\alpha_j ; \alpha_1 ; 1)}{2q} + 2q+1 \frac{\mathcal{F}_q (2q-\alpha_j ; \alpha_1 ; 1)}{2q} \right\} \] (3.22)

where

\[ 2q+1 \frac{T^*_q (a_j ; b_1 ; 1)}{2q} = t_q (a_j ; b_1')(1-a_j)^{-1} \]

\[ \times \left[ \frac{(a_j+2i-3)/2q, (a_j+2i-2)/2q, (a_j-1)/2q;}{2q, a_j/q, (a_j+2q-1)/2q;} \right] \]

\[ \mathcal{F}_{2q} \left[ \frac{(a_j+2q-b_1')/2q, (a_j+b_1')/2q, a_j/q, (a_j+2q-1)/2q;}{a_j/q, (a_j+2q-1)/2q;} \right] \] (3.23)

and \(t_q (a_j, b_1)\) is given by (3.16). As with the definition of \(2q T^*_q - 1\), single terms such as \((a_j+2i-3)/2q\) in the generalised hypergeometric function \(2q+1 \mathcal{F}_q\) in equation (3.23) represent a sequence of \(q\) terms obtained by placing \(i=1, 2, \ldots, q\) and the dash indicates that the term for \(i=j\) is omitted.
In the first limiting case, when \( a=0 \), the products \( 2NC_1 \) and \( 2NC_2 \) have the particularly simple forms

\[
2NC_1 = 2^{-\alpha_1} \csc[(1-\alpha_1)^{\pi}] \csc[(1-\alpha_1)^{\pi}/2]
\]

and

\[
2NC_2 = \csc[(1-\alpha_1)^{\pi}] \cot[(1-\alpha_1)^{\pi}/2]
\]

in agreement with the results of Barnett\(^{(17)}\). When \( a=1 \) the equations (3.19) and (3.20) reduce to

\[
\sigma_{13}^{(I)} = \sigma_{13}^{(II)} \sim \sigma (\ell/r)^{1/2} \sin \phi/2 \quad (-\pi < \phi < \pi)
\]

\[
\sigma_{23}^{(I)} = \sigma_{23}^{(II)} \sim -\sigma (\ell/r)^{1/2} \cos \phi/2 - 1
\]

where the only dependence upon \( g^{(I)} \) and \( g^{(II)} \) is contained in the modified form of the applied stress \( \sigma = [(1+\gamma)\sigma_{23}^A - \sigma_{23}^F] \) given by equation (3.9).

The Wiener-Hopf technique has thus been used in this chapter to find the equilibrium distribution function of a continuously distributed array of screw dislocations piled-up at the welded interface between two different isotropic elastic half-spaces on a plane inclined at an angle \((1-\alpha)^{\pi}/2\) to the interface, \( a \) being a rational number. The number of dislocations in the pile-up has been determined using the relationship (2.26), and the stresses in the neighbourhood of the tip have been evaluated approximately by the method described in Appendix 3.2. The significance of these results is discussed in Section 7.1.
Figure 3.1 The relationship between the rectangular Cartesian axes $Ox_1$ and the set of cylindrical polar coordinates $(r, \phi, z=x_3)$ used in Section 3.3.
Appendix 3.1  The Fifteen Possible Analytic Solutions to the Equation \( \cos \alpha_1 + Y \cos \alpha_1 = 0 \), for Arbitrary \( Y \)

In the following list of solutions the principal values of all inverse cosines should be taken. In order to simplify the writing of the solutions the following notation has been adopted. When symbols \((\pm)\) occur in an expression either all of the upper signs or all of the lower signs must be chosen. On the other hand the symbol \((*)\) is also used, having the same mathematical meaning as \((\pm)\) but where the choice is independent of all other symbols in the expression. The solutions are listed in order of increasing \( q \).

(1) \( a=0 \), take \( q=1 \)  
\[ \alpha_1 = \frac{1}{2} \cos^{-1} Y \]

(2) \( a=1 \), \( q=1 \)  
\[ \alpha_1 = \frac{1}{2} \]

(3) \( a=\frac{1}{2} \), \( q=2 \)  
\[ \alpha_1 = \frac{2}{3} \cos^{-1} \left\{ \frac{1}{4} \left[ \pm (Y^2+8)^{1/2} - Y \right] \right\} \]

(4) \( a=\frac{1}{3} \), \( q=3 \)  
\[ \alpha_1 = \frac{3}{4} \cos^{-1} \left[ \pm \left( \frac{1}{2} (3-Y)^{1/2} \right) \right], \frac{3}{2} \]

(5) \( a=\frac{2}{3} \), \( q=3 \)  
\[ \alpha_1 = \frac{3}{4} \cos^{-1} \left\{ (1+y^2)^{1/2} \cos \left[ \frac{1}{2} (27-2Y^2) (9+Y^2)^{3/2} \right] \right\}, n=1,2,3 \]

where \( \theta = \cos^{-1} \left[ \frac{1}{2} (27-2Y^2) (9+Y^2)^{3/2} \right] \)

(6) \( a=\frac{1}{4} \), \( q=4 \)  
\[ \alpha_1 = \frac{4}{5} \cos^{-1} \left\{ \frac{1}{2} \left[ (1+b)^{1/2} (1-b+(4b^2-2)^{1/2})^{1/2} \right] \right\} \]

where \( b=\frac{1}{2} (10^{1/2} \cos \theta - 1), \theta = \frac{1}{2} \cos^{-1} \left[ (28+27K^2) 10^{-3/2} \right] + \frac{2\pi}{5} \)

and \( K = \frac{1}{4} Y \)
\[ a = \frac{3}{4}, \quad q = 4 \]
\[ \alpha_i = \frac{4}{n} \cos^{-1}\left\{-\frac{1}{2}(K_i(K_i^2 + b) + 2K(K_i^2 + b) + 1/2 \right\} \]
\[ 1(4b^2 - 1)^{1/2} \}
where \( b = \frac{1}{2}\left[(10 + 36K^2)^{1/2}\cos \theta - 1\right] \)
\[ \theta = \frac{1}{2}\cos^{-1}\left[7(4 + 27K^2)(10 + 36K^2) - 3/2\right] \]
\[ \text{and } K = \frac{1}{4} \]

(8) \[ a = \frac{1}{2}, \quad q = 5 \]
\[ \alpha_i = \frac{5}{n} \cos^{-1}\left\{2 - 3/2 \left[5 + (7 + 4y)^{1/2}\right] \right\}, \quad \frac{5}{2} \]

(9) \[ a = \frac{3}{2}, \quad q = 5 \]
\[ \alpha_i = \frac{5}{n} \cos^{-1}\left\{2 - 3/2 \left[5 - y(2y + 5)^{1/2}\right] \right\}, \quad \frac{5}{2} \]

(10) \[ a = \frac{1}{2}, \quad q = 7 \]
\[ \alpha_i = \frac{7}{n} \cos^{-1}\left\{2 - 3/2 \left[5 + y(2y + 5)^{1/2}\right] \right\}, \quad \frac{7}{2} \]
\[ n = 0, 1, 2 \]
where \( \theta = \pi - \cos^{-1}\left[\frac{1}{2}(7 + 27y)^{1/2}\right] \]

(11) \[ a = \frac{3}{2}, \quad q = 7 \]
\[ \alpha_i = \frac{7}{n} \cos^{-1}\left\{2 - 3/2 \left[5 - y(2y + 5)^{1/2}\right] \right\}, \quad \frac{7}{2} \]
\[ n = 0, 1, 2 \]
where \( \theta = \pi - \cos^{-1}\left[\frac{1}{2}(7 - 18y)(7 - 3y)^{-3/2}\right] \]

(12) \[ a = \frac{5}{2}, \quad q = 7 \]
\[ \alpha_i = \frac{7}{n} \cos^{-1}\left\{2 - 3/2 \left[5 + y(2y + 5)^{1/2}\right] \right\}, \quad \frac{7}{2} \]
\[ n = 0, 1, 2 \]
where \( \theta = \pi - \cos^{-1}\left[\frac{1}{2}(7 - 12y + 3y^2 + 2y^3)(7 + y^2)^{-3/2}\right] \]
\( a = \frac{1}{\sqrt{3}}, \theta = 9 \)

\[
\alpha_1 = \frac{9}{n} \cos^{-1} \left( 2^{-3/2} \left[ \frac{9}{2} \pm \left( b - \frac{27}{4} \right)^{1/2} \right] \left[ \frac{27}{2} - b \pm 9 \left( b - \frac{27}{4} \right)^{1/2} \right] \pm 4 \left( \frac{1}{4} b^2 - 9 \gamma \right)^{1/2} \right)^{1/2} \right), \frac{9}{4}
\]

where \( b = 2 \left( 3^{4/3} \gamma + \frac{1}{9} \gamma^2 \right) \cos \frac{\theta}{4} + 9 + \frac{1}{3} \gamma \)

and \( \theta = \cos^{-1} \left[ \frac{9}{2} (1 + \gamma) (3^{4/3} \gamma - 3/2) \right] \)

\( a = \frac{5}{\sqrt{9}}, \theta = 9 \)

\[
\alpha_1 = \frac{9}{n} \cos^{-1} \left( 2^{-3/2} \left[ \frac{9}{2} \pm \left( b - \frac{27}{4} \gamma \right)^{1/2} \right] \left[ \frac{27}{2} - b \pm 9 \left( b - \frac{27}{4} \gamma \right)^{1/2} \right] \pm 4 \left( \frac{1}{4} b^2 - 9 \gamma \right)^{1/2} \right)^{1/2} \right), \frac{9}{4}
\]

where \( b = 2 \left( 3^{4/3} \gamma + \frac{1}{9} \gamma^2 \right) \cos \frac{\theta}{4} + 9 + \frac{1}{3} \gamma \)

and \( \theta = \cos^{-1} \left[ \frac{9}{2} (1 + \gamma) (3^{4/3} \gamma + \frac{1}{9} \gamma^2)^{-3/2} \right] \)

\( a = \frac{7}{\sqrt{9}}, \theta = 9 \)

\[
\alpha_1 = \frac{9}{n} \cos^{-1} \left( 2^{-3/2} \left[ \frac{9}{2} \pm \left( b - \frac{27}{4} \gamma + \frac{1}{9} \gamma^2 \right)^{1/2} \right] \left[ \frac{27}{2} - b + \frac{1}{9} \gamma \pm 7 \gamma \right] \pm 4 \left( \frac{1}{4} b^2 - 9 \gamma \right)^{1/2} \right)^{1/2} \right), \frac{9}{4}
\]

where \( b = 2 \left( 3^{2/3} \gamma + \frac{7}{9} \gamma^2 \right)^{1/2} \cos \frac{\theta}{3} + 9 - \frac{2}{3} \gamma \)

and \( \theta = \cos^{-1} \left[ \frac{9}{2} (1 + \gamma) (3^{2/3} \gamma + \frac{13}{9} \gamma^2 + \frac{7}{9} \gamma^4) (3^{2/3} \gamma + \frac{7}{9} \gamma^2)^{-3/2} \right] \)
Appendix 3.2 Integrals of the Form

\[ I = \int_0^1 \eta^m (\eta^2 - 2\eta r \cos \theta + r^2)^{-1} d\eta \]

It is convenient to denote by \( I_n \) the integral \( I \) for \( m \) in the region \( n-1 < m < n \). Integrating by parts the recurrence relation

\[ I_n = (m-1)^{-1} + r^2 I_{n-2} + r \cos \theta I_{n-1} \quad (A3.2.1) \]

is obtained, and it is therefore necessary to evaluate only the integrals \( I_0 \) and \( I_1 \). By making the change of variable \( \eta = y^{-1} \) \( I_0 \) may be decomposed into the form

\[ I_0 = \int_0^\infty \eta^{-m} (1 + 2r \eta \cos \phi + \eta^2 r^2)^{-1} d\eta \]

\[ + (2i \sin \theta)^{-1} \left[ \int_0^1 \eta^{-m} (\eta - e^{-i\phi})^{-1} d\eta - \int_0^1 \eta^{-m} (\eta - e^{i\phi})^{-1} d\eta \right] \quad (A3.2.2) \]

where \( \phi = \theta - \pi \). The first term is now in the form of a standard integral \(^{(56)}\), provided \( -\pi < \phi < \pi \), whilst the other two terms appear as a special case of the integral representation of the Gauss function \(^{(55)}\), provided \( r < 1 \). Thus

\[ I_0 = r^{m-1} \sin m \phi \csc m \pi \csc \phi \]

\[ - \sum_{n=0}^\infty r^n (n-m+1)^{-1} \sin (n+1) \theta \csc \theta. \quad (A3.2.3) \]

The integral \( I_1 \) may be decomposed into a form similar to that of equation (A3.2.2) without a change of variable, and in fact gives rise to a result identical to that for \( I_0 \) in (A3.2.3), with the same restrictions on \( \phi \) and \( r \). Therefore, by means of (A3.2.1) and (A3.2.3) any of the integrals \( I_n \) may be evaluated analytically.
Two Special Cases of Screw Dislocation Pile-Ups
Near to Plane Boundaries

Two special cases in which the integral equation (2.14) can be solved for all values of the constant \(a\), both rational and irrational, occur when \(Y=1\) and \(Y=-1\), and in both instances a treatment is required which differs to some extent from that given in Chapter 3. The first of these cases, corresponding to a screw dislocation pile-up in a half-space of finite rigidity against a rigid second phase, at first sight seems to be of small physical significance. However, the solutions obtained in the following analysis clearly indicate that when the second phase has finite rigidity the results of the last chapter may be used to assess by interpolation the properties of pile-ups inclined to the boundary at intermediate angles for which analytic treatment is not possible using the present technique. Moreover the mathematical problem is identical to that for two intersecting screw dislocation pile-ups under symmetric loading considered by Smith (23).

The second case when \(Y=-1\) requires considerably different treatment. It corresponds to a dislocation array in a half-space bounded by a free surface, and unlike the cases considered already has little physical significance when the distribution function \(F(x_1)\) is unbounded at the surface, that is when \(x_1=0\). However, if it is bounded at this point and unbounded at \(x_1=\ell\), the model corresponds to an infinitely sharp notch inclined to a free surface, under conditions of antiplane strain, and therefore the
solution to this particular problem is considered here.

4.1 Screw Dislocation Pile-Up Against a Rigid Second Phase

When \( \gamma = 1 \) the function \( K(s) \) given by equation (2.21) may be written directly in the form of a single product, that is

\[
K(s) = 2\pi \cos[(s-1)(1+a)\pi/2] \cos[(s-1)(1-a)\pi/2]/\sin[(s-1)\pi].
\]

Expanding the sines and cosines by means of the infinite product formulae, the factorisation (2.29) may be carried out as before by inspection. Using the infinite product representation of the gamma function \( K_-(s) \) and \( K_+(s) \) may be written in the forms

\[
K_-(s) = 2^{-3/2} e^{-X'(s)} \Gamma[(1-s)/2] \Gamma[(1-s)(1+a)/2] \times \\
\quad \times \left\{ \Gamma[(1-s)(1+a)] \Gamma[(1-s)(1-a)] \right\}^{-1}
\]

\[
K_+(s) = 2^{-3/2} e^{-X'(s)} \Gamma(s) \Gamma[(s-1)(1+a)/2] \Gamma[(s-1)(1-a)/2] \times \\
\quad \times \left\{ \Gamma[(s-1)(1+a)] \Gamma[(s-1)(1+a)] \right\}^{-1}
\]

It is readily shown by means of Stirling's asymptotic formula \(^{(54)}\) for the gamma function that if

\[
X'(s) = - (s-1) \ln 4 \Delta
\]

where \( \Delta = [(1+a)/2](1+a)/2[(1-a)/2](1-a)/2 \)

then \( K_+(s) \) has the necessary algebraic behaviour

\[
\lim_{s \to \infty} K_+(s) \to s^{1/2}
\]

for the application of Liouville's theorem at a later stage,
as in the previous problem.

Assuming a constant applied stress $\sigma_{23}^A$ and a constant frictional stress $\sigma_{23}^F$ then the function $G_+(s)$ will again be given by equation (3.10), where in this case

$$c = 2\pi [G(I)_b]^{-1} \sigma = 2\pi [G(I)_b]^{-1} [2\sin^2 \alpha \pi / 2 \sigma_{23}^A - \sigma_{23}^F]$$

obtained by placing $\gamma = 1$ in (3.9). Also, by identical reasoning to that in Section 3.1 it may be deduced that $J(s) = 0$, when, from (3.11),

$$B_+(s) = G_+(s) / K_+(s)$$

$$= c (2\pi)^{-1} N' \Delta^{-s} \Gamma \left[ 1 \left( \frac{1}{2} (s-1)(1+a)+\frac{1}{2} \right) \right] \Gamma \left[ \left( \frac{1}{2} (s-1)(1-a)+\frac{1}{2} \right) \right] \cdot x \left[ \Gamma (s+1) \right]^{-1}$$

(4.1)

where $N' = \frac{3}{2} \csc \frac{\alpha \pi}{2}$. The distribution function $\Omega(\eta) = F(x)$, obtained by substituting (4.1) into the inversion integral (2.23), has the form

$$F(x_1) = - c \pi^{-1} N' \sum_{m=0}^{\infty} \left[ V_m \left[ 1/(1+a) ; \Delta x_1 / \Delta \right] + V_m \left[ 1/(1-a) ; x_1 \Delta / \Delta \right] \right]$$

(4.2)

where

$$V_m [e;z] = z^{e(m+1)-1} \Gamma [e(2m+1)-1] / \Gamma [e(2m+1)-m] m!.$$

(4.3)

When $a$ is rational (4.2) may be written alternatively as the sum of generalised hypergeometric functions, in agreement with the results of Chapter 3 for this limiting value of $\gamma$. Taking the limit of equation (4.1) as $s \to 1$, the number of dislocations, $n$, in the pile-up is given by the expression

$$n / \ell = c N'/2 \Delta$$

(4.4)
from equation (2.26). Finally, using the results of Appendix 3.2, the stress components $\sigma_{ij}^{(1)P}$ at a point $(r, \phi, z)$ in medium (I) due to the array are given approximately as

$$
\sigma_{ij}^{(1)P} \sim \sigma \csc \frac{\alpha}{2} \left[ \frac{\ell}{r \Delta} \right] a/(1+a) \left\{ \cos a(\phi - \pi) + C \left\{ \sin \alpha \right\} \right\}
$$

(4.5)

for $(1-a)\pi/2 \leq \phi \leq \pi$, and

$$
\sigma_{ij}^{(1)P} \sim \sigma \csc \frac{\alpha}{2} C \left\{ \sin \alpha \right\}
$$

(4.6)

for $-\pi \leq \phi \leq (1+a)\pi/2$. For a given value of $a$, the quantity $C$ is a constant defined by the expression

$$
C = a \pi^{-1} \sum_{m=0}^{\infty} \left\{ v_m \left[ 1/(1+a) ; A \right] + v_m \left[ 1/(1-a) ; A \right] \right\}
$$

(4.7)

where

$$
v_m[e;z] = \frac{e (2m+1)-1}{(e(2m+1)-1) \Gamma [e(2m+1)-1]}
$$

$$
\times \left\{ [e(2m+1)_{-1} \Gamma [e(2m+1)_{-m} m! \right\}^{-1}, \quad (4.8)
$$

The case when $a=0$ and $\gamma=1$, when the pile-up is perpendicular to the boundary, has previously been considered by Chou(14) using the Muskhelishvili theorem. In this instance (4.2) and (4.4) have the particularly simple forms

$$
F(x_1) = 2c \cosh^{-1} (\ell/x_1) n^{-2} \quad \text{and} \quad n/\ell = v/\pi.
$$

It is far more interesting however to compare the present results with those of Smith(23) for two intersecting screw dislocation pile-ups in an infinite homogeneous medium of shear modulus $G$, inclined to each other at an angle $2\pi \beta$ [=$(1-a)\pi$], using Smith's notation, and loaded symmetrically. Referring all stress components to the alternative set of
axes $Ox_1^*$, defined in Figure 4.1, consider a load $\sigma_{ij}^*$ applied at infinity, the only non-zero component of which is $\sigma_{23}^* = -\sigma^*$. The stress acting on each slip plane is $-\sigma^*\cos \pi \beta$ and, making Smith's simplifying assumption that the lattice frictional stress $\sigma^F$ is zero, the distribution function on each plane is given by (4.2) in the form

$$F(x_1) = -\sigma^*(Gb)^{-1}(1-2\beta) \sum_{m=0}^{\infty} \left\{ V_m [1/2(1-\beta); \beta^\beta(1-\beta)^{1-\beta} x_1/\ell] + V_m [1/2\beta; \beta^\beta(1-\beta)^{1-\beta} x_1/\ell] \right\},$$

where the functions $V_m$ are defined in (4.3). This result has not previously been given. Rewriting (4.4) in the present notation, Smith's result for the number of dislocations, $n$, in each slip plane is obtained, namely

$$n = \pi \sigma^* \ell (2Gb)^{-1} \beta (1-\beta)^{1-\beta}.$$

The components $\sigma_{ij}^P$ of the overall stress field due to the arrays at a point $(r, \phi^*, z)$, where $\phi^*$ is defined in Figure 4.1, may be obtained in a similar manner to (4.5) and (4.6). In the region $-(1-\beta)\pi<\phi^*<(1-\beta)\pi$

$$\sigma_{ij}^P(13) \sim \{^+\} \sigma^* \beta^{-\beta}(1-2\beta)/2(1-\beta)(1-\beta)^{1-\beta} x(\ell/r)(1-2\beta)/2(1-\beta) \left\{ \sin[(1-2\beta)\phi^*/2(1-\beta)] + [0] \right\}$$

whilst for $(1-\beta)\pi<\phi^*<\pi$, $-\pi<\phi^*<(1-\beta)\pi$

$$\sigma_{13}^P = 0 \text{ and } \sigma_{23}^P = -\sigma^* C.$$

Here the constant $C$, defined as in (4.7), may be written

$$C = a\kappa^{-1} \sum_{m=0}^{\infty} \left\{ V_m [1/2(1-\beta); \beta^\beta(1-\beta)^{1-\beta}] + V_m [1/2\beta; \beta^\beta(1-\beta)^{1-\beta}] \right\}.$$
Smith has derived the result (4.9) for $\phi^*=0$, omitting the constant term $C$ in his approximation.

4.2 The Infinitely Sharp Notch in Antiplane Strain

Two different approaches are used in this section to find the stress field in an elastic half-space bounded by a free surface and containing a slit notch inclined at an arbitrary angle to the surface. In Section 4.2.1 the notch is represented by a continuous distribution of infinitesimal dislocations confined to the notch plane, and the integral equation expressing the equilibrium conditions is solved using the Wiener-Hopf technique. The series solution obtained by this method is only slowly convergent at points very near to the tip of the notch, and is therefore in an unsuitable form for deriving the crack extension criterion\(^{(57)}\). However the solution for the stress field is exact for all points in the plane of the crack beyond the tip, and the analysis illustrates how the Wiener-Hopf technique may be used when the end conditions on the distribution function differ from those in the problems considered earlier.

For comparison the same problem is solved in Section 4.2.2 using a conformal mapping technique. The mapping function was used originally by Barenblatt and Cherepanov\(^{(58)}\) who considered a similar notch loaded by oppositely directed line forces acting on either face at points where the notch leaves the free surface. By this method it is possible on to obtain/approximate expression for the distribution function at points near to the tip, and the crack extension criterion may then be readily formulated, as shown in Section 4.2.3. Unlike the Wiener-Hopf technique, however, the
the method is restricted to loading in antiplane strain.

4.2.1 The Wiener-Hopf Approach

The physical situation is shown schematically in Figure 4.2, in which n freely-slipping screw dislocations are distributed continuously on the plane $y_2=0$ over the region $0<y_1<\ell$. The surface $x_1=0$ is stress-free, and the dislocations pile-up at the point $y_1=\ell$ under the influence of a uniform stress $\sigma_{13}=\sigma$, referred to axes $Ox_1$, applied at infinity. The model therefore represents an infinitely sharp notch, inclined at an angle $\pi/2$ to the normal to a plane free surface, which is loaded in antiplane strain.

The equilibrium condition in this problem is expressed by the singular integral equation (2.13) in which $\gamma=-1$ and $x_1,x_2$ are replaced by $y_1,y_2$, and a solution is sought which is bounded at $y_1=0$ and unbounded at $y_1=\ell$. By transforming the equation as outlined in Section 2.3 the Wiener-Hopf equation (2.6) is obtained which must be satisfied in this case in the infinite strip $-(1-a)(1+a)<\xi<1$, $-\infty<\xi<\infty$ in the $s=\xi+i\zeta$ plane. In the nomenclature of Chapter 2 this strip is the region (ii) with $\xi_-=(1-a)(1+a)$ and $\xi_+=1$. When $\gamma=1$ equation (2.21) may be written

$$K(s) = 2\pi \sin[(s-1)(1+a)\pi/2] \sin[(s-1)(1-a)\pi/2]/\sin\pi(s-1)$$

and by expanding the sine terms as infinite products, again this function may be factorised by inspection in the manner of (2.29) to give

$$K_+(s) = 2\pi e^{-x'(s)} \Gamma(s-1)/(s-1) \Gamma[(s-1)(1+a)/2] \Gamma[(s-1)(1-a)/2]$$

(4.11)

$$K_-(s) = 4e^{x'(s)} \Gamma(1-s)/(1-a^2) \Gamma[(1-s)(1+a)/2] \Gamma[(1-s)(1-a)/2]$$

(4.12)
where the infinite products have been replaced by gamma functions using Euler's formula. By choosing

\[ \chi'(s) = (1-s) \ln \Delta, \]

where as before \( \Delta = [(1+a)/2]^{(1+a)/2}[(1-a)/2]^{(1-a)/2} \), it may be shown that

\[ \lim_{s \to \infty} K_+(s) = s^{-1/2}, \quad (4.13) \]

apart from a constant multiplying factor, by using Stirling's asymptotic formula. Thus, having established the necessary behaviour of \( K_+(s) \) in this limit, the function \( G_+(s) \) is obtained directly from (3.10) when the applied stress \( \sigma_{13} \) is uniform, giving

\[ G_+(s) = -\kappa' \pi \Delta/s \]

(4.14)

where \( \kappa' = 2\pi \sigma \cos \frac{\pi}{2} (Gb)^{-1} \) and \( G \) is the shear modulus of the material.

So that the form of the function \( J(s) \), defined as in (3.11), may be determined consider the end conditions of the present problem. It is required that the distribution function \( \Omega(\eta) \), where \( \eta=y/l \) in this case, is unbounded at \( \eta=1 \), and so it is reasonable to assume

\[ \Omega(\eta) \sim (1-\eta)^{-M} \text{ as } \eta \to 1, \]

where \( M \) is a constant greater than zero. Therefore

\[ B_+(s) \sim s^{M-1} \text{ as } s \to \infty \]

(4.15)

from the Abelian theorem of Section 2.1. Since in region (iii)

\[ J(s) = K_+(s)B_+(s) - G_+(s), \]

(4.16)
it follows from (4.13), (4.14) and (4.15) that

$$|J(s)| \to |s|^{M-3/2} \text{ as } s \to \infty,$$

and from Liouville's theorem that $J(s) = 0$ provided $M < 3/2$.
Also, since $B_+(s)$ is regular in region (iii), from the Mellin transform theorem in Section 2.1

$$\Omega(\eta) \sim \eta^{(1-a)/(1+a)} \text{ as } \eta \to 0$$

and thus the second end condition, that $B_+(s)$ is bounded at $\eta=0$, is satisfied.

The function $B_+(s)$ is now given uniquely from equations (4.11), (4.14) and (4.16) by the expression

$$B_+(s) = \eta \Delta^{-S} \Gamma [1+(s-1)(1+a)/2] \Gamma [1+(s-1)(1-a)/2]/2\pi \Gamma (s+1)$$

(4.17)

and may be substituted into the integral (2.23) to obtain the dislocation distribution function $\Omega(\eta)$. This integral, taken around the infinite semi-circle enclosing the negative half-plane, may be evaluated by residue theory, yielding the result

$$F(y_1) = \eta \pi^{-1} \sum_{m=0}^{\infty} \left[ W_m [1/(1+a); y_1 \Delta/\ell] + W_m [1/(1-a); y_1 \Delta/\ell] \right]$$

(4.18)

where

$$W_m [b; z] = b z^{2b(m+1)-1} \Gamma [2b(m+1)-1]/\Gamma [2b(m+1)-m] m!$$

and $\eta = 2\pi \sigma (Gb)^{-1}$. The relative displacement, $d$, of the slot surfaces at $x_1=0$ is given by the expression

$$d/\ell = nb/\ell = \sigma / G \Delta$$

(4.19)

obtained from equations (2.26) and (4.17).
Unfortunately the distribution function (4.18) is only slowly convergent as \( y_1 \) approaches \( \ell \), and so the procedure adopted in the previous problems for finding the stress fields approximately at points near to the tip of the array is inappropriate in the present case. However the method outlined in Section 2.3 may be used to find exactly the total stress component \( \sigma_{23}^T \), referred to axes \( Oy_1 \) at points \((y_1 > \ell, 0)\) on the slip plane beyond the end of the pile-up. From (3.6) and (3.11)

\[
H_-(s) = G_+(s)K_-(s) - G(s),
\]

and hence, using (2.27) and (2.28) the stress component \( \sigma_{23}(y_1) \) (referred to \( Oy_1 \)) due to the arrayed dislocations alone may be obtained from the integral

\[
2\pi(Gb)^{-1}\sigma_{23}^P(y_1) = (2\pi i)^{-1} \int_{\xi_0 - i\infty}^{\xi_0 + i\infty} [G_+(s)K_-(s) - G(s)](y_1/\ell)^{-s} ds \quad (x_1 > \ell) \quad (4.20)
\]

where \( \xi_0 < 1 \). This integral may be evaluated round the infinite semi-circle in the right-hand half-plane with the aid of residue theory. In the present case, where the applied stress is constant, by choosing \( \xi_0 < 0 \) the total stress component \( \sigma_{23}^T \) is given by the expression

\[
\sigma_{23}^T(y_1) = Gb(4\pi i)^{-1} \int_{\xi_0 - i\infty}^{\xi_0 + i\infty} G_+(s)K_-(s)(y_1/\ell)^{-s} ds \quad (\xi_0 < 0) \quad (4.21)
\]

obtained by substituting \( G(s) = v' / s \) into the integral (4.20). The functions \( K_-(s) \) and \( G_+(s) \) have already been calculated in equations (4.12) and (4.14) respectively, and the integral (4.19) thus gives
\[ \sigma_{23}^{T} = \sigma \pi \sum_{m=0}^{\infty} (-\ell/y_{1} \Delta)^{m} \times \left\{ \Gamma \left[ \frac{(1+a)(1-m)/2}{1} \right] \Gamma \left[ \frac{(1-a)(1-m)/2}{1} \right] \Gamma (m+1) \right\}^{-1}. \]

In the limiting case when \( a = 0 \), when the slot is perpendicular to the free surface, (4.22) reduces to that obtained by Head and Louat (4) using the Muskhelishvili inversion theorem, namely

\[ \sigma_{23}^{T}(y_{1}) = \sigma y_{1}^{2} (1-\ell^{2})^{-1/2}. \]

However for general values of \( a \) it is not possible to write \( \sigma_{23}^{T}(y_{1}) \) other than the power series (4.22), which is only slowly convergent for values of \( y_{1} \) near to \( \ell \) and is therefore unsuitable for studying the stress field near to the tip. For this reason the same problem is considered in the next section using a conformal mapping technique, where an approximate expression for (4.22) is derived for \( y_{1} \gg \ell \).

### 4.2.2 The Conformal Mapping Approach

Consider a crack, infinite in the Ox3 direction, whose cross-section in the \( x_{1}x_{2} \)-plane is a slit of length \( \ell \) inclined to the Ox2 axis at an angle \( \alpha \pi/2 \), and meeting the free surface \( x_{2} = 0 \) at the origin, as shown in Figure 4.3(a). The material is subject to a constant applied stress \( \sigma_{23} = \sigma \) at infinity, referred to axes Ox1, and the crack faces are stress-free. The transformation

\[ z = \ell(z-1)(1-a)/2 \left[ 1 + \frac{(1-a)}{1+a}z \right] (1+a)/2 \quad (4.23) \]

maps the region above AO1LO2B in the \( z = x_{1} + ix_{2} \) plane in Figure 4.3(b) into the upper half of the \( Z = X_{1} + iX_{2} \) plane.
as shown in Figure 4.4. Undashed and dashed points correspond in the two figures. In particular a point \( P(y_1,0) \) on the crack plane, where \( 0 < y_1 < \ell \) transforms approximately to the point \( P'[0,\{2(y_1-\ell)(1+a)/\ell(1-a)\}^{1/2}] \) in the \( Z \)-plane. Since the system is in antiplane strain the displacements \( u_3 \) are harmonic, and thus, together with the stress components \( \sigma_{13} \) and \( \sigma_{23} \) (referred to \( Ox_1 \)) may be expressed in terms of a single potential function \( \phi(z) \) by the relations

\[
\begin{align*}
    u_3 &= G^{-1} \text{Re}[\phi(z)] \\
    \sigma_{13} - i\sigma_{23} &= G\omega u_2/\omega x_1 - iG\omega u_3/\omega x_2 = \frac{d\phi}{dz}.
\end{align*}
\]

Thus, using the transformation (4.23)

\[
\frac{d\phi}{dZ} = \frac{d\phi}{dz} \frac{dz}{dZ} = \frac{\ell(1-a)}{2} \left[ \frac{1}{1+a} + \frac{1}{1-a} \right] \frac{d\phi}{dz}.
\]

(4.25)

and since \( \frac{d\phi}{dz} = \sigma \) as \( x_1 \to \infty \), the original problem in the \( z \)-plane is equivalent to the trivial problem in the \( Z \)-plane in which \( \frac{d\phi}{dz} = \sigma \ell[(1-a)/(1+a)](1+a)/2 \) as \( x_1 \to \infty \) and \( \omega u_2/\omega x_2 = 0 \) when \( x_2 = 0 \), for all \( x_1 \). The function

\[
\phi = \sigma \ell[(1-a)/(1+a)](1+a)/2 Z
\]

satisfies these conditions and therefore, from (4.26)

\[
\frac{d\phi}{dz} = 2\sigma(\frac{1-a}{1+a})^2(\frac{1-a}{1+a})^{-1} \left[ \frac{1}{1+a} - \frac{1}{1-a} \right] \frac{d\phi}{dz} e^{-i\pi(1-a)/2}.
\]

(4.27)

Referred to the alternative axes \( Oy_1 \) defined in Figure 4.3(a) the component \( \sigma_{23}^m \) of the total stress acting on the crack plane at the point \( P(y_1,0) \) may be obtained from
In the approximate form
\[
\sigma_{23}^T \sim \sigma \left( \frac{1-a}{1+a} \right)^\frac{1}{2} \frac{\ell(1+a)+2(y_1-\ell)(1-a)}{\ell(1-a)+2(y_1-\ell)(1+a)} \frac{1-a}{4} 
\]
\[
x \left\{ \frac{1}{2} \left[ 2(y_1-\ell)(1+a)/\ell(1-a) \right] \cos \left( \frac{1-a}{2} \phi \right) + \sin \left( \frac{1-a}{2} \phi \right) \right\}
\]
where \( \phi = \tan^{-1} \left[ \frac{3}{2} \frac{1}{\ell} \left( y_1-\ell \right)^{\frac{1}{2}} \left[ \ell-2(y_1-\ell) \right]^{-1} (1-a)^{-\frac{1}{2}} \right] \), or

\[
\sigma_{23}^T \sim \sigma \left( \frac{1-a}{1+a} \right)^\frac{a}{2} y_1 \left[ 2(y_1-\ell)/\ell \right]^{-\frac{1}{2}} + O \left[ (y_1-\ell)^{\frac{3}{2}} \right].
\]

Since the points \( O \) and \( O \) in the z-plane transform to points \( O_1 \) and \( O_2 \) in the Z-plane, the relative displacement, \( d \), between \( O \) and \( O \) is readily obtained using (4.24) and (4.26), giving

\[
d = \left[ \text{Re} \left[ \frac{\phi(+0)}{\phi(-0)} \right] \right] /G = \alpha \ell / G \Delta,
\]
where as in the previous sections

\[
\Delta = \left[ (1+a)/2 \right]^{(1+a)/2} \left[ (1-a)/2 \right]^{(1-a)/2}.
\]
This result is identical to equation (4.19) obtained using the Wiener-Hopf technique.

### 4.2.3 The Crack Growth Condition

Smith\(^{(59)}\) has presented Irwin's\(^{(57)}\) growth criterion for a cleavage crack in a form applicable to a crack represented by a linear array of freely-slipping dislocations. If \( \gamma \) is the free surface energy of the material containing the crack, then in the notation of the present problem the criterion may be written

\[
\lim_{y_1 \to \ell} 2\pi(\ell-y_1)[P(y_1)]^2 = 16\gamma / G \beta^2
\]

(4.28)
where $F(y_1)$ is the distribution function of the dislocations representing the notch, and may be determined from the relation

$$F(y_1) = -\frac{2}{b} \frac{\sin \frac{\pi}{2} y_1}{y_1} = -\frac{2}{Gb} \text{Re} \left[ \frac{d\theta}{dz} \right] e^i(1-a)\pi/2 \quad (4.29)$$

At points on the plane $y_2=0$ very near to the notch tip

$$Z \sim 2(\ell_x - y_1)(1+a)/\ell(1-a),$$

and from (4.27) and (4.29) the distribution function in this region has the approximate form

$$F(y_1) = \frac{2\sigma_0(1-a)^{a/2}}{\ell \sqrt{\ell_x - y_1}} \left[ \frac{\ell}{\ell_x - y_1} \right]^{1/2}.$$

Substitution of this expression into (4.28) yields the crack growth criterion

$$\sigma(1-a)^{a/2} = \left( \frac{2YG}{\pi \ell} \right)^{1/2} \quad (4.30)$$

which reduces to the familiar criterion (60) when $a=0$ for the notch perpendicular to the free surface. It is clear from (4.30) that the stress required for crack growth becomes larger as the angle $\alpha/2$ between the surface normal and the plane of the notch increases, and tends to infinity as $a$ tends to 1.

4.3 Summary

In Section 4.1 of this chapter the distribution function of an array of screw dislocations piled-up at an angle $(1-a)\pi/2$ to the plane interface between an elastic and a rigid half-space has been obtained using the Wiener-Hopf technique. Since the mathematical model is essentially identical to that representing two intersecting arrays of
dislocations under symmetric loading, which has been considered by Smith\(^{(29)}\) using a conformal mapping technique, the solutions obtained from the two approaches are compared. Although in this case the latter treatment is only marginally simpler, it is considerably preferable in the problem of a sharp notch in antiplane strain inclined to the free surface of an elastic half-space which has been solved for uniform loading using both techniques in Sections 4.2.1 and 4.2.2. In fact it does not appear possible to derive the crack growth condition, in the manner described in Section 4.2.3, from the results obtained using the Wiener-hopf technique.
Figure 4.1 Schematic illustration of two intersecting screw dislocation pile-ups under symmetrical loading, showing the rectangular Cartesian axes $Ox_1^*$ and cylindrical polar coordinates $(r, \phi^*, z=x_2^*)$ used in the discussion of this problem in Section 4.1.
Figure 4.2  Schematic illustration of the dislocation model used to represent an infinitely sharp notch CL in antiplane strain inclined to the free surface $x_2=0$ at an angle $\alpha \pi/2$. The systems of rectangular Cartesian axes $Ox_1$ and $Oy_1$ are related by a rotation of $\alpha \pi/2$ about $Ox_3=Oy_3$. $n$ positive screw dislocations, distributed continuously on the plane $y_2=0$ in the region $0<y<\ell$, are in equilibrium under a constant applied stress $\sigma_{23}=\sigma$ referred to axes $Ox_1$. 
Figure 4.3  The \( z = x_1 + ix_2 \) plane (a) showing the relationship between the axes \( Ox_1 \) and \( Cy_1 \) used in Section 4.2.2, and (b) showing schematically the notch profile of length \( \ell \) at an angle \( a\pi/2 \) to the normal to the free surface \( x_2 = 0 \).
Figure 4.4  The $z = x_1 + i x_2$ plane obtained from the $z$-plane by the transformation (4.23). Dashed points correspond to undashed points in Figure 4.3(b).
5.1 Introduction

In the preceding chapters the results of Head\(^{27}\) for the interaction between an infinite straight screw dislocation and a plane boundary separating two isotropic elastic half-spaces have been used in deriving the equilibrium integral equations for groups of dislocations piled-up in the neighbourhood of such boundaries. However this analysis, together with the corresponding treatment for the edge dislocation\(^{30}\), can only be applied to boundaries between different materials, or different phases of the same material, and not to grain boundaries. Since the difference in elastic properties of neighbouring grains in a polycrystal arises solely from their relative crystallographic orientation it is necessary to consider two half-spaces, joined by a plane interface, which are elastically anisotropic rather than isotropic in order to investigate the elastic influence of grain boundaries on dislocations.

Very few three-dimensional problems in anisotropic elasticity theory may be solved analytically. Most available solutions are for problems of special symmetry, concerned for example with materials in the form of cylinders under torsion or bending, or with infinite sheets under conditions of plane strain, as discussed for instance by Leknitsky\(^{61}\) and Green and Zerna\(^{62}\). However the state of stress in which the displacement and stress components are invariant in one direction, which, as clearly
illustrated in the preceding chapters of the present work, is of paramount importance in the elastic theory of dislocations and cracks, may be treated as a generalised form of plane strain using complex variable techniques in the manner described by Eshelby, Read and Shockley\(^{(63)}\) in their study of dislocations in anisotropic materials. These solutions, which are for materials of the most general elastic anisotropy, have been presented in an alternative form by Stroh\(^{(64)}\) who also considered the stress fields of cracks infinite in one dimension and the interaction of parallel dislocations. In this chapter solutions to problems of this kind are found when plane boundaries of various types are introduced into the material\(^{(65,48)}\). In Section 5.3 solutions to the standard boundary-value problems are presented for the first time for an elastic half-space in which the stress and displacement components are independent of position in one direction parallel to the boundary. The treatment is then extended in Section 5.4 to composite materials consisting of two different anisotropic elastic half-spaces which are either welded together or may slip freely relative to one another. The theory is entirely general in that it is valid for completely arbitrary stress distributions on either side of the interface, provided that these stresses vanish at infinity. In Section 5.5 the analysis is used to examine the interaction between these boundaries and various configurations of parallel dislocations near to them. Finally the presentation is generalised slightly in Section 5.6 to facilitate its application to specific problems, in particular to boundaries in crystalline materials.

A preliminary treatment of the interaction between a single dislocation and a plane boundary in an anisotropic
5.2 **Generalised Plane Strain in an Infinite Homogeneous Anisotropic Material**

Although the present analysis is based on the general theory of Eshelby et al. (63), the notation of Stroh (64) has been adopted, with some modifications, simply because this enables a systematic procedure to be developed, as discussed in Appendix 5.1, for evaluating the constants introduced here. Stroh's presentation has been seldom employed however and so it is briefly reviewed in this Section. Three different types of suffix are used, those of small Latin or Greek type which may take values 1, 2 or 3, and those of capital Latin type which may also have values 4, 5 or 6. The summation convention is employed for repeated Latin indices, whereas summation over repeated Greek indices will always be shown explicitly. Using this suffix notation the generalised form of Hooke's law for an elastically anisotropic medium may be written in the alternative forms

\[ \sigma_{ij} = c_{ijkl}e_{kl} \]  
\[ e_{ij} = s_{ijkl}c_{kl} \]

where \( \sigma_{ij} \) and \( e_{ij} \) are the components of stress and strain, and \( c_{ijkl} \) and \( s_{ijkl} \) are the elastic stiffness and compliance constants respectively. The elastic strains \( e_{ij} \) are related to the displacement components \( u_i \) by the expressions
and so the equations of elastic equilibrium may be written in the equivalent forms

\[ \sigma_{ij}/\partial x_j = 0, \quad c_{ijkl}\partial^2 u_k/\partial x_j \partial x_l = 0. \quad (5.4, 5.5) \]

If the stress and displacement components are independent of the \( x_3 \) coordinate, solutions to these sets of equations may be sought which are functions of the complex variable \( z = x_1 + px_2 \), where \( p \) is a complex constant. In particular, if \( f \) is an analytic function of \( z \), the expressions

\[ u_i = A_i f(z) \]

are solutions to equation (5.5) provided \( p \) satisfies the sextic equation

\[ |c_{ilk1} + p(c_{i2k1} + c_{ilk2}) + p^2c_{i2k2}| = 0. \quad (5.6) \]

Eshelby et al. have shown that solutions to (5.6) always occur in complex conjugate pairs labelled \( p_{\alpha} \) and \( \bar{p}_{\alpha} \) chosen so that \( \text{Im}(p_{\alpha}) > 0 \). Consequently \( u_i \) may be written in the more general form

\[ u_i = \sum_{\alpha} A_{i\alpha} f_{\alpha}(z_{\alpha}) \quad (5.7) \]

where \( A_{i\alpha} \) and \( f_{\alpha} \) are the forms of \( A_i \) and \( f \) which correspond to the particular solution \( p_{\alpha} \), and \( z_{\alpha} = x_1 + p_{\alpha} x_2 \). Throughout the present work, where complex expressions such as (5.7) occur, only the real part has physical significance. Using equations (5.1), (5.3) and (5.7) the stress components \( \sigma_{i1} \) and \( \sigma_{i2} \) are given by the formulae

\[ e_{ij} = \frac{1}{2}(\partial u_i/\partial x_j + \partial u_j/\partial x_i) \quad (5.3) \]
\[
\sigma_{i1} = \sum_{\alpha} \alpha i_{\alpha} \delta_{x_2}[f_{\alpha}(z_{\alpha})]
\]
\[
\sigma_{i2} = \sum_{\alpha} \alpha i_{\alpha} \delta_{x_1}[f_{\alpha}(z_{\alpha})]
\]
where
\[
I_{i\alpha} = (c_{i2k1} + p_{\alpha} c_{i2k2}) A_{k\alpha} = -(p_{\alpha}^{-1} c_{ilk1} + c_{ilk2}) A_{k\alpha}.
\]

The component \( \sigma_{33} \), which is excluded from (5.8) may be obtained in terms of the other stress components using the fact that \( e_{33} = 0 \) in equation (5.2).

The constants \( A_{i\alpha} \) and \( I_{i\alpha} \) are the \( i \)th components of vectors associated with the solution \( p_{\alpha} \) to the sextic equation (5.6). It is possible, and in the present analysis convenient, to treat each set of nine constants as though they formed the elements of a 3x3 matrix, to which the normal rules of matrix algebra apply.

5.3 The Classical Boundary-Value Problems for a Half-Space

There are two types of boundary-value problem associated with the elastic half-space \( x_2 > 0 \). In the first problem the plane boundary \( x_2 = 0 \) is subjected to an applied stress \( \sigma_{i2}(x_1,0) = \beta_i(x_1) \), whereas in the second it is constrained so that the displacements \( u_i(x_1,0) \) at the boundary have given values \( r_i(x_1) \). In this section the solutions of these two problems are discussed for the case when, prior to the application of the boundary conditions, the stress field and displacements in the region \( x_2 > 0 \) are invariant in the \( x_3 \)-direction and are described by a set of functions having the form

\[
f_0(z) = \ln z + O(1/z) \quad (5.10)
\]
so that the stress components vanish at infinity in the \( x_1x_2 \)-plane.

To each point \((x_1, x_2)\) in the region \(x_2 > 0\), on any plane \(x_2 = \text{constant}\), there corresponds one point on each of the three \(z_\alpha\)-planes. Also, since by definition \(\text{Im}(p_\alpha) > 0\), these points are all contained in the half-planes \(\text{Im}(z_\alpha) > 0\). Suppose that the functions \(f_{0\alpha}(z_\alpha)\) describe the stresses and displacements in the region \(x_2 > 0\) in the absence of the boundary \(x_2 = 0\), that is when the medium is assumed to be infinite and homogeneous. It is necessary to determine the set of functions \(f_{1\alpha}(z_\alpha)\), holomorphic for \(x_2 > 0\), such that the combined potentials

\[
f_\alpha(z_\alpha) = f_{0\alpha}(z_\alpha) + f_{1\alpha}(z_\alpha)
\]

describe a state of stress which satisfies the appropriate boundary conditions on the plane \(x_2 = 0\). To this end it is convenient to define in the region \(\xi > 0\) a set of functions \(k_\iota\) of the complex variable \(z = \xi + i\zeta\) as follows:

\[
k_\iota(z) = \sum \alpha f_{1\alpha}(z) \quad (\zeta > 0).
\]

Since the normal rules of matrix algebra may be applied to the array \(L_{\iota\alpha}\), this expression may be inverted to give

\[
f_{1\alpha}(z) = M_{\alpha \iota} k_\iota(z) \quad (5.11)
\]

where the \(M_{\alpha \iota}\) are the elements of the matrix reciprocal to \(L_{\iota\alpha}\), such that

\[
\sum \alpha L_{\iota\alpha} M_{\alpha \beta} = \delta_{\iota \beta} \quad \text{and} \quad M_{\alpha \iota} L_{\iota \beta} = \delta_{\alpha \beta}.
\]

The definition of the functions \(k_\iota(z)\) may be extended to the region \(\zeta < 0\) by the relation
where the notation $k_i(z) = k_i(\overline{z})$ has been used, these functions being the analytic continuations of the $k_i(z)$ across the regions of the boundary on which the applied stress is zero. However, when $z$ lies in $\zeta<0$, $\overline{z}$ is in the region $\zeta>0$ for which the relations

$$k_i(\overline{z}) = -k_i(z) \quad (\zeta>0) \quad (5.13)$$

therefore hold.

Using the equations (5.11) and (5.13) the actual stress components $\sigma_{12}$ in the half-space $x_2>0$ may be written as

$$\sigma_{12} = \frac{1}{2\pi} \sum_{\alpha} \left[ L_{i\alpha} \dot{f}_{0\alpha}(z_{\alpha}) + \overline{L}_{i\alpha} \dot{f}_{0\alpha}(\overline{z}_{\alpha}) + L_{i\alpha} M_{\alpha j} k_j'(z_{\alpha}) - \overline{L}_{i\alpha} \overline{M}_{\alpha j} k_j'(\overline{z}_{\alpha}) \right] \quad (5.14)$$

by taking the real part of equation (5.8). The dashes denote first derivatives. Taking the limit as $x_2 \to 0$, $\sigma_{12} \to \rho_i$ equation (5.14) becomes

$$\left\{ k_i'(x_{1}) \right\}^+ - \left\{ k_i'(x_{1}) \right\}^- = -\sum_{\alpha} \left[ L_{i\alpha} \dot{f}_{0\alpha}(x_{1}) + \overline{L}_{i\alpha} \dot{f}_{0\alpha}(x_{1}) \right] + 2\rho_i(x_{1}) \quad (5.15)$$

where $\left\{ \right\}^+$ and $\left\{ \right\}^-$ denote the limiting forms of $K_i(z_{\alpha})$ as $x_2 \to +0$ and $x_2 \to -0$ respectively. Because of the assumed form of $f_{i\alpha}$, and the definition of $k_i(z)$ in the whole of the $z$-plane, the formulae of Plemelj may be used with (5.15) to give unique expressions for $k_i'(z)$, and hence for the complete potential functions $f_{\alpha}(z_{\alpha})$ which take the form...
The definite integral may be evaluated using residue theory.

By defining a set of functions
\[ \ell_i(z) = \sum_{\alpha} A_{i\alpha} f_{1\alpha}(z) \]
a method analogous to that already discussed may be used in the solution of the second boundary-value problem, for the case when the surface \( x_2 = 0 \) has given displacements \( r_i(x_1) \). In this instance

\[ f_{\alpha}(z_{\alpha}) = f_{0\alpha}(z_{\alpha}) - \sum_{\beta} B_{\alpha i\beta} \tilde{F}_{\beta\alpha}(z_{\alpha}) \]

\[ + (\pi i)^{-1} M_{\alpha i} \int_{-\infty}^{\infty} r_i(t)(t-z_{\alpha})^{-1} dt \]  \hspace{1cm} (5.17)

where \( B_{\alpha i} \) is the matrix reciprocal to \( A_{i\alpha} \).

An important application of the solution (5.16) is to the stress-free surface, for which \( \rho_i(x_1) = 0 \) and the integral vanishes.

5.4 The Interface between Two Elastically Different Half-Spaces

5.4.1 Introduction

Consider two half-spaces labelled I and II, having in general different anisotropic elastic properties, which are joined along the plane \( x_2 = 0 \) so that I occupies the region \( x_2 > 0 \). In the following analysis quantities pertaining to media I and II will be indicated by superfixes \((I)\) and \((II)\) respectively, and referred to the same set of coordinate axes unless otherwise stated. Provided that, in the absence of the boundary, both media contain stress
singularities described by functions $f_{0\alpha}^{(I)}$ and $f_{0\alpha}^{(II)}$ which are of the same form as in (5.10), then the approach discussed in the previous section may be used to solve the boundary-value problems for the two different kinds of interface, when the two half-spaces are either welded together or allowed to slip freely. The displacements $u_i$ and the tractions $\sigma_{12}$ are all transmitted across the welded interface whereas only components $u_2$ and $\sigma_{22}$ are continuous across the freely-slipping boundary. The problem of a boundary which permits a limited amount of slip to occur is more complicated, involving interfacial dislocations, and is not considered here.

Because of the symmetry of these problems it is convenient to introduce the general superfixes $(g)$ and $(h)$, where

$$
g = I, h = II \text{ when either } \text{Im}(z_\alpha) > 0 \text{ or } \zeta > 0
$$

$$
g = II, h = I \text{ when either } \text{Im}(z_\alpha) < 0 \text{ or } \zeta < 0
$$

to avoid needless repetition of expressions. Two sets of functions $f_{l\alpha}^{(g)}(z^{(g)})$, defined and holomorphic in either half-space, are sought so that the functions

$$f_{\alpha}^{(g)}(z^{(g)}) = f_{0\alpha}^{(g)}(z^{(g)}) + f_{l\alpha}^{(g)}(z^{(g)}) \quad (5.18)$$

describe the stress and displacement fields which satisfy the appropriate boundary conditions. As in Section 5.3 the functions $k_i^{(g)}(z)$ and $\kappa_i^{(g)}(z)$ are defined by the relations

$$f_{l\alpha}^{(g)}(z) = \Omega^{(g)} k_i^{(g)}(z), \quad f_{l\alpha}^{(g)}(z) = \Omega^{(g)} \kappa_i^{(g)}(z). \quad (5.19a,b)$$
as in (5.12), i.e. \( k_i^{(h)}(z) = -k_i^{(g)}(z) \), to give the relations

\[
k_i^{(g)}(\overline{z}) = -k_i^{(g)}(\overline{z})
\]

which are analogous to equations (5.13). Consequently complete expressions for the stresses and displacements in each half-space, obtained by taking the real parts of (5.7) and (5.8), may be written

\[
\sigma_{12}^{(g)} = \frac{1}{2} \sum_\alpha \left[ L_{i\alpha}^{(g)} f_\alpha^{(g)}(z_\alpha^{(g)}) + \overline{R_{i\alpha}^{(g)} f_\alpha^{(g)}(z_\alpha^{(g)})} \right] + \sum_\alpha \left[ L_{i\alpha}^{(g)} M_{\alpha j}^{(g)} k_j^{(g)}(z_\alpha^{(g)}) + \overline{R_{i\alpha}^{(g)} M_{\alpha j}^{(g)} k_j^{(g)}(z_\alpha^{(g)})} \right] \tag{5.20}
\]

and

\[
u_1^{(g)} = \frac{1}{2} \sum_\alpha \left[ A_{i\alpha}^{(g)} f_\alpha^{(g)}(z_\alpha^{(g)}) + \overline{\overline{R_{i\alpha}^{(g)} f_\alpha^{(g)}(z_\alpha^{(g)})}} \right] + \sum_\alpha \left[ A_{i\alpha}^{(g)} M_{\alpha j}^{(g)} k_j^{(g)}(z_\alpha^{(g)}) + \overline{\overline{R_{i\alpha}^{(g)} M_{\alpha j}^{(g)} k_j^{(g)}(z_\alpha^{(g)})}} \right]. \tag{5.21}
\]

Similar expressions for \( \sigma_{12}^{(g)} \) and \( u_1^{(g)} \) may be obtained in terms of the functions \( k_i^{(g)}(z) \) by using (5.19b) instead of (5.19a).

### 5.4.2 The Welded Interface

In the case of the welded interface, taking the limit as \( x_2 \to 0 \), \( \sigma_{12}^{(I)} = \sigma_{12}^{(II)} \) in (5.20) gives the relation

\[
-2 \text{Re} \sum_\alpha \left[ L_{i\alpha}^{(I)} f_\alpha^{(I)}(x_1) - L_{i\alpha}^{(II)} f_\alpha^{(II)}(x_1) \right] = \left\{ k_i^{(I)}'(x_1) + k_i^{(II)}'(x_1) \right\}^+ - \left\{ k_i^{(I)}'(x_1) + k_i^{(II)}'(x_1) \right\}^- \tag{5.22}
\]

from which the unique solutions

\[
k_i^{(g)}'(z) + k_i^{(h)}'(z) = -\sum_\alpha \left[ R_{i\alpha}^{(g)} f_\alpha^{(g)}'(z) - L_{i\alpha}^{(h)} f_\alpha^{(h)}'(z) \right] \tag{5.23}
\]
may be obtained using the Macelj formulae. When the second boundary condition, that \( u_1^{(I)} = u_1^{(II)} \) as \( x_2 \to 0 \), is applied using (5.21), the resulting equation

\[
-2\text{Re} \sum_{\alpha} [A_{i\alpha} f^{(I)}(x_1) - A_{i\alpha} f^{(II)}(x_1)]
\]

\[
= \left[ \bar{w}^{(I)}(I)k_j(x_1) + \bar{w}^{(II)}(I)k_j(x_1) \right]^+ - \left[ \bar{w}^{(I)}(I)k_j(x_1) + \bar{w}^{(II)}(I)k_j(x_1) \right]^-, \tag{5.24}
\]

where

\[
\bar{w}_{ij} = \sum_{\alpha} A_{i\alpha} M_{\alpha j}, \tag{5.25}
\]

cannot be solved in exactly the same way as (5.22). However, if equation (5.24) is multiplied by \((2\pi i)^{-1}(x_1-z)^{-1}dx_1\) and both sides are integrated between the limits \( x_1 = \pm \infty \), the properties of the resulting Cauchy integrals permit the equation to be split into two parts, one corresponding to each half-space, whose solutions may be written as

\[
\bar{w}^{(g)}(z) = \bar{w}^{(h)}(z), \tag{5.26}
\]

Solving equations (5.23) and (5.26) simultaneously for \( k_{\alpha}(z) \), and using (5.18) and (5.19), the functions \( f^{(g)}(z) \) may be written as

\[
f^{(g)}(z) = f^{(g)}(z) - \sum_{\alpha} \mathcal{M} \delta_{\alpha i} \partial_{z_{\alpha}} \bar{f}_{\alpha}(z) + \sum_{\beta} \mathcal{M} \delta_{\alpha i} \partial_{z_{\alpha}} \bar{f}_{\alpha}(z) = 0 \tag{5.27}
\]

where

\[
\mathcal{M} = \frac{i}{2} [\bar{w}^{(g)} - \bar{w}^{(h)}],
\]

\( G_{ij}^{(g,h)} \) is the matrix reciprocal to
and \( \delta_{ij} \) is the Kronecker delta.

5.4.3 The Freely-Slipping Interface

For the freely-slipping interface the following boundary conditions must be satisfied:

\[
\begin{align*}
    u_2^{(I)} &= u_2^{(II)}, \quad \sigma_{22}^{(I)} = \sigma_{22}^{(II)}, \\
    \sigma_{12}^{(I)} &= 0 = \sigma_{12}^{(II)} = \sigma_{32}^{(I)} = \sigma_{32}^{(II)}.
\end{align*}
\] (5.28, 5.29)

Conditions (5.28) will be fulfilled provided that the functions \( k_i^g(z) \) and \( k_i^h(z) \) satisfy the equations

\[
\begin{align*}
    w_{2i}^g k_i^g(z) + \bar{w}_{2i}^h k_i^h(z) &= -\sum_\alpha \left[ \frac{A_i^g(z)}{L_{2\alpha} f_0^g(z)} - \frac{A_i^h(z)}{L_{2\alpha} f_0^h(z)} \right] \quad (5.30)
\end{align*}
\]

and

\[
\begin{align*}
    k_2^g(z) + k_2^h(z) &= -\sum_\alpha \left[ \frac{L_i^g(z)}{L_{2\alpha} f_0^g(z)} - \frac{L_i^h(z)}{L_{2\alpha} f_0^h(z)} \right] \quad (5.31)
\end{align*}
\]

which correspond to equations (5.23) and (5.26), and which were derived in a similar way. Furthermore the conditions (5.29) will be satisfied if

\[
\begin{align*}
    k_i^g(z) &= -\sum_\alpha \left[ \frac{L_i^g(z)}{L_{2\alpha} f_0^g(z)} \right] \\
    k_i^h(z) &= +\sum_\alpha \left[ \frac{L_i^h(z)}{L_{2\alpha} f_0^h(z)} \right] 
\end{align*}
\] (i=1,3) (5.32)

which are solutions to (5.15) when \( \rho_i(x_1)=0 \). The six equations (5.30), (5.31) and (5.32) may be solved simultaneously for the functions \( k_i^g \) and using (5.18) and (5.19) the functions \( f_{\alpha}^g \) may be written in the form
\[ f_\alpha(z_\alpha') = f_{\alpha 0}(z_\alpha') - \sum_{\beta} M_{\alpha i} \tilde{L}_{ij} \tilde{L}_{0 \beta}(z_\alpha') \]
\[ + \sum_{\beta} M_{\alpha i} \tilde{H}_{ij} \tilde{L}_{j \beta} f_{\beta 0}(z_\alpha'). \]

(5.33)

5.4.4 Discussion

By inspection of the solutions (5.16), (5.27) and (5.33) to the boundary-value problems for the free surface, the welded and the slipping interfaces respectively it is clear that they may all be written in the general form

\[ f\alpha(z\alpha') = f\alpha_0(z\alpha') \]
\[ - \sum_{\beta} M_{\alpha i} K_{ij}(g,h) \tilde{L}_{ij} \tilde{L}_{0 \beta}(z_\alpha') \]
\[ + \sum_{\beta} M_{\alpha i} \tilde{L}_{ij} \tilde{L}_{0 \beta} f_{\beta 0}(z_\alpha'). \]

(5.34)

where

\[ K_{ij}(g,h) = \delta_{ij} \]

(5.35)

for the free surface,

\[ K_{ij}(g,h) = \delta_{ij} - \delta_{ij22} h_{2j} \]

(5.36)

for the slipping interface, and

\[ K_{ij}(g,h) = g_{ij}(g,h) \]

(5.37)

for the welded interface. Thus, in the examples considered in Section 5.5 equation (5.34) is used and the solutions given in terms of \( K_{ij}(g,h) \) for the general plane interface.

All of these solutions are expressed entirely in terms of the constants \( L_{i \alpha}, M_{ij} \) and \( W_{ij} \). If however the functions \( f_{\alpha 0} \) had been defined in Section 5.4.2 by the equation
(5.19b) rather than (5.19a) a solution would have been obtained, alternative and equivalent to that for the welded boundary given by (5.34) and (5.36), but with the constants \( L_{i \alpha}, M_{\alpha i}, \) and \( W_{ij} \) replaced by \( A_{i \alpha}, B_{\alpha i}, \) and \( V_{ij} = \sum_{\beta} L_{i \alpha} B_{\alpha j} \), respectively. Nevertheless it is not possible to express the free surface and freely-slipping boundary solutions (5.35) and (5.37) simply in terms of this alternative notation. In fact, by interchanging matrices in this way, the solution corresponding to (5.35) would be for a half-space with a rigidly constrained boundary [cf. equation (5.17)] satisfying the conditions

\[
    u_k = 0, \text{ when } x_2 = 0,
\]

whilst that analogous to equation (5.37) would be for a composite material in which the conditions

\[
    u_2^{(I)} = u_2^{(II)}, \quad \sigma_{22}^{(I)} = \sigma_{22}^{(II)},
\]

and

\[
    u_1^{(I)} = 0 = u_1^{(II)} = u_3^{(I)} = u_3^{(II)}, \text{ when } x_2 = 0,
\]

are satisfied. Physically this solution corresponds to a welded interface which may deform only in a direction normal to itself. Since however these two problems are of little practical application the examples discussed in the remainder of this chapter are based entirely on the generalised solution (5.34).

As discussed in Appendix 5.1, it is easier to calculate the constants \( A_{i \alpha} \) in terms of the elastic stiffnesses \( c_{ijkl} \), using the analysis of Eshelby et al.\(^{63}\), and the \( L_{i \alpha} \) in terms of the elastic compliances \( s_{ijkl} \) as described by Stroh\(^{64}\). In view of the applicability of equation (5.34), in practice use of Stroh's presentation is preferable in problems of this type.
5.5 The Interaction between Straight Dislocations and Plane Boundaries

5.5.1 Introduction

The preceding analysis may be used to investigate the interactions between planar boundaries and certain types of stress singularities having stress and displacement fields which are invariant in one direction parallel to the boundary. One such singularity of particular interest is the infinite straight dislocation, whose elastic properties in a homogeneous anisotropic medium have been discussed by Eshelby et al. (63) and Stroh (64). For a dislocation, with Burgers vector components $b_i$, lying parallel to $Ox_3$ and passing through the point $(X_1, X_2)$, Stroh has shown that the function $f_{0\alpha}(z_\alpha)$ may be written

$$f_{0\alpha}(z_\alpha) = (2\pi)^{-1}M_{\alpha j}d_j \log(z_\alpha - Z_\alpha) \quad (5.38)$$

where $Z_\alpha = X_1 + \rho_\alpha X_2$, and the constants $d_j$ are defined in the medium labelled $\alpha$ by the relation

$$b_i = \tilde{H}_{ij}^{(g,g)}d_j^{(g)}.$$

Furthermore Stroh has analysed the interactions between two such dislocations which are parallel, using the method of forming one dislocation in the presence of the other. If the dislocations, parallel to $Ox_3$, and passing through the points $(x_1^{(1)}, x_2^{(1)})$ and $(x_1^{(2)}, x_2^{(2)})$, have Burgers vector components $b_i^{(1)}$ and $b_i^{(2)}$ respectively, it may be shown that the force on dislocation 1 due to the presence of 2 has
components parallel to \( O x_1 \) and \( O x_2 \) given by the expressions

\[
P_1^{(1)} = (2\pi r)^{-1} b_1^{(1)} d_j^{(2)} \sum_{\alpha} L_{i\alpha} / \alpha(\Psi)^{-1} \alpha M_{\alpha j} \quad (5.39)
\]

and

\[
P_2^{(1)} = (2\pi r)^{-1} b_1^{(1)} d_j^{(2)} \sum_{\alpha} L_{i\alpha} \alpha / \alpha(\Psi)^{-1} \alpha M_{\alpha j} \quad (5.40)
\]

Here

\[
r = \sqrt{[X_1^{(1)} - X_1^{(2)}]^2 + [X_2^{(1)} - X_2^{(2)}]^2},
\]

\[
\Psi = \arctan \left[ \frac{X_2^{(1)} - X_2^{(2)}}{X_1^{(1)} - X_1^{(2)}} \right]^{-1}
\]

and

\[
/ \alpha(\Psi) = \cos \Psi + \alpha(\sin \Psi). \quad (5.41)
\]

In the following examples the influence of planar boundaries on dislocation-dislocation interactions of this type are considered, and the approximate interpretation of these effects in terms of image dislocations, analogous to image charges in electrostatics, is discussed. There are two general types of interaction to be considered, where the dislocations are positioned either in the same half-space or on opposite sides of the boundary. In the present chapter these situations are considered separately, for, because their effects are additive, problems involving more general distributions of dislocations throughout a bicrystal may be analysed in terms of these basic interactions, as for instance in Chapter 6.

5.5.2 Two Dislocations in One Half-Space

Consider the two dislocations 1 and 2 described above, situated in medium g in a composite material in which the plane boundary \( x_2^2 = 0 \) separates media g and h. The stress fields produced by these dislocations may be obtained by
substituting appropriate expressions of the form of (5.38) into equation (5.34), whence by means of (5.8) algebraic formulae for \( \sigma_{12}^{(1)} \) and \( \sigma_{12}^{(2)} \), due to dislocations 1 and 2 respectively, may be written down. In particular on the plane \( x_2 = x_2^{(1)} \) the dislocations give rise to stress components

\[
\sigma_{12}^{(1)} = (2\pi)^{-1} d_{1}(1, g)[x_1 - x_1^{(1)}]^{-1} \\
- (2\pi)^{-1} \sum_{\alpha, \beta} L(g) \mu_{\alpha \beta}(g, h) \mu_{\alpha \beta}(g) d_{\alpha \beta}(1, g) \\
\times \left\{ [x_1 - x_1^{(1)}] + [p_{\alpha}(g) - p_{\beta}(g)] x_2^{(1)} \right\}^{-1},
\]

\[
\sigma_{12}^{(2)} = (2\pi)^{-1} \sum_{\alpha, \beta} L(g) \mu_{\alpha \beta}(g) d_{2}(2, g) \\
\times \left\{ [x_1 - x_1^{(2)}] + [p_{\alpha}(g) - p_{\beta}(g)] x_2^{(2)} \right\}^{-1} \\
- (2\pi)^{-1} \sum_{\alpha, \beta} L(g) \mu_{\alpha \beta}(g, h) \mu_{\alpha \beta}(g) d_{\alpha \beta}(2, g) \\
\times \left\{ [x_1 - x_1^{(2)}] + [p_{\alpha}(g) x_2^{(1)} - p_{\beta}(g) x_2^{(2)}] \right\}^{-1}.
\]

If dislocation 1 is created in the presence of both the boundary and the other dislocation it is possible to calculate the contribution of their interaction to the total energy of 1. The resultant interaction force experienced by this dislocation may then be found from the gradient of this interaction energy at the centre of the dislocation core. The total energy of 1 per unit length may be calculated by the integral

\[
V(1) = \int_{R+X_1^{(1)}}^{x_1^{(1)}} dx_1 \int_{0}^{b_1^{(1)}} \sigma_{12}^{(1)} |_{x_2 = x_2^{(1)}} db_1^{(1)} (5.43)
\]

where in this case \( \sigma_{12}^{(1)} = \sigma_{12}^{(1)} + \sigma_{12}^{(2)} \) as given in (5.42), and
R and \( r_0 \) are the conventional outer and inner radii of the dislocation. The force experienced by the dislocation due to this interaction has components perpendicular and parallel to the interface given by

\[
F_\perp(1) = -aV(1)/aX_2(1), \quad F_\parallel(1) = -aV(1)/aX_1(1) \quad (5.44)
\]

respectively. Using the notation

\[
\begin{align*}
    r_1 &= \left[ (X_1(1)-X_1(2))^2 + (X_2(1)-X_2(2))^2 \right]^{1/2}, \\
    r_2 &= \left[ (X_1(1)+X_1(2))^2 + (X_2(1)+X_2(2))^2 \right]^{1/2}, \\
    r_3 &= 2X_2(1), \\
    \psi &= \arctan\left[ \frac{X_2(1)-X_2(2)}{X_1(1)-X_1(2)} \right] \left[ \frac{X_1(1)-X_1(2)}{X_2(1)-X_2(2)} \right]^{-1}, \\
    \phi &= \arctan\left[ \frac{X_2(1)+X_2(2)}{X_1(1)-X_1(2)} \right] \left[ \frac{X_1(1)-X_1(2)}{X_2(1)+X_2(2)} \right]^{-1},
\end{align*}
\]

the components \( F_\perp(1) \) and \( F_\parallel(1) \) may be written in the following form:

\[
\begin{align*}
F_\perp(1) &= (2\pi r_1)^{-1}b_i(1)d_j(2,g) \Sigma L_i(g)(g) \left[ \mu(\alpha)(\Psi) \right]^{-1}M_{ij}(g) \\
&\quad - (2\pi r_2)^{-1}b_i(1)d_j(2,g) \Sigma L_i(g)(g) \left[ \mu(\alpha)(\phi)(1-\epsilon_{\alpha\beta}) \right]^{-1} \\
&\quad \times M_{\alpha k}k_{k\ell}k_{\ell\beta}M_{ij}(g) \\
&\quad - (2\pi r_3)^{-1}b_i(1)k_{ij}(g,h)d_j(1,g) \quad (5.46)
\end{align*}
\]

and

\[
\begin{align*}
F_\parallel(1) &= (2\pi r_1)^{-1}b_i(1)d_j(2,g) \Sigma L_i(g)(g) \left[ \mu(\alpha)(\Psi) \right]^{-1}M_{ij}(g) \\
&\quad - (2\pi r_2)^{-1}b_i(1)d_j(2,g) \Sigma L_i(g)(g) \left[ \mu(\alpha)(\phi)(1-\epsilon_{\alpha\beta}) \right]^{-1} \\
&\quad \times M_{\alpha k}k_{k\ell}k_{\ell\beta}M_{ij}(g) \\
&\quad - (2\pi r_3)^{-1}b_i(1)k_{ij}(g,h)d_j(1,g) \quad (5.47)
\end{align*}
\]

where \( k_{ij}(g,h) \) is a function of the dislocation interface and \( g \) are the relevant parameters.
where \( e_{\alpha\beta} = [p_{\alpha} + \nabla_{\beta}] x_{\alpha}^{(2)} [\phi_{\alpha}(\phi), r_{2}]^{-1} \).

It is instructive to compare these expressions with those in (5.39) and (5.40) for the components of the interaction force between two parallel dislocations in the absence of any boundary. The first terms in (5.46) and (5.47) are identical in form to \( F_{2}^{(1)} \) and \( F_{1}^{(1)} \) respectively, and obviously represent the dislocation-dislocation interaction in the present example. The functions \( c_{\alpha\beta} \), which are zero for isotropic materials, are small compared to unity in all but the very anisotropic materials. If to a first approximation they are neglected, the second terms in \( F_{2}^{(1)} \) and \( F_{1}^{(1)} \) reduce to the form of \( F_{2}^{(1)} \) and \( F_{1}^{(1)} \) for the interaction between dislocation 1 and a dislocation positioned at \( (x_{1}^{(2)}, -x_{2}^{(2)}) \) in an infinite homogeneous medium of material \( g \), with Burgers vector components \( b_{i}^{(2')} = \chi_{i}^{(g, h)} b_{j}^{(2')}, \) where

\[
\chi_{i}^{(g, h)} = \Re \left[ H_{ik}^{(g, h)} K_{k\ell}^{(g, h)} G_{\ell\jmath}^{(g, h)} \right].
\]

The third term in (5.46) has exactly the form of \( F_{2}^{(1)} \) for the case when \( \Psi = \pi/2 \), representing the radial component of the interaction force between 1 and a dislocation at \( (x_{1}^{(1)}, -x_{2}^{(1)}) \), again in an infinite homogeneous medium of material \( g \), but having Burgers vector components \( b_{i}^{(1')} = \chi_{i}^{(g, h)} b_{j}^{(1')} \). However, such a dislocation configuration would interact with a tangential component

\[
- (2\pi r_{2})^{-1} b_{i}^{(1')} k_{i\jmath}^{(g, h)} d_{i\jmath}^{(1, g)} \Sigma_{\alpha\jmath}^{(g, h)} p_{\alpha}^{(g)} - l_{\alpha\jmath}^{(g)}
\]

which is absent from equation (5.47). In view of these analogies it is possible to represent approximately the
interactions of two parallel dislocations with a plane boundary by a system of image dislocations in an infinite homogeneous medium, as shown schematically in Figure 5.1.

When the boundary is a free surface, the image dislocations have Burgers vectors \( \mathbf{b}(1) \) and \( \mathbf{b}(2) \), equal in magnitude and antiparallel to the Burgers vectors of the corresponding dislocations 1 and 2. In the other cases the image dislocations have Burgers vectors with components of the form

\[
- \mathbf{b}_i + \text{Re} \{ H_{12}^{(g,g)} H_{22}^{(g,h)} - H_{2k}^{(g,g)} H_{kj}^{(g,g)} \} \mathbf{b}_j
\]

for the slipping boundary, and

\[
- \text{Re} \{ H_{ik}^{(g,g)} H_{kj}^{(g,h)} G_{ij}^{(g,g)} \} \mathbf{b}_j
\]

for the welded boundary, which are smaller in magnitude than for the free surface, and except in the limiting isotropic case have in general orientations different from those of the actual dislocations.

5.5.3 Two Dislocations Separated by a Plane Boundary

If the dislocations are situated on either side of the plane boundary, for instance if 1 and 2 are in media \( g \) and \( h \) respectively, the notation used in the previous example may be employed here. In this case however the stress acting on the plane \( x_2 = x_2^{(1)} \) is, from (5.34) and (5.38),
\[ \sigma_{12}^{(1)} = (2\pi r_1)^{-1} d_{ij}^{(2,1)} [x_i - x_j^{(1)}]^{-1} \]

\[ - (2\pi r_1)^{-1} \sum_{\alpha, \beta} L_{\alpha \beta}^{(g)} M_{\alpha \beta}^{(g)} [k_{\alpha \beta}^{(g)} x_{i j}^{(1)}]^{-1} \]

Using this expression for \( \sigma_{12}^{(1)} \) in the integral (5.43) and taking the gradients of the resulting expression as in (5.44), the components of the resulting expression for the interaction force on dislocation 1 due to the presence of the boundary and the other dislocation may be written

\[ F_{1 \parallel}^{(1)} = (2\pi r_1)^{-1} b_i^{(1)} d_{i j}^{(2,1)} \sum_{\alpha, \beta} L_{\alpha \beta}^{(g)} [k_{\alpha \beta}^{(g)} (\Psi) (1 + e_{\alpha \beta}^*)]^{-1} \]

\[ \times [M_{\alpha \beta}^{(g)} k_{\alpha \beta}^{(g)} M_{\alpha \beta}^{(h)} L_{\alpha \beta}^{(h)} M_{\alpha \beta}^{(h)}] \]

\[ - (2\pi r_2)^{-1} b_i^{(1)} b_{i j}^{(g,h)} d_{i j}^{(1, g)} \] \hspace{1cm} (5.48)

and

\[ F_{1 \perp}^{(1)} = (2\pi r_1)^{-1} b_i^{(1)} d_{i j}^{(2,1)} \sum_{\alpha, \beta} L_{\alpha \beta}^{(g)} [k_{\alpha \beta}^{(g)} (\Psi) (1 + e_{\alpha \beta}^*)]^{-1} \]

\[ \times [M_{\alpha \beta}^{(g)} k_{\alpha \beta}^{(g)} M_{\alpha \beta}^{(h)} L_{\alpha \beta}^{(h)} M_{\alpha \beta}^{(h)}] \] \hspace{1cm} (5.49)

Here the notation introduced in (5.45) has been employed and

\[ e_{\alpha \beta}^* = [p_{\alpha}^{(g)} - p_{\beta}^{(h)}] x_2^{(2)} [r_1 k_{\alpha \beta}^{(g)} (\Psi)]^{-1}. \]

The second term in (5.48) is identical to the third term in the expression for \( F_{1 \parallel}^{(1)} \) in the previous example, and so an identical image representation may be used. However, if the term \( e_{\alpha \beta}^* \), which is zero in isotropic materials, is neglected in the first terms of (5.48) and (5.49), the
resulting expressions have the form of (5.39) and (5.40) for the interaction of dislocation 1 with a second dislocation at \((x_1^{(2)}, x_2^{(2)})\) whose Burgers vector has components

\[ b_{i}'^{(2)} = b_{i}^{(2)} - \sum_{j} \kappa_{ij} b_{j}^{(2)}. \]  

(5.50)

Consequently the interaction in this case may be represented approximately by the system of dislocations shown in Figure 5.2 in an infinite homogeneous medium. It is interesting to note that dislocation 1 sees 2 in the same position, but with an apparent Burgers vector modified as in (5.50).

5.6 Related Groups of Interfaces

5.6.1 Extension of the General Theory

The analysis of Section 5.4, which is applicable to arbitrary stress distributions provided these are invariant in the Ox^-direction, has been restricted to the specific interface \(x_2 = 0\). Thus in applications of this theory the orientation of the boundary determines the system of axes to be used, to which all stress and strain components must be referred. Often however this will not be the most convenient choice of axes for describing a given stress field. The purpose of this section is to generalise the foregoing theory so that in each half-space a system of axes Ox_1 may be chosen referred to which the interface is a plane of the form \(x_2 \cos \theta - x_1 \sin \theta = 0\), where \(\theta\) is defined as in Figure 5.3. This modified presentation allows complete freedom of choice of axes without significantly complicating the analysis.
By rationalising the complex variable

\[ x_\alpha = z_\alpha \left[ f_\alpha(\Theta) \right]^{-1} = z_\alpha \left[ \cos \Theta + p_\alpha \sin \Theta \right]^{-1} \]

it is clear that to all points for which \( x_\alpha \cos \Theta > x_\alpha \sin \Theta \) on any plane \( x_3 = \) constant there corresponds a point on each half-plane \( \text{Im}(x_\alpha) > 0 \). Consider the function \( f_\alpha(x_\alpha) \) defined by

\[ f_\alpha(x_\alpha) = f_\alpha(z_\alpha) \]

in terms of which the stresses \( \sigma_{ij} \) and displacements \( u_i \) may be written

\[ \sigma_{il} = -\sum_{\alpha} L_{i\alpha} p_\alpha a_{ij} / a_{ij}(x_\alpha), \quad \sigma_{l2} = \sum_{\alpha} L_{i\alpha} a_{ij} / a_{ij}(x_\alpha) \]

and

\[ u_k = \sum_{\alpha} f_{i\alpha k} / f_{i\alpha}(x_\alpha). \]

Let \( \sigma_{ij} \) and \( v_i \) be the stress and displacement components referred to a new set of axes \( Oy_i \), obtained from \( Ox_i \) by a rotation of \( \Theta \) about \( Ox_3 \). Then

\[ \sigma_{i2} = \sum_{\alpha} L_{i\alpha} / a_{ij}(x_\alpha) \]

\[ v_i = \sum_{\alpha} f_{i\alpha} / f_{i\alpha}(x_\alpha) \]

where

\[ L_{i\alpha} = a_{ij} L_{j\alpha}, \quad f_{i\alpha} = a_{ij} f_{j\alpha} \]

and

\[ a_{ij} = \begin{pmatrix} \cos \Theta & \sin \Theta & 0 \\ -\sin \Theta & \cos \Theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \]

is the rotation matrix relating the two sets of axes.
Written in this form the problem is now identical to that discussed in Section 5.4, but in \( x \)-space rather than in \( z \)-space. Suppose that \( \Theta \) has the values \( \Theta(I) \) and \( \Theta(II) \) in media I and II, which therefore occupy half-spaces
\[ [x_2 \cos \Theta(I) - x_1 \sin \Theta(I)] > 0 \quad \text{and} \quad [x_2 \cos \Theta(II) - x_1 \sin \Theta(II)] < 0 \]
respectively, and that functions of \( \Theta \) bearing surfaces \( (I) \) and \( (II) \) are evaluated at the appropriate values of \( \Theta \).

Adopting the notation
\[ \begin{align*}
  \varphi = I, \ h = II & \quad \text{when} \ x_2 \cos \Theta(I) > x_1 \sin \Theta(I) \\
  \varphi = II, \ h = I & \quad \text{when} \ x_2 \cos \Theta(II) < x_1 \sin \Theta(II)
\end{align*} \]

it is possible to write down the solutions \( f^{(g)} ((\varphi) \Theta) \)
\[ = \sum_{\alpha} f^{(\alpha)} (z_{\alpha}) \] in the form
\[ f^{(\varphi)} (z_{\alpha}) = f^{(\alpha)} (z_{\alpha}) \]

\[ - \sum_{\alpha} \mathcal{M}^{(\varphi)}_{\alpha i} \mathcal{H}^{(\alpha)}_{ij} \mathcal{L}^{(\varphi)}_{jk} \mathcal{L}^{(\alpha)}_{k\beta} \left[ \frac{z_{\alpha}}{\alpha} \right] \left( \frac{z_{\alpha}}{\beta} \right) \left( \frac{z_{\alpha}}{\alpha} \right)^{-1} \]

\[ + \sum_{\beta} \mathcal{M}^{(\varphi)}_{\alpha i} \left[ \delta_{ij} - \mathcal{H}^{(\alpha)}_{ij} \mathcal{L}^{(\alpha)}_{ij} \right] \mathcal{L}^{(\beta)} \left[ \frac{z_{\beta}}{\beta} \right] \left( \frac{z_{\beta}}{\beta} \right)^{-1} \]

\[ \times f^{(\beta)} \left( \frac{z_{\beta}}{\beta} \right) \]

\[ (5.51) \]

where
\[ \mathcal{M}^{(\varphi)}_{\alpha i} = \mathcal{M}^{(\varphi)}_{\alpha j} a_{ij}. \]

Defining the constants
\[ \mathcal{J}_{ij}^{(\varphi, \alpha)} = \frac{1}{2} \left[ a_{ik} \mathcal{W}_{k\ell} a_{j\ell} - a_{ik} \mathcal{W}_{k\ell} a_{j\ell} \right] \]
and \[ \mathcal{K}_{ij}^{(g,h)} = \left[ \mathcal{G}_{ij}^{(g,h)} \right]^{-1} \]
\[ = \frac{i}{\pi} \left[ \mathcal{a}_{ik} \mathcal{W}_{kl} \mathcal{a}_{jk}^{*} - \mathcal{a}_{ik} \mathcal{W}_{kl} \mathcal{a}_{jk}^{*} \right], \]
the generalised matrix \[ \mathcal{K}_{ij}^{(g,h)} \] may be written as
\[ \mathcal{K}_{ij}^{(g,h)} = \delta_{ij} \]
for the free surface,
\[ \mathcal{K}_{ij}^{(g,h)} = \delta_{ij} - \delta_{i2} \left[ \mathcal{K}_{22}^{(g,h)} \right]^{-1} \mathcal{K}_{2j}^{(g,h)} \]
for the freely-slipping interface, and
\[ \mathcal{K}_{ij}^{(g,h)} = \mathcal{G}_{ik}^{(g,h)} \mathcal{G}_{kj}^{(g,h)} \]
for the welded interface.

In the case of the slipping and welded interfaces equation (5.51) relates the solution to the generalised boundary-value problem in any one composite material to that in another which has identical anisotropic elastic properties except that in each half-space the material has been rotated about the axis \( Ox_3 \), as shown schematically in Figure 5.4. This expression is of great importance in applications of the theory as it both extends the usefulness of a given analytical solution and also often reduces the amount of computation necessary in numerical treatments.
5.6.2 A Simple Application

To illustrate the use of this analysis consider the interaction of a single dislocation in medium \( \varrho \) with the plane boundary. If the dislocation is positioned at \( b_i (x_1, x_2) \) with Burgers vector components \( \mathbf{b}_i \) it gives rise to a stress field along the plane \( x_2 = x_2 \) with components

\[
\sigma_{12} = (2\pi)^{-1} d_i^j (x_1 - x_1)^{-1}
\]

\[
- (2\pi)^{-1} \sum_{\alpha, \beta} L_{i\alpha} M_{\beta j} K_{jk} \bar{m}_\beta (g, \mathbf{h}) \mathcal{L} (g) (g) (g) (g)
\]

\[
x \left[ (x_1 + \mathbf{p}_\alpha x_2) \mathbf{P}_\beta (\mathbf{r}) (\mathbf{r}) (g)^{-1} - \mathbf{P}_\beta (g) \right]^{-1}
\]

using (5.8), (5.38) and (5.51). The part of the energy of the dislocation due to the proximity of the boundary, obtained by substituting the second term of (5.52) into integral (5.43), may be written

\[
\Delta V = - (4\pi)^{-1} \sum_{\alpha, \beta} b_i \mathbf{L}_{i\alpha} M_{\beta j} K_{jk} \bar{m}_\beta (g, \mathbf{h}) \mathcal{L} (g) (g) (g)
\]

\[
x \ln \left[ \frac{r_{\beta} (g) + (\mathbf{p}_\alpha - \mathbf{P}_\beta) Y_2}{r_{\beta} (g) + (\mathbf{p}_\alpha - \mathbf{P}_\beta) Y_2} \right]
\]

where

\[
Y_1 = a_{ij} x_j.
\]

The force acting normal to the interface may be obtained by taking the gradient

\[
F = - \frac{\partial (\Delta V)}{\partial Y_2} = - (4\pi Y_2)^{-1} b_i \mathbf{L}_{i\alpha} K_{jk} \bar{m}_\beta (g, \mathbf{h}) \mathcal{L} (g) (g).
\]

(5.53)
When \( \phi^{(\rho)} = \phi^{(\kappa)} \), equation (5.53) reduces to
\[
F_{\perp} = - (4\pi Y_2)^{-1} b_i K_{ij} \phi^{(\rho)} \phi^{(\kappa)}
\]
for each of the three kinds of interface, which is identical in form to the interaction of a single dislocation with the interface \( x_2 = 0 \), obtained by placing \( b^{(2)} = 0 \) in either (5.46) or (5.48). The physical significance of this result, which remains true for arbitrary distributions of dislocations, is that the magnitude of the image force on a dislocation near to a plane boundary is a function only of the separation of the dislocation and boundary, and of the elastic constants of the component half-spaces. It is independent of the orientation of the boundary plane about the dislocation line, this orientation affecting only the direction in which the force acts.

5.7 Discussion

A variety of boundary-value problems associated with elastically anisotropic half-spaces have been solved for the most general distributions of stress provided that these are invariant in one direction parallel to the boundary, and vanish at infinity in all other directions. To illustrate their application these solutions have been used to investigate the interactions of pairs of dislocations with free surfaces, and welded and freely-slipping interfaces between elastically different half-spaces. It has been shown that these interactions may be represented approxi-
The interactions are of particular importance in anisotropic crystalline materials for which the welded and freely-slippering interfaces serve as idealised models of grain boundaries at low and high temperatures respectively. A dislocation parallel to a nearby grain boundary experiences a force acting normally to, and inversely proportional to its separation from, the boundary. The magnitude of this force is also a function of the misorientation between component grains, but is independent of the boundary orientation. Examples of these interactions in metals with the hexagonal close packed crystal structure are discussed in Section 7.1. As pointed out in Section 1.4 the present analysis using anisotropic elasticity theory is essential to a detailed study of the Hall-Petch relation, especially in the light of the preliminary analysis of Chou and Barnett of a screw dislocation array piled-up at a grain boundary. The generalisation of their model to include more realistic problems is considered in the next chapter based on the results derived above.
Figure 5.1 The approximate representation of the interaction between a pair of dislocations 1 and 2, having Burgers vectors \( \mathbf{b}^{(1)} \) and \( \mathbf{b}^{(2)} \) respectively, when they are situated on the same side of a plane boundary \( x_2 = 0 \) in an elastically anisotropic medium. In the presence of the boundary the force on 1, which has components \( F^{(1)} \) and \( F_{||}^{(1)} \), is approximately the same as that arising from its interaction with dislocation 2 and the "image" dislocations 1' and 2', with Burgers vectors \( \mathbf{b}^{(1')} \) and \( \mathbf{b}^{(2')} \), when the boundary is absent. Expressions for the components of \( \mathbf{b}^{(1')} \) and \( \mathbf{b}^{(2')} \), as well as definitions of \( r_1 \), \( r_2 \), \( r_3 \), \( \Psi \) and \( \phi \), are given in Section 5.5.2.
Figure 5.2  The approximate representation of the interaction between a pair of dislocations 1 and 2 when they are on opposite sides of the boundary $x_2=0$, rather than on the same side as in Figure 5.1. In this case the force on 1 is approximately the same as that due to an image dislocation $l'$, of Burgers vector $\mathbf{b}^{(1')}$, and a modified dislocation $2'$, in the position of 2 but with Burgers vector $\mathbf{b}^{(2')}$, when the medium is homogeneous. Expressions for the components of $\mathbf{b}^{(2')}$ are given in Section 5.5.3, whilst all other quantities are the same as in Figure 5.1.
Figure 5.3 The relationship between the sets of axes $Ox_1$ and $Cy_1$ used in Section 5.6, which differ by a rotation of $\theta$ about the axis $Ox_2=Oy_2$. 

$$x_2 \cos \theta - x_1 \sin \theta = 0$$
Figure 5.4  Diagrams (a) and (c) represent schematically two composite media, whose solutions for the boundary-value problems are related by the analysis of Section 5.6, and whose orientations are related by the rotations $\theta(I)$ and $\theta(II)$ shown in diagram (b).
Appendix 5.1  Evaluation of Constants

It was pointed out in Section (5.4) that the solutions discussed in this chapter for the free surface, and welded and freely-slipping interfaces are expressed entirely in terms of the constants $L_{i\alpha}$, $M_{\alpha i}$ and $W_{ij}$. Therefore the most convenient method is sought of evaluating these quantities, which are all functions of the elastic constants of the material.

In the treatment of Eshelby et al.\(^\text{(63)}\) all quantities are expressed in terms of the elastic stiffnesses $c_{ijkl}$. In particular the $L_{i\alpha}$ are given by equations (5.9) using values of $p_{\alpha}$ from (5.6) and values of $A_{i\alpha}$ obtained by solving the homogeneous equations

$$[c_{ijkl} + p_{\alpha}(c_{ilk2} + c_{i2k1}) + p_{\alpha}^2 c_{i2k2}]A_{k\alpha} = 0.$$ \hfill(5.9)

The matrix elements $W_{ij}$ can only be obtained in terms of the $c_{ijkl}$ by inverting the matrix

$$V_{ij} = c_{i2j1} + c_{i2k2} \Sigma_{\alpha} A_{k\alpha} p_{\alpha} B_{\alpha j}$$

$$= - c_{ij} - c_{ilk2} \Sigma_{\alpha} A_{k\alpha} p_{\alpha}^{-1} B_{\alpha j}$$

obtained by multiplying equation (5.9) by $B_{\alpha j}$. It is clear that this treatment is more suitable for calculating the set of constants $A_{i\alpha}$, $B_{\alpha i}$ and $V_{ij}$ rather than the set $L_{i\alpha}$, $M_{\alpha i}$ and $W_{ij}$ which are required for the present work.

Stroh\(^\text{(64)}\) has derived a method of evaluating the constants $p_{\alpha}$ and $L_{i\alpha}$ in terms of the elastic compliances $s_{ijkl}$. Using the shortened suffix notation\(^\text{(70)}\) he defines a set of reduced compliances
\[ S_{MN} = s_{MN} - s_{M3} s_{N3} / s_{33} \]

in terms of which the sextic equation (5.6) may be written in the alternative form

\[ S^1 S^2 - S^3 S^4 = 0, \quad (A5.1) \]

where

\[
\begin{align*}
S^1 &= p_\alpha^4 S_{11} - 2p_\alpha^3 S_{16} + p_\alpha^2 (2S_{12} + S_{66}) - 2p_\alpha S_{26} + S_{22} \\
S^2 &= p_\alpha^2 S_{55} - 2p_\alpha S_{45} + S_{44} \\
S^3 &= p_\alpha^3 S_{15} - p_\alpha^2 (S_{14} + S_{56}) + p_\alpha (S_{25} + S_{46}) - S_{24}.
\end{align*}
\]

Also the constants \( L_{i\alpha} \) may be obtained by solving equations

\[
\begin{align*}
S^1 L_{2\alpha} - S^3 L_{3\alpha} &= 0, \\
S^2 L_{2\alpha} - S^4 L_{3\alpha} &= 0, \quad (A5.1.2) \\
L_{1\alpha} + p_\alpha L_{2\alpha} &= 0,
\end{align*}
\]

and it remains to find suitable expressions for the elements \( W_{ij} \).

The strains \( e_M \) may be written either in terms of the \( L_{i\alpha} \), using equations (5.2) and (5.8) giving

\[
e_M = S_{MN} \nu_N
\]

\[
= \sum_\alpha \left[ (p_\alpha^2 S_{M1} - p_\alpha S_{M6} + S_{M2}) L_{2\alpha} - (p_\alpha S_{M5} - S_{M4}) L_{3\alpha} \right] f_\alpha'(z_\alpha),
\]

or in terms of the \( A_{i\alpha} \) using equations (5.7) in the definition (5.3). Eliminating the \( e_M \) between these two sets of equations, and solving for \( A_{k\alpha} \), the expressions
\[ A_{1\alpha} = (p_\alpha S_{11} - p_\alpha S_{16} + S_{12})L_{2\alpha} - (p_\alpha S_{15} - S_{14})L_{3\alpha}, \]
\[ A_{2\alpha} = (p_\alpha S_{12} - S_{26} + p_\alpha S_{22})L_{2\alpha} - (S_{25} - p_\alpha S_{24})L_{3\alpha}, \]
\[ A_{3\alpha} = (p_\alpha S_{15} - p_\alpha S_{56} + S_{25})L_{2\alpha} - (p_\alpha S_{55} - S_{45})L_{3\alpha}. \]

are obtained, which are the inversions of equations (5.9).

Finally, by multiplying these equations by \( M_{\alpha j} \), and summing over \( \alpha \), the desired components \( W_{ij} \) are given in the convenient form

\[
W_{1j} = S_1(2j) - S_1(1l)p_{ij} \\
W_{2j} = -S_2(1j) + S_2(2k)q_{kj} \quad \text{(i=1,3 and k=2,3)} \]
\[ W_{3j} = S_5(2j) - S_5(1l)p_{ij} \]
\[ = -S_4(1j) + S_4(2k)q_{kj} \]

(A5.1.3)

Here the notation

\[ S_M(ij) = S_{MN} \]

has been used, where \( N \) is the reduced form of the indices \((ij)\), together with the reciprocal matrices

\[ p_{ij} = \Sigma p_\alpha p_\alpha^{-1} M_{\alpha j} \quad \text{and} \quad q_{ij} = \Sigma p_\alpha p_\alpha^{-1} M_{\alpha j}. \]

Consequently, in applying the analysis presented above it is advisable to evaluate the constants involved in terms of the elastic compliances \( s_{ijkl} \) using equations (A5.1.1), (A5.1.2) and (A5.1.3).
CHAPTER 6

Screw Dislocation Pile-Ups in
Elastically Anisotropic Two-Phase Materials

6.1 Introduction

Based on an intuitive approximation (68) for the interaction between a screw dislocation and a plane boundary in an elastically anisotropic two-phase medium Armstrong and Head (50) carried out the first study of screw dislocation pile-ups in such materials. Both phases were assumed to have cubic symmetry. The significance of their results is doubtful for several reasons. Their assumed boundary/dislocation interaction was identical in form to the isotropic results given in equations (2.11) and (2.12) except that \( \gamma \) is defined by the expression

\[
\gamma = \frac{[E^{(II)} - E^{(I)}]}{[E^{(II)} + E^{(I)}]} - 1
\]

where \( E^{(I)} \) and \( E^{(II)} \) are the anisotropic energies of the dislocation at infinity in media (I) and (II) respectively. Although this definition of \( \gamma \) is correct in some very symmetric cases, the forms of the stresses due to the dislocation are considerably in error. Moreover it may be clearly seen from the results of the last chapter that the constants \( \gamma \) are in less symmetric cases considerably different. The dislocation distribution was calculated numerically using a discrete model of a pile-up perpendicular to the plane boundary, and thus the results shed little light on the functional dependence of the distribution and resultant stress fields on the elastic properties of the component phases.
Chou and Barnett\(^{(49)}\) presented the first rigorous analysis of a pile-up of this type. They essentially combined the results of Chou for (i) the interaction of a screw dislocation with a plane boundary between two half-spaces of orthorhombic symmetry\(^{(69)}\) and (ii) the equilibrium distribution of stacked screw dislocation arrays in a homogeneous anisotropic material of orthotropic symmetry\(^{(71)}\) with Barnett's\(^{(17)}\) treatment of the single pile-up problem in an isotropic two-phase material, which was discussed in detail in Chapter 3. Using an infinite sequence of identical, equally-spaced and continuously distributed dislocation arrays on planes normal to the boundary in medium (I) they obtained analytic expressions for both the dislocation distribution function and the components of stress in the undislocated second phase (II). In particular, at points on the plane of the pile-up and a small distance \(x\) from its tip the stresses \(\sigma_{i3}^{(II)}\) (\(i=1,2\)) are of the form

\[
\sigma_{i3}^{(II)} \propto \frac{\tanh \pi \ell/h \sigma_{i3}^{(I)}}{\tanh \pi x/h \sigma_{i3}^{(II)}} \left[ \frac{\pi \ell}{h} \gamma \right]^{c}, \tag{6.1}
\]

where \(h\) is the spacing between adjacent arrays, \(\ell\) is their length and \(\sigma_{i3}^{(II)} = \left[ \sigma_{44}^{(II)}/\sigma_{55}^{(II)} \right]^{1/2}\). The constant \(c\) is related to the elastic constants by the expression \(c = \pi^{-1} \cos^{-1} \gamma\) where \(\gamma = \left[ G^{(II)} G^{(I)} \right]^{-1/2}\). From this analysis the corresponding results for a single pile-up may be obtained as the limiting case when \(h \to \infty\) in (6.1), yielding the dependency

\[
\sigma_{i3}^{(II)} \propto \left[ \frac{\sigma_{i3}^{(II)}}{\sigma_{i3}^{(I)}} \right]^{c}. \tag{6.2}
\]

The results are useful for comparing the effects of isolated dislocation pile-ups at boundaries with those due to an
infinitely broad slip band, but their applicability is limited for two reasons. Firstly they are restricted to dislocation pile-ups on planes normal to the grain boundary, whereas in practice arbitrary orientations are observed. Although very broad slip bands held-up at grain boundaries are often observed in experimental work on bicrystals \(^{(72,73)}\), these are usually inclined to the boundary at angles considerably different from \(90^\circ\) and the usefulness of the results of Chou and Barnett in making even qualitative predictions in these cases is doubtful. Secondly the symmetry requirements on each half-crystal greatly restrict the number of bicrystals to which the analysis can be applied, even for materials of high symmetry. This is illustrated in Figure 6.1 for hexagonal materials where the six types of bicrystal possessing the appropriate orthorhombic symmetry are shown. In fact only in the cases (a) is the full analysis of Chou and Barnett required, the integral equation for cases (b) and (c) being identical to that for a pile-up in an infinite homogeneous solid. Moreover, when applying the results to specific hexagonal materials most if not all of the dislocations defined in Figure 6.1 are not observed in practice.

For bicrystals of this symmetry an analysis \(^{(21)}\) has been presented recently, based on the isotropic solutions given in Chapter 3 of the present work, of an isolated screw dislocation pile-up on a plane inclined at an angle other than \(\pi/2\) to the interface. Although this treatment overcomes the first limitation discussed above it is still subject to the same symmetry requirements. For this reason, in Section 6.2, the solution is generalised to include pile-ups in bicrystals in which the dislocation lines are parallel to two-fold symmetry axes in each half-crystal. Unlike
the problem of Chou and Barnett\textsuperscript{(49)} the analysis in these cases may not be readily extended to infinite sequences of identical pile-ups.

Finally, in Section 6.3, using the results of Chapter 5 it is demonstrated that the distribution function for pile-ups normal to the boundary between two half-spaces of orthorhombic symmetry\textsuperscript{(49)} remains unchanged in form even when the undislocated half-crystal possesses no symmetry elements whatsoever. Although in this section attention is restricted to an isolated pile-up it is a straightforward task to generalise the analysis for an infinite sequence of such arrays.

6.2 Screw Dislocation Pile-Ups in Bicrystals of Two-Fold Symmetry

The symbols used in this section are illustrated in Figure 6.2. To simplify the diagram use has been made of the superscript notation \( c \) introduced in Section 5.6.1, where for instance axes \( O x^c_1 \) represent two sets of axes \( O x^c_1(I) \) and \( O x^c_1(II) \) related to \( O y_1 \) by rotations of \( \omega^c(I) \) and \( \omega^c(II) \) respectively about \( O y_3 \). The interface \( y_2 = 0 \) separates the two half-spaces (I) and (II) both of which possess a two-fold symmetry axis parallel to \( O y_3 \), and whose elastic constants are referred to axes \( O x^c_1(I) \) and \( O x^c_1(II) \) respectively. In materials of this symmetry the elastic constants \( s_{14}, s_{15}, s_{24}, s_{26}, s_{34}, s_{35}, s_{46} \) and \( s_{56} \), in the reduced suffix notation\textsuperscript{(70)}, are zero, when the sextic equation (A5.1.1) reduces to the form \( S_1(c)S_2^*(c) = 0 \). The calculation of constants defined in Chapter 5 has been considered in detail by Stroh\textsuperscript{(64)} for this special case. Throughout this section all components of stress and positions of dislocations will be
referred to axes $Ow_1$, related to $Oy_1$ by a rotation of $\Psi(g) + \omega(g)$ about $Oy_3$, and two sets of cylindrical polar coordinates $(r, \theta(g), z=w_3')$, where the angles $\theta(g)$ are defined in Figure 6.2, will be used to describe the single point $P$ at which the stress is calculated.

Consider a single screw dislocation, parallel to $Ow_3$ and of Burgers vector $b=(0,0,-b)$, situated at the point $(0,W_2)$ in the $w_1w_2$-plane. In order to simplify the expressions for the stress components in each half-space due to this dislocation it is convenient to define the following quantities:

\[
\begin{align*}
\beta_{\mu}^{(g)} &= \cos^{-1}\left[\frac{p_{32}^{(g)}}{B_{\mu}^{(g)}}\cos \mu\right], \\
\delta_{\mu}^{(g)} &= \sin^{-1}\left[\frac{p_{32}^{(g)}}{D_{\mu}^{(g)}}\sin \mu\right],
\end{align*}
\]

\[
R(I) = rB_{\theta}^{(I)}/B_{\Psi}^{(I)}, \quad R(II) = rB_{\theta}^{(II)}/B_{\Psi}^{(II)},
\]

where

\[
B_{\mu}^{(g)} = [(\sin \mu)^2 + p_{31}^{(g)} \cos \mu]^2 + p_{32}^{(g)} \cos^2 \mu,\]

\[
D_{\omega}^{(g)} = [(\cos \omega)^2 + p_{31}^{(g)} \sin \omega]^2 + p_{32}^{(g)} \sin^2 \omega,\]

\[
D_{\Psi}^{(g)} = [(\cos \Psi)^2 - p_{31}^{(g)} \sin \Psi]^2 + p_{32}^{(g)} \sin^2 \Psi,\]

and $p_{31}^{(g)}$ and $p_{32}^{(g)}$ are the real and imaginary parts respectively of the solutions

\[
p_{3}^{(g)} = p_{31}^{(g)} + ip_{32}^{(g)} = s_{45}^{(g)} + is_{44}^{(g)} s_{55}^{(g)} - s_{45}^{2},\]

(6.2)

to the sextic equation (A5.1.1) in each half-space. Then, using the analysis of Section 5.6.1, the stress components $\sigma_{13}^{(g)}$ at the point $P$ due to the dislocation at $(0,W_2)$ may be
\[ \sigma_{13}^{(I)} = \frac{G(I)b}{2\pi} \left\{ \frac{R(I)\cos(\beta(I) - \beta(I)) + W_2}{R(I)^2 - 2R(I)W_2\cos(\beta(I) + \beta(I)) + W_2^2} \right\}, \]

\[ \sigma_{23}^{(I)} = -\frac{G(I)b\Delta(I)}{2\pi R(I)^2 \left\{ \frac{R(I)\cos(\beta(I) - \beta(I)) + W_2}{R(I)^2 - 2R(I)W_2\cos(\beta(I) + \beta(I)) + W_2^2} \right\}}, \]

\[ \sigma_{13}^{(II)} = \frac{G(I)b}{2\pi (1 + \gamma)} \frac{R(II)D(II)}{R(I)D(II)} \left\{ \frac{R(II)\cos(\beta(I) - \beta(I)) + W_2\cos(\beta(I) + \beta(I))}{R(II)^2 - 2R(II)W_2\cos(\beta(I) + \beta(I)) + W_2^2} \right\}, \]

\[ \sigma_{23}^{(II)} = -\frac{G(I)b\Delta(I)}{2\pi R(I)^2 \left\{ \frac{R(II)\cos(\beta(I) - \beta(I)) + W_2\cos(\beta(I) + \beta(I))}{R(II)^2 - 2R(II)W_2\cos(\beta(I) + \beta(I)) + W_2^2} \right\}}. \]

(6.3)

In writing the stress components in this form it has been assumed that the inequality \( s_{44} s_{55} > s_{45}^2 \) holds for both materials (I) and (II), when the constants \( G(\phi) \) and \( \gamma \) may be defined as

\[ G(\phi) = \left[ s_{44}(\phi)s_{55}(\phi) - s_{45}(\phi)^2 \right]^{-1/2} \]

and

\[ \gamma = \left[ G(II) - G(I) \right] \left[ G(II) + G(I) \right]^{-1}. \]
The convenience of this notation becomes apparent in the limiting case when materials (I) and (II) are both isotropic, when \( B_{\mu}^{(I)} = D_{\mu}^{(I)} = 1 \), \( R(I) = R(II) = r \), \( G(I) \) and \( G(II) \) become the isotropic shear moduli of the media and values of \( \beta_{\mu}^{(I)} \) and \( \delta_{\mu}^{(I)} \) are obtained by replacing \( \beta \) and \( \delta \) by their subscripts, i.e. \( \beta_{\mu}^{(I)} = \delta_{\mu}^{(I)} = \mu_{\mu}^{(I)} \). The expressions (6.2) may then be compared directly with those given in (2.11) and (2.12), taking into account the different reference axes used in the two cases.

Consider now n screw dislocations of Burgers vector \( \mathbf{b} \) distributed continuously on the plane \( \omega_{1} = 0 \) in the region \( 0 < \omega_{2} < \ell \). For simplicity it will be assumed that a constant stress \( \sigma_{13}^{(I)} = \sigma^{A} = G(I)v A / 2\pi \) applied at infinity is uniform throughout the bicrystal, and that the friction stress opposing the motion of the dislocations may be represented by a constant stress \( \sigma_{13}^{(I)} = \sigma^{F} = G(I)v F / 2\pi \) acting on the dislocated region of the plane \( \omega_{1} = 0 \), where \( \sigma^{F} < \sigma^{A} \). Following the procedure outlined in Section 1.2 and using the expression for \( \sigma_{13}^{(I)} \) in (6.2) the equation of equilibrium for all the dislocations in the array may be written

\[
\int_{0}^{\ell} F(w_{2}) \left\{ \left[ w_{2} - w_{2} \right]^{-1} + \frac{\gamma}{2} \left[ w_{2} + w_{2} \right] e^{i2(\beta_{\omega}^{(I)} + \beta_{\omega}^{(I)}) - 1} \right\} \left[ \left[ w_{2} + w_{2} \right] e^{-i2(\beta_{\omega}^{(I)} + \beta_{\omega}^{(I)}) - 1} \right] \, dw_{2} + \sigma = 0
\]

where \( \sigma = \sigma^{A} - \sigma^{F} \).

The solution to the singular integral equation (6.4) may be obtained in an identical manner to that discussed in Section 3.1 for values of \( \theta^{(I)} \) and \( \omega^{(I)} \) satisfying the condition
or

\[ \tan \theta(I) = \frac{p(I)^2 [\tan p I - \tan(I)] - p(I) [p(I) - \tan(I)]\tan(p I)}{[p(I)^2 + \tan(I)\tan(p I)] + p(I)\tan(p I)} \]

where \( p \) and \( q \) are integers. If \( \alpha_i \) \((i=1,2...q)\) are the solutions of the equation

\[ \cos \alpha_i + \gamma \cos(\beta(I) + \beta(I))\alpha_i = 0 \]

in the range \( 0<\alpha_i<q \), the distribution function \( F(W_2) \) is given by equation (3.15) and the number of dislocations, \( n \), in the pile-up by (3.18). Using (6.3) with the results of Appendix 3.2 the non-zero stress components at a point \( P(r<\ell, \theta(I)) \) in half-crystal (I) due to the piled-up dislocations may be written

\[
\sigma_{13}^{(I)} \sim 2\sigma N \left\{ c_1 \cos[(1-\alpha_1)(\beta(I) - \beta(I))] + \gamma \cos[(1-\alpha_1)(\beta(I) - \beta(I)) - \alpha_1(2\beta(I) + \delta(I)\pm\pi)]\right\} \frac{\ell}{R(I)} \]

\[
+ c_2 \{ 1 - \gamma \cos(\beta(I) + \delta(I)) \}, \tag{6.5}
\]

and

\[
\sigma_{23}^{(I)} \sim 2\sigma N \frac{D(I)}{B(I)} \left\{ c_1 \sin[(1-\alpha_1)(\beta(I) - \beta(I)) + (\beta(I) - \delta(I))] + \gamma \sin[(1-\alpha_1)(\beta(I) - \delta(I)) - \alpha_1(\beta(I) + \delta(I) + \delta(I))]\right\} \frac{\ell}{R(I)} \]

\[
\times \left\{ 1 - \gamma \sin(\beta(I) - \delta(I)) + \gamma \sin(\beta(I) + \delta(I) + \delta(I)) \right\}, \tag{6.6}
\]

where \( 0<(\beta(I) - \beta(I))<2\pi, 0<(\beta(I) - \delta(I))<2\pi \), and positive and negative signs should be taken when

(a) \( 0<(\beta(I) - \beta(I))<\pi \) and \( \pi<(\beta(I) - \beta(I))<2\pi \) respectively in

(6.5)
(b) \(0 < \beta_\theta^{(I)} - \delta_\psi^{(I)} < \pi\) and \(\pi < \beta_\theta^{(I)} - \delta_\psi^{(I)} < 2\pi\) respectively in (6.6).

The constants \(N\), \(C_1\) and \(C_2\) are defined by equations (3.14), (3.21) and (3.22) respectively. Similarly in medium (II) at the point \(P(r < \ell, \theta^{(II)})\)

\[
\sigma_{13}^{(II)} P \sim 2\sigma N(1+\gamma) \frac{B_{\psi^{(II)}} D_{\psi^{(II)}}^{(I)}}{B_{\psi^{(II)}} D_{\psi^{(II)}}^{(II)}}
\]

\[
x \left[ \cos[(1-\alpha_1)(\beta_\theta^{(II)} - \delta_\psi^{(II)} - \pi) + \alpha_1(\beta_\alpha^{(II)} + \delta_\psi^{(II)} + \delta_\omega^{(II)})] \right]
\]

\[
x [\ell/R^{(II)}]^{1-\alpha_1}
\]

\[
- C_2 \cos(\beta_\theta^{(II)} + \delta_\omega^{(II)} - \delta_\psi^{(II)})
\]

and

\[
\sigma_{23}^{(II)} P \sim -2\sigma N(1+\gamma) \frac{B_{\psi^{(II)}} D_{\psi^{(II)}}^{(I)}}{B_{\psi^{(II)}} D_{\psi^{(II)}}^{(II)}}
\]

\[
x \left[ \sin[(1-\alpha_1)(\beta_\theta^{(II)} - \delta_\psi^{(II)} - \pi) + \alpha_1(\beta_\alpha^{(II)} + \delta_\psi^{(II)} + \delta_\omega^{(II)})] \right]
\]

\[
x [\ell/R^{(II)}]^{1-\alpha_1}
\]

\[
- C_2 \sin(\beta_\theta^{(II)} + \delta_\omega^{(II)} - \delta_\psi^{(II)})
\]

where \(0 < (\beta_\theta^{(II)} - \beta_\psi^{(II)}) < 2\pi\) and \(0 < (\beta_\theta^{(II)} - \delta_\psi^{(II)}) < 2\pi\alpha\)

6.3 **Screw Dislocation File-Ups against a Second Phase of General Anisotropy**

As explained in Section 6.1 the following analysis is a generalisation of the problem treated by Chou and Barnett(49). Consider an infinite solid consisting of two half-spaces (I) and (II), of orthorhombic and triclinic symmetries respectively referred to the same set of axes \(Ox_1\), and welded together along the boundary \(x_2 = 0\). The
situation is illustrated in Figure 6.3. In reduced notation the off-diagonal elements of the elastic compliance matrix $s_{ij}$ are all zero except for $s_{12}$, $s_{13}$ and $s_{23}$ in medium (I) and are all non-zero in medium (II), whilst the diagonal elements are non-zero and independent in both media.

To calculate the stress field components at a point $P(r, \theta, z)$ due to a right-hand screw dislocation parallel to $Ox_3$ in medium (I) it is again convenient to introduce a notation similar to that used on the previous section, namely

$$\beta_{\alpha}(g) = \cos^{-1}\left[\frac{p_{\alpha}(g)}{B_{\alpha}(g)} \cos \theta\right],$$

$$R_{\alpha}(g) = r B_{\alpha}(g) P(I)^{-1},$$

where

$$B_{\alpha}(g) = \left[(\sin \theta + p_{\alpha}(g) \cos \theta)^2 + p_{\alpha}(g) \cos^2 \theta\right]^{1/2},$$

and

$$p_{\alpha}(g) = p_{\alpha 1} + i p_{\alpha 2} \quad (p_{\alpha 1}, p_{\alpha 2} \text{ real})$$

are the solutions to the sextic equation (A5.1.1) in medium (g). By further defining the constants

$$\lambda_i(\alpha) = \lambda_{i1}(\alpha) + i \lambda_{i2}(\alpha) = \left. L_{i\alpha}^II (II) M_{\alpha j}^II \delta_{jj} \right. [K(I, II)]$$

$$\times [s_{44}(I)/s_{55}(I)]^{-1/2},$$

$$\nu_i(\alpha) = \nu_{i1}(\alpha) + i \nu_{i2}(\alpha) = \left. L_{i\alpha}^II M_{\alpha j}^II \delta_{jj} \right. [K(I, II)]$$

$$\times [s_{44}(I)/s_{55}(I)]^{-1/2}$$

and

$$\gamma = \gamma_1 + i \gamma_2 = - K_{33}^{(I, II)} \quad (i=1, 2, 3)$$

where $\lambda_{i1}, \lambda_{i2}, \nu_{i1}, \nu_{i2}, \gamma_1$ and $\gamma_2$ are all real, $K_{ij}^{(I, II)}$
and \( L_{i\alpha}^{(g)} \) are defined in (5.37) and (5.9) respectively, 
\( M_{\alpha i}^{(g)} \) is the matrix reciprocal to \( L_{i\alpha}^{(g)} \) and \( \delta_{ij} \) is the Kronecker delta, then from (5.34) the non-zero components of stress due to the single dislocation at \((0, X_2)\) may be written

\[
\sigma_{13}^{(I)} = G(I) b \left[ \frac{R_3^{(I)} \cos \theta_3}{2\pi} \right] \frac{R_3^{(I)} \cos \theta_3 - X_2}{R_3^{(I)} + X_2^2} X_2 - \frac{1}{2} R_3^{(I)} X_2 \cos \theta_3 + X_2^2 + \frac{y_2 R_3^{(I)} \sin \theta_3}{R_3^{(I)} + X_2^2} \right], \quad (6.9)
\]

\[
\sigma_{23}^{(I)} = -G(I) b \left[ \frac{R_3^{(I)} \sin \theta_3}{2\pi} \right] \frac{R_3^{(I)} \sin \theta_3}{R_3^{(I)} + X_2^2} X_2 - \frac{1}{2} R_3^{(I)} X_2 \cos \theta_3 + X_2^2 + \frac{y_2 R_3^{(I)} \sin \theta_3}{R_3^{(I)} + X_2^2} \right] \quad (6.10)
\]

and

\[
\sigma_{11}^{(II)} = G(I) b \sum_{\alpha} \lambda_{11}(\alpha) R_\alpha^{(II)} \sin \theta_\alpha^{(II)} + \lambda_{12}(\alpha) R_\alpha^{(II)} \cos \theta_\alpha^{(II)} - X_2^2 \frac{R_\alpha^{(II)} - 2 R_\alpha^{(II)} X_2 \cos \theta_\alpha^{(II)} + X_2^2}{R_\alpha^{(II)} + X_2^2} \right], \quad (6.11)
\]

\[
\sigma_{12}^{(II)} = G(I) b \sum_{\alpha} \nu_{11}(\alpha) R_\alpha^{(II)} \sin \theta_\alpha^{(II)} + \nu_{12}(\alpha) R_\alpha^{(II)} \cos \theta_\alpha^{(II)} - X_2^2 \frac{R_\alpha^{(II)} - 2 R_\alpha^{(II)} X_2 \cos \theta_\alpha^{(II)} + X_2^2}{R_\alpha^{(II)} + X_2^2} \right]. \quad (6.12)
\]

Here \( G(I) = [\begin{array}{cc} s_{44}^{(I)} & s_{55}^{(I)} \end{array}]^{-1/2} \) and \( b \) is the magnitude of the Burgers vector. The component \( \sigma_{23}^{(II)} \) excluded from (6.11) and (6.12) must be obtained as described in Section 5.2.

As in the previous section it will be assumed that
a constant stress \( \sigma_{13}^{(I)} = \sigma^A = G(I)b c^A/2\pi \) applied at infinity
acts uniformly throughout medium (I), and that dislocations moving in the plane \( x_1 = 0 \) experience a constant frictional stress \( \sigma_{13}^{(I)} = -\sigma^F = -G^{(I)}bc^F/2\pi \) opposing their motion, both stresses being referred to axes Ox_1. Using the continuous distribution approximation the equilibrium condition for an array of right-hand screw dislocations within the interval \( 0 \leq x_2 \leq \ell \) on the plane \( x_1 = 0 \) may be written in terms of their distribution function \( F(x_2) \) using equation (6.9) as

\[
\int_0^\ell F(x_2) \left[ (x_2-x_2)^{-1} + \frac{1}{2}(x_2+x_2)^{-1} \right] dx_2 + \mathcal{C} = 0
\]

where \( \mathcal{C} = \mathcal{C}^A - \mathcal{C}^F \). This equation is identical in form to that solved by Barnett (17) and treated as a special case in Chapter 3 of the present work. The distribution function may thus be written

\[
F(x_2) = \frac{\mathcal{C}}{\pi \sin \pi x_2} \sinh[c \cosh^{-1}(\ell/x_2)] \quad (6.13)
\]

where \( c = n^{-1} \cos^{-1} \gamma_1 \), whilst the number of dislocations, \( n \), in the pile-up is given by the expression

\[
n/\ell = \frac{\mathcal{C}c}{(1-\gamma_1^2)^{1/2}}. \quad (6.14)
\]

Expanding (6.13) as a power series, the results of Appendix 3.2 may be used to obtain approximate expressions for the stress components due to the pile-up at points \( P(r \ll \ell, \theta, z) \) near to its tip. In medium (I) the non-zero stress components are
\[
\sigma_{13}^I \sim \frac{c}{2\sin\alpha\sin\gamma/2} \left\{ \cos[c(\beta_{\Theta_3} - \pi)] - \gamma_1 \cos[c(\beta_{\Theta_3} - \pi \pm \pi)] 
+ \gamma_2 \sin[c(\beta_{\Theta_3} - \pi \pm \pi)] \right\} [2\ell/R_{\alpha}^I]^\circ -2(1+\gamma_1)\cos\gamma/2 ,
\]
(6.15)

and
\[
\sigma_{23}^I \sim \frac{c}{2\sin\alpha\sin\gamma/2} \left\{ \sin[c(\beta_{\Theta_3} - \pi)] - \gamma_1 \sin[c(\beta_{\Theta_3} - \pi \pm \pi)] 
- \gamma_2 \cos[c(\beta_{\Theta_3} - \pi \pm \pi)] \right\} [2\ell/R_{\alpha}^I]^\circ -2\gamma_2\cos\gamma/2 ,
\]
(6.16)

where \(0 \leq \Theta \leq 2\pi\) and positive and negative signs are to be taken in regions \(0 < \Theta < \pi\) and \(\pi < \Theta < 2\pi\) respectively. Similarly in medium (II)

\[
\sigma_{11}^{II} \sim \frac{c}{2\sin\alpha\sin\gamma/2} \sum_{\alpha} \left\{ \lambda_{11}(\alpha)\sin[c(\beta_{\Theta_\alpha} - \pi)] 
+ \lambda_{12}(\alpha)\cos[c(\beta_{\Theta_\alpha} - \pi)] \right\} [2\ell/R_{\alpha}^{II}]^\circ -2\lambda_{12}(\alpha)\cos\gamma/2 ,
\]
(6.17)

and
\[
\sigma_{22}^{II} \sim \frac{c}{2\sin\alpha\sin\gamma/2} \sum_{\alpha} \left\{ \nu_{11}(\alpha)\sin[c(\beta_{\Theta_\alpha} - \pi)] 
+ \nu_{12}(\alpha)\cos[c(\beta_{\Theta_\alpha} - \pi)] \right\} [2\ell/R_{\alpha}^{II}]^\circ -2\nu_{12}(\alpha)\cos\gamma/2 .
\]
(6.18)

When the second half-crystal also has orthorhombic symmetry relative to the axes Ox, which is the case considered by Chou and Barnett (49) the distribution function \(F(x_2)\) and the number of dislocations, \(n\), are still given by equations (6.13) and (6.14), in which the constant \(\gamma\) has the simple form

\[
\gamma = \left[ G^{II} - G^{I} \right] \left[ G^{II} + G^{I} \right]^{-1}
\]

where
\[
G(g) = [g_{44}^I g_{55}^I]^{-1/2} .
\]
Similarly the stress components in medium (I) are given by (6.15) and (6.16) in which, since $\gamma$ is real, $\gamma_2 = 0$. The greatest simplification occurs however in the expressions for the stress components in medium (II), where, using equations (6.17) and (6.18), they become

$$
\sigma_{13}^{(II)} \sim \frac{\gamma(1+\gamma)}{2 \sin \gamma \sin \gamma/2} \frac{p_{32}^{(II)}}{p_{32}^{(I)}} \left\{ \frac{\cos[c(\beta_{3}^{(II)} - \pi)] [2 \ell p_{32}^{(I)}/r]^c}{[\sin^2 \theta + p_{32}^{(II)}]^{c/2} \cos^2 \theta]^{c/2}} - 2 \cos \gamma/2 \right\} \quad (6.19)
$$

and

$$
\sigma_{23}^{(II)} \sim \frac{-\gamma(1+\gamma)}{2 \sin \gamma \sin \gamma/2} \frac{1}{p_{32}^{(I)}} \frac{\sin[c(\beta_{3}^{(II)} - \pi)] [2 \ell p_{32}^{(II)}/r]^c}{[\sin^2 \theta + p_{32}^{(II)}]^{c/2} \cos^2 \theta]^{c/2}} \ . \quad (6.20)
$$

The constants $p_{32}^{(g)}$ are given by the expressions

$$
p_{32}^{(g)} = \left[ s_{44}^{(g)}/s_{55}^{(g)} \right]^{1/2} .
$$

When $\theta = \pi$ (6.19) and (6.20) reduce to the results of Chou and Barnett\(^{(49)}\).

6.4 Summary

As discussed in Section 6.1 the existing model of a screw dislocation pile-up in an anisotropic bicrystal due to Chou and Barnett\(^{(49)}\) is of very limited application since it requires that the component half-spaces have orthorhombic symmetry. In Section 6.2 this model is generalised, using the analysis of Chapters 3 and 5 to include dislocation pile-ups inclined at angles other than $\pi/2$ to the plane interface between half-spaces having at least two-fold symmetry in the direction of the dislocation lines. For a pile-up perpendicular to the boundary the model is gener-
alised still further in Section 6.3 to include an array in a material of orthorhombic symmetry blocked at the interface with a half-crystal of triclinic symmetry. Thus the present analysis is of far wider application to real materials than that presented by Chou and Barnett.
Figure 6.1  Schematic illustration of the six cases of bicrystals formed from materials with hexagonal crystal structure which satisfy the symmetry requirements in the analysis of Chou and Barnett (49). Basal planes are indicated by the hexagons and all orientations of the \( \mathbf{a} \)-vectors in these planes are permissible. The piled-up screw dislocations may be on either side of the boundary ABCD with Burgers vectors \( \mathbf{b} \) as shown. No account is taken of the further restrictions due to the observed deformation modes of the materials comprising the bicrystals. The significance of the classification "non-degenerate", "semi-degenerate" and "degenerate" is discussed in Section 6.1.
(a) **Non-degenerate**, \( \gamma \neq 0 \), \( p_3^{(I)} \neq p_3^{(II)} \)

![Diagram](image)

(b) **Semi-degenerate**, \( \gamma = 0 \), \( p_3^{(I)} \neq p_3^{(II)} \)

![Diagram](image)

(c) **Degenerate**, \( \gamma = 0 \), \( p_3^{(I)} = p_3^{(II)} \)

![Diagram](image)

*Figure 6.1*
Figure 6.2 Illustration defining the notation used in Section 6.2. To simplify the diagram use has been made of the superscript notation \( ^{\phi} \) introduced in Section 5.6.1, where for instance the axes \( O_{x_{1}}^{^{\phi}} \) represents two sets of axes \( O_{x_{1}}^{(I)} \) and \( O_{x_{1}}^{(II)} \) related to \( O_{y_{1}} \) by rotations of \( \omega(I) \) and \( \omega(II) \) respectively about \( O_{y_{2}} = O_{x_{2}}^{^{\phi}} \).
Figure 6.3 The bicrystal in which screw dislocation pile-ups are discussed in Section 6.3, showing the relationship between the cylindrical polar coordinates \((r, \theta, z=x_2)\) and the rectangular Cartesian axes \(Ox_1\). The half-crystals (I) and (II) possess orthorhombic and triclinic symmetry respectively, and attention is restricted to pile-ups on the plane \(x_1=0\) only.
CHAPTER 7

Conclusion

7.1 Results of the Present Work

The purpose of this thesis has been to extend existing models of slip bands held-up at grain boundaries as a step to improving the current theories of polycrystalline plasticity. A linear array of continuously distributed infinitesimal dislocations in an elastic medium has been used throughout to represent a slip band in a real crystal, and grain boundaries have been regarded as the plane welded interface between two elastically different half-spaces. Describing the distribution of the dislocations by a function $F$ the condition that each dislocation in the array is in equilibrium under the combined effect of the applied load and internal stresses (including the image and compatibility stresses discussed in Section 1.3) may be written as a singular integral equation as outlined in Section 1.2. If the leading dislocation is blocked causing the other dislocations to pile-up behind it a solution for $F$ is sought which is unbounded at the blocked dislocation and bounded at the free end of the pile-up. Existing solutions to such problems are discussed in Section 1.4.

When the plane of a screw dislocation pile-up is inclined to the boundary between two different isotropic half-spaces at an angle $(1-a)\pi/2$, as shown in Figure 2.2, the equilibrium integral equation has the form of (2.13) which may be solved for rational values of the constant $a$ using the Wiener-Hopf technique with Mellin transforms as in Chapter
This technique, which has been used only once before to solve pile-up problems, is discussed in detail in Chapter 2. By writing \( a = pq^{-1} \), where \( p \) and \( q \) are integers, the distribution function \( F \) is expressed in equation (3.15) in terms of a set of \( q \) constants \( \alpha_i(i=1,2,...,q) \) which are functions of the quantities \( a \) and \( \gamma \), where \( \gamma \) depends on the ratio of the shear moduli of the component half-crystals and is defined in equation (1.8). Analytic expressions for \( \alpha_i \) are listed in Appendix 3.1. Since this solution appears as the sum of generalised hypergeometric series a recurrence relation is developed in Appendix 3.2 to enable the stresses due to the pile-up to be determined in a straightforward way, and approximate expressions for these stresses at points very near to the pile-up tip are given as equations (3.19) and (3.20).

Assuming, in terms of the discussion in Section 1.3, that the pile-up is external to a large inclusion, so that \( \sigma_c \), the stress tending to move the dislocations, is given by (3.9) and the applied load gives rise to the stresses (3.8) in each half-crystal, contours of constant shear stress \( \sigma_23^A \), referred to the axes \( Ox_1 \) of Figure 2.2, have been plotted in Figures 7.1 to 7.6 based on equations (3.19) and (3.20). In each case the applied stress \( \sigma_23^A \) has been taken as being 10 times greater than the frictional stress \( \sigma_23^F \) opposing the motion of the dislocations in the pile-up, and the corresponding curves for a pile-up in a homogeneous medium are shown as broken lines. Also the lines OA represent the plane of the pile-up whilst the plane of the boundary is indicated by the lines BOC. Figures 7.1 and 7.2 illustrate the nature of these stresses in different regions of the material surrounding the tip of the array for the case when \( \gamma = -1/4 \) and \( a = 1/2 \). The corresponding curves for \( \gamma = 1/4, a = 1/2 \) and \( \gamma = -1/4, a = 0 \) are
shown in Figures 7.3, 7.4 and 7.5, 7.6 respectively.

According to relations (3.19) and (3.20) the pile-up stresses vary with $r$, the distance from the pile-up tip, as $r^{-\alpha_1}$, where $\alpha_1$ is the member of the set $\alpha_i$ lying in the range $0<\alpha_1<1$ and is plotted as a function of $a$ for $\gamma = 0.8, 0.4, 0, -0.4$ and -0.8 in Figure 7.7 using the results of Appendix 3.1. This graph clearly illustrates that $\alpha_1$ is most strongly dependent upon $\gamma$ when $a=0$ and is independent of $\gamma$ for $a=1$. Moreover when $\gamma>0$, that is when material (II) has a greater shear modulus than material (I), $\alpha_1 > 1/2$ and the stresses consequently fall off less rapidly with increasing distance from the pile-up tip than in a homogeneous medium ($\gamma=0$), whilst the converse is true for $\gamma<0$. This effect can be clearly seen in Figures 7.1 to 7.6. In medium (II) the variation of the stresses with the angle $\phi$, defined as in Figure 2.2, is of the form $\cos(1-\alpha_0)\phi$, but since the shape of the stress contours for $\gamma=\pm 1/4$ varies little from that of the contours for $\gamma=0$ the influence of $\gamma$ is small in this respect. Because of the term $\cos[(1-\alpha_1)\phi-\alpha_1(a+1)\pi]$ in (3.19) the influence of this constant is slightly more marked in medium (I). Far more important is the effect of $\gamma$ on the magnitudes of $\sigma_{23}^{(I)}$ and $\sigma_{23}^{(II)}$, especially when $a=0$ as may be seen from Figures 7.5 and 7.6, arising partly from the form of the constants $2N\sigma_1$ and $2N\sigma_2$ and partly from the assumed form of $\sigma$. It follows therefore that the effects due to the inhomogeneity of the material are most apparent for pile-ups normal to the plane boundary, and that the inclusion of the elastic compatibility stresses is important in calculations of this type.
The number of dislocations, \( n \), in the pile-up is given by (3.18) and a plot of \( [2\pi G(I)b] \frac{\sigma \varepsilon}{n} \) against \( \gamma \) based on this equation is shown in Figure 7.8 for \( a=0 \), 0.5 and 1. It is interesting that the variation of \( n \) with \( a \) is so much greater in the range \( 1/2 < a < 1 \) than when \( 0 < a < 1/2 \).

In Chapter 4 the problem solved originally by Smith using a conformal mapping procedure of two intersecting screw dislocation pile-ups under symmetrical loading is treated by means of the Wiener-Hopf technique. The stress fields in the region of the intersection are given by equations (4.9) and (4.10) in rather more detail than previously, and show that, referred to axes \( O_x^1 \) in Figure 4.1, the shear stresses \( \sigma_{13}=0 \) and \( \sigma_{23}=-C\sigma \), where \( C \) is a constant of order unity, in the material between the two pile-ups. This result illustrates clearly the stress relaxation that occurs in the material inside a deformation twin immediately behind its tip, except that normally the dislocations would be of edge orientation. The solution of this problem is important to the present work since the governing integral equation is identical in form to (2.13) for the limiting case when \( \gamma=1 \), corresponding to a pile-up at an arbitrary angle to the boundary against a rigid second phase. The fact that the distribution function given by equation (4.2) varies continuously with the orientation parameter \( a \) indicates that the solutions to the problem considered in Chapter 3 when \( a \) is irrational may be obtained by interpolation between results for rational values of \( a \).

The second problem considered in Chapter 4 is that of a slit notch in the surface of a semi-infinite solid.
inclined to the plane surface at an arbitrary angle. Although an exact solution to the problem can in principle be found using the Wiener-Hopf technique as described in Section 4.2.1, the result is in an unsuitable form for considering the stresses immediately beyond the notch tip. For this reason the problem has been solved alternatively in Section 4.2.2 using a conformal mapping technique and the crack growth criterion established in Section 4.2.3 with the use of these results.

Strictly speaking the model of two elastically isotropic half-spaces welded together, on which the analysis of Chapter 3 is based, can only be used as an idealised model of a composite solid formed either from different materials or from different phases of the same material. Because the image forces on dislocations in polycrystals arise solely from the anisotropy of the elastic properties of the component grains it is clearly necessary to treat the corresponding model of a two-material medium using anisotropic in preference to isotropic elasticity theory. In Chapter 5 boundary-value problems associated with elastic half-spaces of the most general anisotropy, namely when the boundary is a stress-free surface or a freely-slipping or welded interface between two half-spaces, have been solved for the case when the stresses in the solid are invariant in one direction parallel to the boundary and vanish at infinity in all directions normal to this. The image forces on one of a pair of dislocations have been determined when the dislocations are either in the same half-space (Section 5.5.2) or separated by the boundary (Section 5.5.3). In Section 5.6.1 the solutions to the boundary-value problems have been generalised to
facilitate their application to specific problems, and as a result it has been proved in Section 5.6.2 that the magnitude of the image force on a dislocation near to a plane boundary depends on the elastic constants of the component half-spaces referred to the same set of axes, but for a given separation of the dislocation and the boundary is independent of the orientation of the boundary about the direction of the dislocation line.

To demonstrate the magnitude of the image forces in polycrystals consider bicrystals of materials having the hexagonal close packed structure shown in Figure 7.9. The small hexagons drawn in both diagrams indicate the basal planes, but because of the six-fold symmetry of these materials the present results are valid for all orientations of the $a$-axes in these planes. Referring to the bicrystal in Figure 7.9(a) as "soft" because of the continuity of the slip plane at the boundary and that in Figure 7.9(b) as "hard", quantities pertaining to them will be denoted by surfaces $S$ and $H$ respectively. The general form of the magnitude $F$ of the image force may be written

$$F = [\gamma_e G_e b_e (1-\nu)^{-1} + \gamma_s G_s b_s (4\pi r)^{-1} \text{ (7.1)}$$

where $b_e$ and $b_s$ are respectively the edge and screw components of the Burgers vector of the dislocation a distance $r$ from the boundary, and $\gamma_e$ and $\gamma_s$ are constants. For both bicrystals

$$G_e/(1-\nu) = s_{11} (s_{11}^2 - s_{12}^2)^{-1/2}$$

$$x [2(s_{11}s_{33} - s_{13}^2)^{1/2}(s_{11}^2 - s_{12}^2)^{1/2} + 2s_{13}(s_{11}s_{12} + s_{11}s_{44})^{-1/2}$$
where the shortened suffix notation $s_{MN}$ has been used for the elastic compliance constants $s_{ijkl}$. In Table 7.1, values of $\gamma^S_0$ and $\gamma^S_1$ for arbitrary $\Theta_1$, and $\gamma^H_0$ and $\gamma^H_1$ for $\Theta_1 + \Theta_2 = 90^\circ$ are listed for six h.c.p. metals at 298°C calculated using the elastic constants quoted by Tyson \((74)\).

The strongest interactions occur for zinc and cadmium in each case, and with the exception of zirconium edge and screw dislocations interact in opposite senses with boundaries in the hard bicrystals. The effect of temperature on $\gamma^H_0$ and $\gamma^H_1$ is shown in Table 7.2 for titanium indicating that these quantities increase by a factor of approximately 7 in the range 4°C to 1023°C. A more detailed description of these effects has been given by Tucker \((75)\).

Finally, using the results of Chapter 5, the solutions obtained in Chapter 3 for screw dislocations piled-up at a plane boundary have been generalised to include certain cases when the materials on either side of the boundary are elastically anisotropic. Solutions are obtained in Section 6.2 for the stress field and dislocation distribution function of pile-ups inclined to the plane boundary at an angle $(1-n)\pi/2$ when $n$ is rational, provided that the dislocation lines are parallel to two-fold symmetry axes in each half-crystal. In Section 6.3 corresponding solutions have been obtained for a pile-up perpendicular to the boundary in a half-space of orthorhombic symmetry welded to a half-space exhibiting the most general anisotropy.
The two suggested mechanisms for yield in polycrystals which embody a linear array of dislocations piled-up at a grain boundary were discussed in Section 1.5. Hall assumed that yield occurred when the stress intensification ahead of the tip of a blocked slip band in one grain was sufficient to activate a pre-existing source on the other side of the boundary, whilst Petch suggested that fresh dislocations were nucleated at the boundary when the stress exerted by the slip band reached a critical value. It was pointed out in that section that the results of Barnett and Chou and Barnett for the stress fields of screw dislocation pile-ups perpendicular to plane boundaries between elastic half-spaces of finite rigidity indicate that, if the Hall model of yielding were operative in a polycrystal, the dependence of yield stress on grain size would differ from that of the well-established Hall-Petch relationship (1.19). In Section 7.2.1 this suggestion is examined in detail in the light of the results obtained in the present work, and it is demonstrated that the observed yield stress-grain size relationship can be interpreted in terms of the elastically isotropic model used in Chapter 3 of a slip band held up at a grain boundary. Chou's conclusion that the rival Petch model for yielding ahead of a pile-up at a grain boundary gives rise to an exact Hall-Petch relationship is discussed in Section 7.2.2.
7.2.1 The Hall Mechanism

In comparing the yield stresses of a bicrystal of the type considered in Chapter 3 with those of a homogeneous medium it is most instructive to use the simplest form of the Hall mechanism of slip initiation at grain boundaries in which it is assumed that both the slip planes and the slip directions are parallel in adjacent grains. Moreover the influence of the self-stress of the source on the dislocation distribution in the pile-up is neglected. The model is shown schematically in Figure 7.10. Because the results of the previous chapter for pile-ups against boundaries in elastically anisotropic materials are not sufficiently general to encompass all situations in a real polycrystal a pseudo-anisotropic treatment is employed in this section. A given anisotropic solid composed of two welded half-spaces (I), containing the dislocation pile-up, and (II) is replaced by the isotropic model of Chapter 3 with

\[ \gamma = \Re [H_{2i}^{(I,I)}K_{ij}^{(I,II)}G_{ij}^{(I,I)}]. \]

The constants \( H_{2i}^{(I,I)} \) and \( G_{ij}^{(I,I)} \) are defined as in equation (5.27) and \( K_{ij}^{(I,II)} \) is defined in (5.37). This form of \( \gamma \) is based on the expression (5.46) for the image force on a screw dislocation in an elastically anisotropic bicrystal. Referred to axes \( Ox_1 \), suppose that when the load \( \sigma_{23} \) applied at infinity is equal to the yield stress \( \sigma_{23}^Y \) the stress acting at \( S \) reaches the critical value \( \sigma_{23}^S \) needed to operate the source. Because of the elastic compatibility stresses discussed in Section 1.3 it is important to distinguish between the two cases when the model represents a pile-up within and external to a large inclusion. Using equations
and assuming a constant frictional stress $\sigma_{A}^{\alpha}$ opposes the motion of the dislocations in the pile-up, the yield stress $\sigma_{23}^{Y}$ is given by the equations

$$
\sigma_{23}^{Y} = \frac{2NC_{1}(1+\gamma)\sigma_{23}^{F} + [\sigma_{23}^{S}-2NC_{2}(1+\gamma)\sigma_{23}^{F}](\rho/\ell)^{1-\alpha_{1}}}{2NC_{1}(1-\gamma^{2}) + [(1+\gamma\cos\phi)-(2NC_{2}(1-\gamma^{2})](\rho/\ell)^{1-\alpha_{1}}}
$$

(7.2)

when the pile-up is inside the inclusion, and

$$
\sigma_{23}^{Y} = \frac{2NC_{1}(1+\gamma)\sigma_{23}^{F} + [\sigma_{23}^{S}-2NC_{2}(1+\gamma)\sigma_{23}^{F}](\rho/\ell)^{1-\alpha_{1}}}{2NC_{1}(1+\gamma)(1-\gamma\cos\phi)+(1+\gamma)[1-2NC_{2}(1-\gamma\cos\phi)](\rho/\ell)^{1-\alpha_{1}}}
$$

(7.3)

when it is outside. It is of interest to note that when $\alpha=0$ the two equations are identical, whilst when $\alpha=1$ $\sigma_{23}^{Y}(\gamma)$ given by (7.2) is identical to $\sigma_{23}^{Y}(\gamma)$ given by (7.3). Estimating for iron at $300^\circ\text{K}$ that $\sigma_{23}^{S}\approx 5 \times 10^{10}$ dyne cm$^{-2}$ (44) and $\sigma_{23}^{F}\approx 5 \times 10^{8}$ dyne cm$^{-2}$ (76), plots of $\sigma_{23}^{Y}/\sigma_{23}^{F}$ against $(\rho/d)^{1/2}$ using (7.2) and (7.3), where $d=2\ell$ is taken to be the average grain diameter, are shown in Figures 7.11 for $\gamma=1/4$ and 7.12 for $\gamma=-1/4$ when $\alpha=0$, 0.5 and 1. In Figures 7.11(b) and 7.12(b) the arithmetic average of these plots is shown as the continuous curve marked A but have been omitted from 7.11(a) and 7.12(a) to avoid complication. For the purpose of comparison the curve for the pile-up in a homogeneous medium ($\gamma=0$) is shown on each graph as the broken line. The deviations from the $d^{-1/2}$ relationship are greatest for $\alpha=0$ and zero for $\alpha=1$ as is to be expected from the variation of $\alpha_{1}$ with $\gamma$ shown in Figure 7.7.

A striking feature of these curves is the much greater dependence of the yield stress on the relative orientation of the slip plane and
the grain boundary when the pile-ups are external to the
inclusion. In the range of $\rho/\ell$ considered

$$2NC_1(1-Y^2) \geq [(1+Y\cos\alpha) - 2NC_2(1-Y^2)](\rho/\ell)^{1-\alpha}$$

and $2NC_1(1+Y)(1-Y\cos\alpha) \geq (1+Y)[1-2NC_1(1-Y\cos\alpha)](\rho/\ell)^{1-\alpha}$

and thus the strong dependency of $\sigma_{23}^Y$ on $\alpha$ in (7.3) arises
from the term $(1-Y\cos\alpha)^{-1}$ which is absent from (7.2). It
is clear therefore that this feature is entirely due to
the elastic compatibility stresses and emphasises their
importance in these calculations.

It is necessary to take an average of either equations
(7.2) or (7.3) for all possible values of $\alpha$ and $\gamma$ to obtain
a Hall-Petch-type equation for the material based on this
particular yield mechanism. Although comparison of such
an average theoretical relationship with that observed can
be only qualitative, owing to the limitation of the analysis
to screw dislocation pile-ups and the lack of generality
of the yield mechanism itself, quantitative comparison
with the relationship derived using the same mechanism
in a homogeneous medium is instructive. The averaging
process may be carried out in two stages. Firstly, for
a given value of $\gamma$, the average form of (7.2) or (7.3)
is sought for values of $\alpha$ between 0 and 1. Since all
values of $\alpha$ are equally possible, it is assumed in the
present treatment that the arithmetic mean of $\sigma_{23}^Y(\alpha=0)$
and $\sigma_{23}^Y(\alpha=1)$ serves as an approximation to the average
form of $\sigma_{23}^Y$ for a given value of $\gamma$, an assumption which
to some extent is supported by Figures 7.11 and 7.12.

The second stage of this process, averaging over permissible
values of $Y$ requires more detailed treatment. It is first necessary to determine the distribution $D(Y)$ of values of $Y$ in a given polycrystal, calculated such that there are $D(Y)dY$ grain boundaries with values in the range $Y$ to $Y+dY$. A possible form of $D(Y)$ for a real crystal is shown as curve A in Figure 7.13 whilst that for a homogeneous crystal has the form of a δ-function (curve B). Clearly the exact form of A would require detailed computation based on the analysis of Chapter 5, but for the purposes of the present calculation $D(Y)$ is assumed to be the segment of the curve $D(Y) = 1-Y^2$ between the extreme values $Y_{\min}$ and $Y_{\max}$ at which curve A vanishes. The reasons for this particular choice of $D(Y)$ are that the average of $\sigma_{23}^Y$ may be obtained analytically and also that when the actual distribution function is available this could be represented by an amalgamation of segments of this type.

Using (7.2) and (7.3) with the distribution function $C$ of Figure 7.13 the average yield stress $<\sigma_{23}^Y>$ is given by

$$<\sigma_{23}^Y> = \frac{[2\sigma^F(\alpha - \frac{\sin \pi \alpha}{n}) + \sigma S j(\alpha)]_{\alpha_{\max}}^{\alpha_{\min}}}{[\alpha - \frac{\sin 2\pi \alpha}{2n}]_{\alpha_{\min}}^{\alpha_{\max}}} \quad (7.4)$$

for pile-ups inside an inclusion, and

$$<\sigma_{23}^Y> = \frac{[2\sigma^F(\alpha + \sigma S j(\alpha))]_{\alpha_{\min}}^{\alpha_{\max}}}{[\alpha - \frac{\sin 2\pi \alpha}{2n}]_{\alpha_{\min}}^{\alpha_{\max}}} \quad (7.5)$$

for pile-ups outside an inclusion, where
\[ j(\alpha) = \left( \frac{\dot{\rho}}{d} \right)^{\alpha} \left\{ \frac{\log\left( \frac{\dot{\rho}}{d} \right) \cos \frac{\pi \alpha}{2} + \frac{\dot{\rho}}{d} \sin \frac{\pi \alpha}{2}}{[\log(\dot{\rho}/d)]^2 + (\frac{\dot{\rho}}{d})^2} - \frac{\log\left( \frac{\dot{\rho}}{d} \right) \cos \frac{3\pi \alpha}{2} + \frac{\dot{\rho}}{d} \sin \frac{3\pi \alpha}{2}}{[\log(\dot{\rho}/d)]^2 + (\frac{\dot{\rho}}{d})^2} \right\} \]

and \( \alpha_{\text{max}} = \pi^{-1} \cos^{-1} \gamma_{\text{max}}, \alpha_{\text{min}} = \pi^{-1} \cos^{-1} \gamma_{\text{min}} \). Taking \( \gamma_{\text{max}} = 0.4, \gamma_{\text{min}} = 0 \) for iron, based on the approximate results of Armstrong and Head\(^{(50)}\), and values of \( \sigma_{23}^S \) and \( \sigma_{23}^P \) used in Figures 7.11 and 7.12, \( \sigma_{23}^F / \sigma_{23}^F \) has been plotted in Figure 7.14 as a function of \((\rho/d)^{1/2}\) for pile-ups both inside (curve C) and outside (curve B) the inclusion. The horizontal axis of this graph has also been calibrated in terms of \( d^{-1/2} \) and \( d \) by taking \( \rho = 2 \times 10^{-5} \) cm based on the estimate of Stroh\(^{(77)}\). The limiting curves A, for the case when \( \gamma_{\text{max}} = \gamma_{\text{min}} = 1/2 \) and the medium is homogeneous, and D, when \( \gamma_{\text{max}} = 1 \) and \( \gamma_{\text{min}} = -1 \), have also been included. For \( \rho < 1 \) mm the deviations of curves B, C and D are not sufficiently large to be detectable outside the limits of experimental error, as may be seen for instance by inspection of the results of Cracknell and Petch\(^{(76)}\). Since the model of a pile-up inside a large inclusion is physically a more realistic representation of a slip band in one grain of a polycrystal than a pile-up external to the inclusion, curve C is taken here as an estimate of the Hall-Petch relationship in polycrystalline iron in preference to B. By taking the curve to be linear for \( \rho < 1 \) mm the slope of this portion is approximately 20\% greater than that of A, and the extrapolated intercept with the \( \sigma_{23}^F / \sigma_{23}^F \)-axis is \( \sim 1.8 \) compared with 1 for A. In the case of D the increase in slope is approximately 50\% and the intercept is at \( \sigma_{23}^F / \sigma_{23}^F \sim 3.7 \).

The averaging technique can be criticised for its oversimplicity, but in the absence of a reliable distribution
function \( D(Y) \) there is little point in seeking greater accuracy at this stage. It is unlikely that a more rigorous approach would invalidate the principal conclusion to be reached from the present calculations, namely that, when account is taken of the difference in elastic properties of neighbouring grains in a polycrystal a theoretical yield stress-grain size relationship compatible with that observed experimentally may be derived using the Hall model of yielding by averaging the results for individual pairs of grains. Furthermore the effects considered here could contribute as much as 20\% to the observed Hall-Petch slope \( k \) and slightly less than 50\% to the constant \( \sigma^0 \) in equation (1.19). The latter effect may explain why, when \( \sigma^0 \) is interpreted as the Peierls stress on the dislocations in the pile-up, the value is somewhat higher than expected (76).

7.2.2 The Petch Mechanism

The results of Koehler (78), which were used by Petch (43) to derive his cleavage strength-grain size relationship, indicate that tensile stresses \( \sigma^T \) exist ahead of an array of \( n \) edge dislocations pressed against an obstacle under the influence of an applied stress \( \sigma \) of the form

\[ \sigma^T \propto n\sigma. \]

The conclusion of Cottrell (37) that the leading dislocation must experience a shear stress \( \sigma^S = n\sigma \) due to the obstacle if the array is to remain stationary suggests that the obstacle must experience an equal and opposite shear stress due to the array, in keeping with Koehler's results. If the presence of the obstacle in no way affects the elastic properties of the solid, then by assuming that the array
when a critical value of $\psi$ is achieved, a Hall-Petch relation for yield may be formulated as described in Section 1.5.

When the obstacle is the plane boundary between two different elastic half-spaces the piled-up dislocations are in equilibrium under a non-uniform shear stress due to the presence of the image dislocations, and it is necessary to use Smith's formula (1.16) for $\sigma^S$. Considering for simplicity the case of a pile-up perpendicular to the boundary, $\sigma^S$ is given by

$$\sigma^S = \frac{G(I)b}{2n} \int_0^L F(x)dx[\sigma - \gamma \int_0^L \frac{F(x')dx'}{(x+x')}],$$

from (1.16) and (2.13). These results arise from the form of the image forces on the dislocations. As the leading dislocation reaches the boundary, the force on it is assumed to be infinitely repulsive for $\gamma>0$, infinitely attractive for $\gamma<0$ and zero for $\gamma=0$. Thus it is itself in equilibrium with the image stresses when $\gamma>0$ and does not require an additional stress to be exerted by the obstacle to keep it stationary. In contrast when $\gamma<0$ an infinite stress is required to overcome the attractive image forces on the dislocation. It is apparent therefore that, contrary to the supposition of Chou (51,79), the Petch mechanism cannot be incorporated in this particular model of a polycrystal.

Recently Pacheco and Mura (80,81) have studied the interaction of a screw dislocation and a plane boundary, taking into account the non-Hookean effects due to the change in lattice parameter on the slip plane at the bound-
Using the Peierls model of a dislocation in preference to the elastic model employed in the present work they have shown that the stress $\sigma^B$ on the dislocation when it is in medium (I) a distance $r$ from the boundary has the approximate form

$$\sigma^B = -\frac{G(I)b}{\alpha n^2} \left[ \frac{\gamma_2 \tan^{-1} \frac{2r}{a}}{a} - \frac{\gamma^* \gamma^*}{4r^2/a^2 + 1} \right] 
(7.6)$$

where

$$\gamma^* = \left[ a^{(II)} - a^{(I)} \right] \left[ a^{(II)} + a^{(I)} \right]^{-1},$$

$$2a^{-1} = a^{(I)}^{-1} + a^{(II)}^{-1},$$

and $a(I)$ and $a(II)$ are the lattice parameters in the slip plane in media (I) and (II) respectively. Clearly it would be very difficult to apply these results directly to a dislocation pile-up, but the elastic model may be adapted in the following way to embody the essential features of the interaction, namely that as $r \to 0$, $\sigma^B$ tends to the finite limit

$$\sigma^B \to -\frac{G(I)b}{\alpha n^2} (2\gamma - \gamma^*),$$

and as $r \to \infty$

$$\sigma^B \to -\frac{\gamma G(I)b}{4\pi r}$$

in agreement with Head's relationship for an elastic dislocation. If the image stress $\sigma^B^*$ on an elastic dislocation is assumed to be of the modified form

$$\sigma^B^* = -\frac{\gamma G(I)b}{4\pi(r+e)}$$

where $e = \alpha n(2\gamma - \gamma^*)$ which is of the same order of magnitude as $b$, $\sigma^B^*$ and $\sigma^B$ have identical forms in the limits $r \to \infty$ and $r \to 0$. The equilibrium equation for the pile-
up may then be written

\[ \frac{G(I)b}{2\pi} \int_{-e}^{e} F(x')[(x-x')^{-1}+\gamma(x+x')^{-1}]dx' = \sigma(x), \quad (7.7) \]

when \( \alpha = 0 \). Comparing this equation with (2.13) it appears that the stress on the leading dislocation of an array held up at the boundary based on the model of Pacheco and Mura is approximately the same as the stress on the leading dislocation of an array of the same length but based on Head's model and held up a distance \( e \) from the boundary. Boiko and Fed'erson have treated this problem for \( \ell = \infty \) but their results are obviously of no use in deriving a yield stress-grain size relationship. It is evident, however, from Smith's analysis of a pile-up held up a distance \( h \) from a rigid elliptical cylindrical inclusion that when \( h \) is of the order of \( b \) the dislocations assume an equilibrium configuration only marginally different from that when \( h = 0 \). It is concluded therefore that the results of the previous section based on Hall's mechanism slightly overestimate the effect of the difference in elastic properties of neighbouring grains on the Hall-Petch relationship, and that a comparable analysis based on the Petch mechanism will not be possible until the solution to the integral equation (7.7) is available.

### 7.3 Outstanding Problems Associated with the Present Work

The model of a slip band held up at a grain boundary in a polycrystalline material used in Chapters 3 and 6 is that of a single linear array of continuously distributed infinitesimal dislocations in an infinite elastic medium
composed of two half-spaces welded together. There are four principal objections to this model. Firstly that, by treating a dislocation in a two-phase material as a purely elastic entity, a form of image force is assumed which tends to infinity as the dislocation nears the boundary. As discussed in Section 7.2.2 this feature makes it impossible to derive a yield stress-grain size relationship based on the Petch mechanism (43), and it is suggested that in a more realistic model the distribution function of the dislocations piled-up at the interface will resemble that for a pile-up of dislocations blocked a small distance, of the order of magnitude of their Burgers vector, from the plane boundary in the purely elastic model. To the author's knowledge the solution to this problem has not been reported. The second objection is that the model is at present limited to antiplane strain. Although the distribution functions of edge dislocation pile-ups normal to plane boundaries in elastically isotropic two-phase media have been derived (20) no subsequent attempt appears to have been made to calculate the tip stresses. This objection is all the more serious in the light of the results given in Table 7.1 which demonstrate that edge and screw dislocations in elastically anisotropic bicrystals can experience oppositely directed image forces. Thirdly, since the results of Section 7.2.1 illustrate clearly the importance of the elastic compatibility stresses, the necessity to investigate dislocation pile-ups within cylindrical inclusions of finite radius is apparent. Finally no allowance has been made for the probable finite width of a slip band in a real crystal. Using a pair of identical screw dislocation arrays situated one above the other and separated by a
distance $h$ as a model which embodies this feature Smith has shown that the stress singularity at the tip of each array has the same inverse-square-root character as for a single array, but of magnitude dependent upon $h$. If these dislocations are piled-up against a grain boundary then ignoring image effects Smith's model is applicable only to a slip band orientated normal to the boundary. For other orientations the band would have a 'chisel-shaped' tip and the distributions in each array would differ. For large deviations from $\pi/2$ stresses considerably different from those due to a single pile-up might occur, the lagging array crowding together the dislocations at the tip of the leading array and thus enhancing the stress intensification in the adjacent grain. It is suggested therefore that the generalisation of Smith's model in this respect would be of interest to the problem of yield propagation in polycrystals.

All of the above objections could greatly affect the yield stress dependence on grain size based on either of the mechanisms discussed in the last two sections, and it has not been considered worthwhile to use a more rigorous averaging technique than that used in Section 7.2.1. Moreover the distribution of values of $Y$ within a given polycrystal is unknown at present, and since prior knowledge of this distribution is fundamental to a further development of this work its investigation is deemed worthwhile.
Table 7.1  Values of constants $\gamma_{e}^{S}$, $\gamma_{s}^{S}$, $\gamma_{e}^{H}$ and $\gamma_{s}^{H}$ in equation (7.1) for certain h.c.p. metals at 298°K.

<table>
<thead>
<tr>
<th>Metal</th>
<th>$\gamma_{e}^{S}$</th>
<th>$\gamma_{s}^{S}$</th>
<th>$\gamma_{e}^{H}$</th>
<th>$\gamma_{s}^{H}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cd</td>
<td>-0.204</td>
<td>0</td>
<td>-0.164</td>
<td>0.154</td>
</tr>
<tr>
<td>Zn</td>
<td>-0.230</td>
<td>0</td>
<td>-0.134</td>
<td>0.060</td>
</tr>
<tr>
<td>Mg</td>
<td>0.010</td>
<td>0</td>
<td>-0.010</td>
<td>0.007</td>
</tr>
<tr>
<td>Zr</td>
<td>0.035</td>
<td>0</td>
<td>0.007</td>
<td>0.022</td>
</tr>
<tr>
<td>Ti</td>
<td>0.027</td>
<td>0</td>
<td>0.101</td>
<td>-0.072</td>
</tr>
<tr>
<td>Be</td>
<td>0.035</td>
<td>0</td>
<td>0.031</td>
<td>-0.059</td>
</tr>
</tbody>
</table>

Table 7.2  Values of constants $\gamma_{e}^{H}$ and $\gamma_{s}^{H}$ in equation (7.1) for titanium at various temperatures

<table>
<thead>
<tr>
<th>Temperature</th>
<th>$\gamma_{e}^{H}$</th>
<th>$\gamma_{s}^{H}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4°K</td>
<td>0.052</td>
<td>-0.032</td>
</tr>
<tr>
<td>298°K</td>
<td>0.101</td>
<td>-0.072</td>
</tr>
<tr>
<td>723°K</td>
<td>0.236</td>
<td>-0.155</td>
</tr>
<tr>
<td>1023°K</td>
<td>0.341</td>
<td>-0.219</td>
</tr>
</tbody>
</table>
Figures 7.1 to 7.6

Contours of constant shear stress $\sigma_{23}$ due to a right-handed screw dislocation pile-up on plane OA against the plane boundary BOC separating two isotropic elastic half-spaces. As discussed in Section 7.1 the curves are based on equations (3.19) and (3.20), and results for

(i) $a=1/2$, $\gamma=-1/4$ are shown in Figures 7.1 and 7.2,
(ii) $a=1/2$, $\gamma=1/4$ are shown in Figures 7.3 and 7.4, and
(iii) $a=0$, $\gamma=-1/4$ are shown in Figures 7.5 and 7.6

by the continuous curves. The corresponding contours for a pile-up in a homogeneous medium ($\gamma=0$) are shown by broken lines.
Figure 7.2
Figure 7.4
Figure 7.5
Figure 7.7  The variation of the constant $\alpha_1$ with $a$ calculated using the analytic expressions in Appendix 3.1.
Figure 7.8 The variation of \( \frac{2\pi}{d(I)_{\text{b}} \cdot \sigma \ell/n} \) with \( \gamma \) calculated from equation (3.18), where \( \sigma \) is the stress tending to move an array of \( n \) dislocations distributed continuously over a region \( \ell \) of the slip plane and blocked at the grain boundary.
Figure 7.9 (a) "Soft" and (b) "Hard" bicrystals of materials of hexagonal close packed structure discussed in Section 7.1 and used in the calculation of Tables 7.1 and 7.2. Basal planes in each half-crystal are indicated by hexagons.
Figure 7.10 The model of the Hall mechanism used in Section 7.2.1 to calculate the yield stress–grain size relationship in polycrystalline solids. Neighbouring grains (I) and (II) are represented by two elastically isotropic half-spaces of different shear moduli welded together along the plane interface AOB. Referred to the rectangular Cartesian axes Ox, the blocked slip band is represented by a piled-up array of screw dislocations parallel to Ox on the plane x=0 in medium (I) and it is supposed that slip is initiated in medium (II) when the stress intensification due to the pile-up is sufficient to activate a source S, a distance OS=ρ from the boundary, which is of screw orientation and operates in the plane x=0.
Figures 7.11 and 7.12

Plots of $\frac{\sigma_{23}}{\sigma_{23}^F}$ against $(p/d)^{1/2}$, where $\sigma_{23}$ and $\sigma_{23}^F$ are the yield and friction stresses respectively, $d$ is the average grain diameter and $p$ is defined in Figure 7.10. The continuous curves (except those labelled "A") are calculated from equation (7.2) in graphs (a) and from equation (7.3) in graphs (b), assuming $\gamma = 1/4$ in Figure 7.11, $\gamma = -1/4$ in Figure 7.12 and $\sigma_{23}^S = 100\sigma_{23}^F$ in both cases. Broken lines correspond to the equations (7.2) and (7.3) for the case when $\gamma = 0$ and the medium containing the pile-up is homogeneous. The curves labelled "A" in graphs (b) are obtained by taking the arithmetic average of curves for $a = 0, 0.5$ and $1$ shown on the same plots.
Figure 7.11
Figure 7.12
Figure 7.15 The distribution of values of $\gamma$ in a polycrystal as discussed in Section 7.2.1.

$D(\gamma) = 1 - \gamma^2$
Figure 7.14 The yield stress-grain size relationships obtained by averaging equations (7.2) and (7.3) by the procedure developed in Section 7.2.1, in which the meaning of curves A, B, C, D is discussed.
References

(26) Head, A.K., Phil. Mag. 44, 92 (1953).
(29) Head, A.K., Phil. Mag. 44, 92 (1953).
(43) Stroh, A.N., Phil. Mag. 46, 198 (1955).
(47) Tucker, M.O., Phil. Mag. 12, 1141 (1969).


(64) Stroh, A.N., Phil. Mag. 2, 625 (1958).


(74) Tyson, W., Acta Met. 15, 574 (1967).
(81) Pacheco, E.S. and Mura, T., to be published (1969).