REACTIONS OF SOLIDS CONTAINING DISLOCATIONS

THE EFFECT OF DISLOCATIONS ON THE LINEAR RESPONSE OF ELASTIC HETEROGENEOUS SOLIDS

by

Salah M. H. el Helbawi
Department of Mechanical Engineering
Masters of Engineering

ABSTRACT

In this thesis, the influence of mobile line dislocations, anchored to slip planes in an otherwise isotropic elastic matrix, on the quasi-static linear elastic response of an idealized polycrystalline aggregate of close-packed crystals, is discussed. The formulation incorporates the inactivated Frank-Read source as its fundamental mechanism and examines its effect on the response characteristics, through the use of statistical correlation theory. The independent parameters used in the correlation analysis are the slip plane orientation and the direction of the dislocation line segments which differ from crystal to crystal in a random fashion. The relation between this linear theory derived on the basis of the conservation of energy in the absence of dissipation, and its extension into non-linear ranges of response, along with its relation to other theories currently being discussed in the literature, are investigated.

SUMMARY

In this thesis, the influence of mobile line dislocations, anchored to slip planes in an otherwise isotropic elastic matrix, on the quasi-static linear elastic response of an idealized polycrystalline aggregate of close-packed crystals is discussed. The dislocation mechanisms are discussed in Chapter II. The formulation incorporates the inactivated Frank-Read source, discussed in Chapter III, as its fundamental mechanism and examines its effect on the response characteristics through the use of statistical correlation theory. The independent parameters used in the correlation analysis are the slip plane orientation and the direction of the dislocation line segments, which differ from crystal to crystal in a random fashion. The relation between this linear theory, derived on the basis of the conservation of energy in the absence of dissipation is discussed in relation to four cases frequently encountered in the current literature. This is shown in Chapter V.

The present work is considered an important step in the redefinition of certain basic concepts pertaining to the proper use of materials since it leads to a specification of the limitations on the linear elastic response of polycrystalline metals containing dislocations.

ACKNOWLEDGEMENTS

The author wishes to express his sincere thanks to his research supervisor, Dr. J. W. Provan. The successful completion of this thesis depended significantly on his many useful ideas and on the numerous informal discussions with him. The author would also like to acknowledge the help of Dr. D. R. Axelrad for important suggestions offered on several occasions during the course of this work. Sincere thanks to Miss Rhonda Curley who diligently typed this thesis. This project was supported by a National Research Council of Canada grant. This financial help is gratefully acknowledged.

TABLE OF CONTENTS

LIST OF SYMBOLS

δ_{ij}	The Kronecker delta; equal 1 if $i = j$ and equal 0 if $i \neq j$.
ε_{ij}	The linear strain tensor.
$\underset{\sim}{\varepsilon}$, $\underset{\sim}{\varepsilon}^2$	As defined in the correlation functions given by Equations (5.16).
ζ	The self-energy of a dislocation.
η	A parameter containing the dislocation density.
θ	The θ-coordinate in the cylindrical coordinate system.
κ	A constant defined by Equation (2.9).
λ	The Lamé coefficient.
μ	The Lamé coefficient or the shear modulus.
ν	Poisson's ratio.
ξ	Coordinates of a bowed out dislocation.
ρ	The dislocation density cm/cm^3.
σ_{ij}	The linear stress tensor.
σ_{mm}	The spherical components of σ_{ij}.

σ'_{ij} The deviatoric components of σ_{ij}.

$\underset{\sim}{\sigma}$, $\underset{\sim}{\sigma}^2$ As defined in the correlation functions given by Equations (5.16).

τ The ratio of mobile dislocations.

υ The volume of a crystal.

ϕ The angle made by a zigzaged dislocation to the base line joining the pinning points.

χ The Airy stress function.

$\underset{\sim}{\Psi}$ A vectorial geometric quantity.

ω_{ij} The direction cosines of the z_i coordinates with respect to the reference coordinate system x_i.

ℓ The length of an anchored dislocation segment.

Γ_{ijkl} The orientation tensor.

$\underset{\sim}{\Gamma}$, $\underset{\sim}{\Gamma}^2$ As defined in the correlation functions given by Equations (5.16).

Δ Designates an increment.

Λ The total length of the dislocation line in a crystal.

Ω^k_{ij} Designated the slip directions in a crystal.

$\underset{\sim}{b}$ Designates the Burgers vector.

d A distance.

$\underset{\sim}{m}$ The unit vector along a dislocation line.

n Number of crystals in the mesoscopic region.

$\underset{\sim}{n}$ The unit vector normal to a slip plane

r A radius.

u_i The displacement in the i-th direction.

x_i Designates the Cartesian coordinates of the reference frame.

z_i Designates the Cartesian coordinates attached to the center of mass of a crystal.

$A,\ldots,E$ Tensor quantities defined by Equations (5.18).

C_{ijkl} The fourth order material isotropic tensor.

E_c Compressive energy.

E_e Extension energy.

E_m Misfit energy.

F The force per unit length on a dislocation line.

R Designates the correlation functions and the product moments, defined by Equations (5.16).

S The misfit area.

T The line tension in a bowed out dislocation.

U^n The free energy stored in a mesocopic region.

V The macroscopic volume of a specimen.

SUPERSCRIPTS

$.^{\alpha}$ Designates a crystal in the mesoscopic region.

$.^{\gamma}$ Denotes a crystal influencing the state of stress in the α-th crystal.

$.^{n}$ Designates the mesoscopic region.

$.^{k}$ Designates the k-th slip direction.

SUBSCRIPTS

$.\beta$ Takes the value 2 or 3.

$.i,..,n$ Dummy indices, take the value 1, 2, 3.

$.p,..,s$ Dummy indices, take the value 1, 2, 3.

$._o$ Designates the cut-off radius.

OTHER SYMBOLS

$\cdot_{,}$	Denotes partial differentiation.
$\underset{\sim}{\cdot}$	Denotes a vectorial quantity.
$\bar{\cdot}$	Denotes the average of a quantity.
$\langle\cdot\rangle$	Designates the average of a random process.
$\cdot^{*}$	Designates the fluctuating components of a random process.
$\lvert\cdot\rvert$	Designates the absolute value.

Note:

Symbols are defined where they first appear in the text.

LIST OF FIGURES

CHAPTER I

INTRODUCTION

Metals are made up of crystals separated from each other by boundaries. Each crystal is a three-dimensional network of atoms, arranged in unit cells possessing an order which tends to reduce their volume to a minimum. A perfect crystal is one in which these unit cells are arranged on a periodic space lattice throughout the macroscopic volume. Due to reasons as yet not fully understood, the lattices of actual crystals are never perfect, being disturbed by the presence of vacancies, line imperfections, such as dislocations in addition to the grain boundaries which are themselves surface defects. Further, impurity atoms frequently penetrate the lattice structure causing further distortions in it. Apart from these geometrical defects, lattice vibrations cause additional unaccountable deviations of the observed response characteristics in comparison with those theoretically predicted by assuming that the crystal lattice is perfect.

The scatter frequently encountered in experimental data is, to a great extent, due to inadequacies in the phenomenological laws and theories pertaining to elasticity

and plasticity. These laws either neglect non-linear effects on the response of a solid or are designed to smooth them out over macroscopic regions of the material specimen. In this manner local mechanisms and their effects on the theoretical response are not taken into account. Extensions and modifications of the classical continuum theory known as higher order continuum theories have been developed for the purpose of accounting for such nonlinearities in the response behaviour of metals. However, these theories are frequently too vague and ill-defined to be of use in the solution of problems for which they were formulated. Moreover such an approach frequently obscures the physical phenomena involved and requires a special formulation for each. However, as defects exist in crystal lattices, their effects must be included in any formulation which describes the material response.

For this purpose, dislocations will be considered as the main mechanism for the description of the nonlinear response of solids. It is fortunate in this respect that dislocations have long range stress fields. Furthermore, beyond a few lattice vectors away from a dislocation line, the atomic displacements are small compared with the inter-atomic distances. It becomes unnecessary therefore to deal directly with the atomic structure of dislocations, hence allowing the use of linear elasticity for the description of their local effects,

i.e., the individual crystal is assumed to be made up of an isotropic elastic matrix observing the laws of perfect linear elasticity in which a three-dimensional network of dislocations is embedded. Segments of this network, lying in slip planes, are anchored to inter-stitial atoms. From the analysis of the deformation of these segments and that of the elastic matrix, a quasi-static linear elastic response of the polycrystalline metal is then derived. In this way, the overall mechanical response will be correlated to the response of crystals containing dislocations.

In order to introduce the subject matter of this thesis, a brief review of dislocation theory is given in Chapter II. Chapter III is concerned entirely with a discusion of the Frank-Read mechanism due to its importance in the formulation of the proposed theory. The proposed mathematical model is then treated in Chapters IV and V, before certain conclusions are drawn in Chapter VI.

CHAPTER II

DISLOCATION MECHANISM

As already pointed out in the Introduction, dislocations are of great significance in determining the mechanical response characteristics of solids. The existence of dislocations was first conjectured as a means by which the magnitude of the yield stress in solids could be estimated. It was experimentally observed that, in general, yield stresses in crystals appeared in a scatter several orders of magnitude less than the theoretical stress calculated on the assumption that all atoms in a shear plane slip simultaneously. Since the shear stress is never uniformly distributed, and due to the visualization of the atoms to be flexibly coupled (linear chain model), the assumption of simultaneous slip had to be discarded. Instead of this assumption, it was then hypothesized that a boundary separates the slipped from the unslipped regions. The line defining this boundary was then termed a *dislocation line*. See, for instance, A. H. Cottrell (1953).

For the definition of a dislocation, consider a circuit drawn to pass through the atoms in a perfect lattice. It will be necessarily closed. However, if this circuit, also termed the *Burgers circuit*, does not close by an amount equal to a lattice vector, called the *Burgers vector*, it is said to encircle a dislocation. The dislocation has everywhere the same

Burgers vector and can only end at the boundary of the crystal. If these dislocations end within the crystal, they have to form closed loops or three-dimensional networks. *See H. G. van Bueren [1960].* An elementary length of a dislocation loop of unit vector $\underset{\sim}{m}$ and Burgers vector $\underset{\sim}{b}$ lying in a slip plane whose unit normal is $\underset{\sim}{n}$ is said to move *conservatively*, if the direction of motion is $\underset{\sim}{n} \times \underset{\sim}{m}$. See Figure 2.1. Two distinct cases in this category can be discerned. In the first, the dislocation is called a *screw dislocation* when the Burgers vector $\underset{\sim}{b}$ lying in the slip plane $\underset{\sim}{n}$ is parallel to the unit vector $\underset{\sim}{m}$. See Figure 2.2a. In the second case, the dislocation is called an *edge dislocation* when the Burgers vector $\underset{\sim}{b}$ lying in the slip plane $\underset{\sim}{n}$ is perpendicular to unit vector $\underset{\sim}{m}$. See Figure 2.2b. Any dislocation of Burgers vector $\underset{\sim}{b}$ lying in the slip plane $\underset{\sim}{n}$ can be decomposed into a screw and an edge dislocation.

When a dislocation of Burgers vector $\underset{\sim}{b}$ lying in the slip plane $\underset{\sim}{n}$ moves such that the condition $\underset{\sim}{n}.\underset{\sim}{b} = 0$ is not satisfied, the motion is said to be *non-conservative*, since the density of the atoms in the slip plane does not remain constant.

The ease with which a dislocation moves depends on its *width*, W. W is defined as the width of the transition between the slipped and the unslipped areas of the crystal.

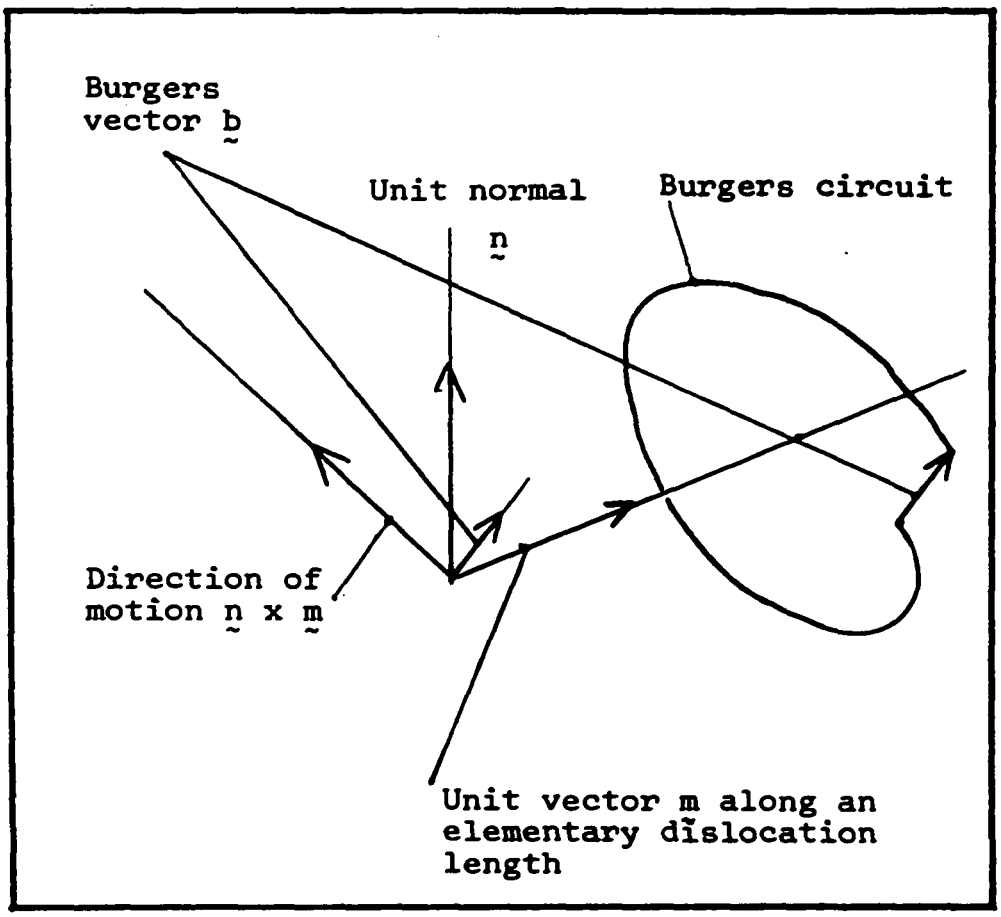

Figure 2.1

Dislocation Line

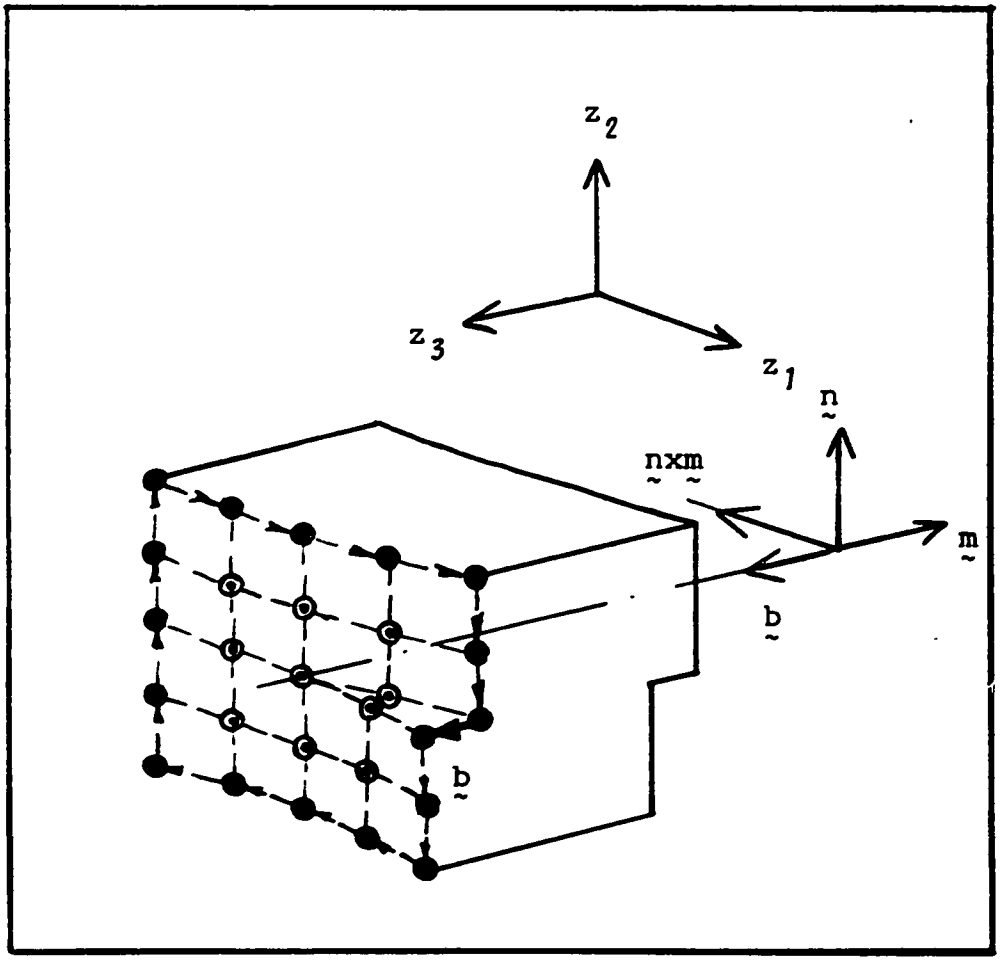

Figure 2.2a

Screw Dislocation

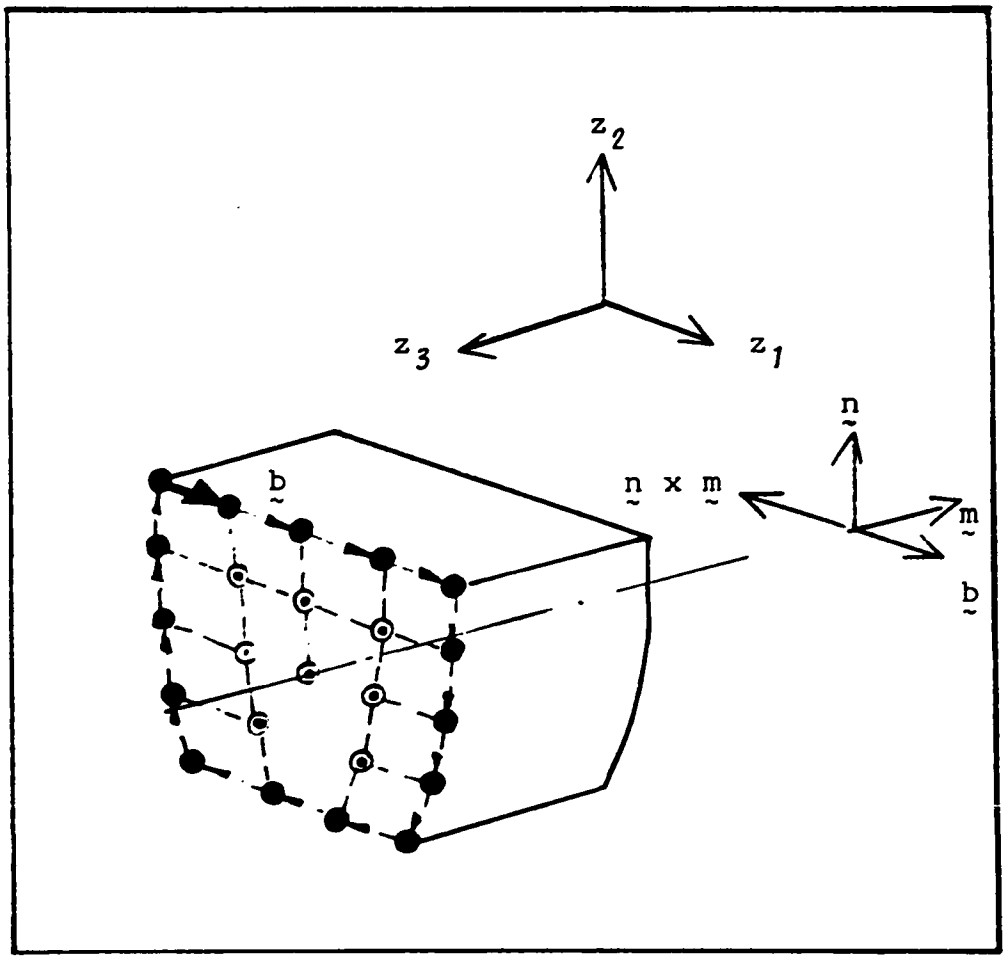

Figure 2.2b

Edge Dislocations

See Figure 2.3. The force required to move a dislocation one Burgers vector in a slip plane is inversely proportional to its width. If the width is infinitely large, an infinitesimally small force is required due to the fact that the atomic displacements are infinitesimally small and occur in the interatomic potential wells. The actual width of dislocations in real crystals is due to the balance between the *compressive energy* E_c in the top half of the crystal plus the *extension energy* E_e in the bottom half of the crystal and the *misfit energy* E_m across the slip plane.

If a Burgers circuit, of radius r is drawn around a screw dislocation of Burgers vector $\underset{\sim}{b}$ and magnitude b, the shear stress, obtained by multiplying the shear strain $b/2\pi r$ by the shear modulus μ, is seen to be proportional to $1/r$. This indicates that dislocations have a long range influence and it is justifiable to use linear elasticity at large distances away from the core. The dependence of the stress on $1/r$ is assumed invalid within a cut-off radius of about 5b from the core due to the fact that the displacements are large and linear elasticity will not apply. Accordingly, in developing the equations for the stress and strain fields of dislocations, the Navier equilibrium displacement equations of isotropic linear elasticity, in the absence of body forces can be used. These equations are:

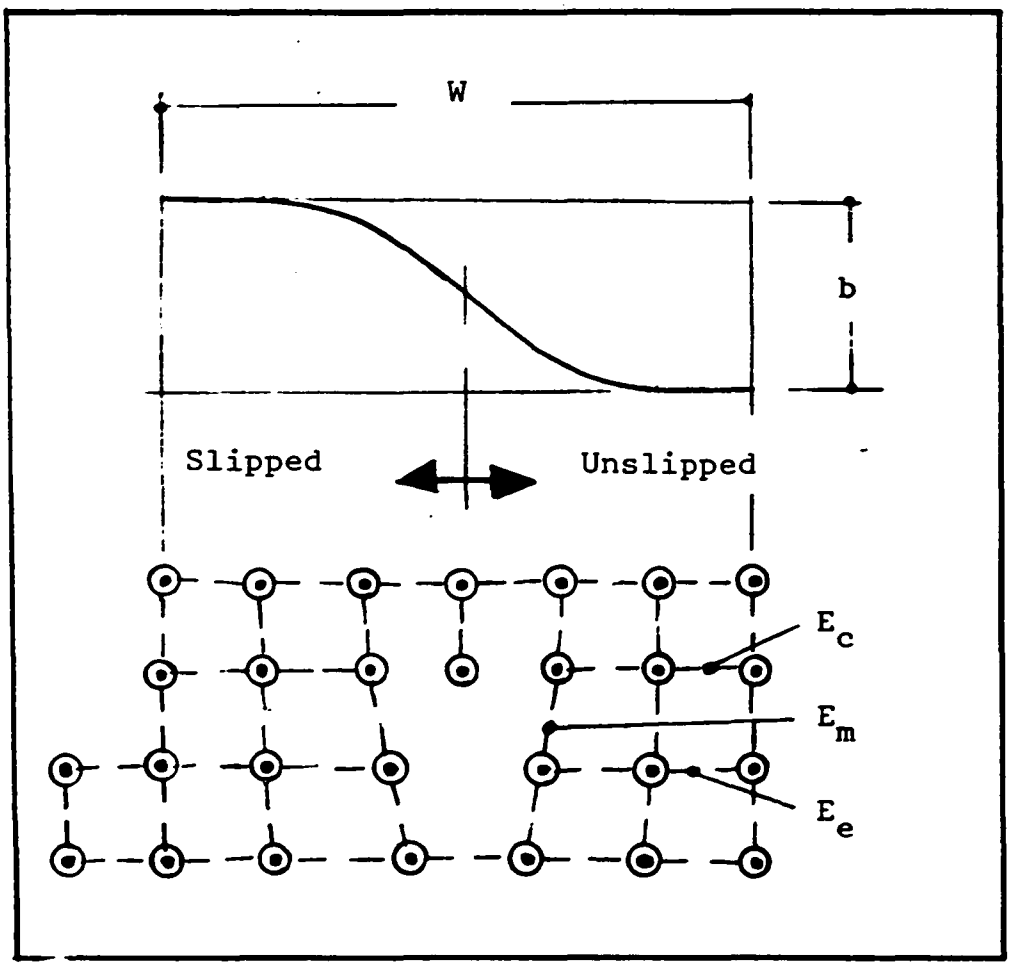

Figure 2.3

Width of a Dislocation

$$\mu\, u_{i,jj} + (\lambda+\mu)\, u_{j,ji} = 0 \qquad (2.1)$$

where λ and μ are the Lamé coefficients, u_i is the displacement in the i-th direction, Latin indices have the range 1, 2, 3, the summation convention applies, and a comma before Latin indices denotes differentiation with respect to the Cartesian coordinates indicated. The solution has to satisfy the condition that the forces opposing the relative displacement of the atoms are periodic, with a period b, rather than increasing monotonically.

Drawing a Burgers circuit around a straight screw dislocation whose unit vector $\underset{\sim}{m}$ coincides with the z_3 axis, the displacements are found to be multi-valued functions of position. The discontinuity b in the displacement is constant in the z_3 direction and the only linear strain components ε_{ij} dependent on u_3 are ε_{13} and ε_{23}, whilst all other strains vanish. In polar co-ordinates the surviving component of the strain is $\varepsilon_{\theta z}$ and is periodic with an increment of 2π. The simplest solution that satisfies Equation (2.1) is an inverse trigonometric function of the following form:

$$u_3 = b\theta/2\pi = b/2\pi \tan^{-1}(z_2/z_1), \qquad (2.2)$$

where z_i are indicated in Figure 2.2a. From Equation (2.2) it may be seen that the displacement is evenly distributed around the dislocation line. It is then a matter of substitution to write down the non-vanishing components of the stress and strain. Since all elastic deformations are accompanied by a corresponding strain energy, the *self-energy* ζ of a dislocation is defined as the energy stored in its elastic field per unit length, i.e.:

$$\zeta = \tfrac{1}{2} \int \sigma_{ij}\varepsilon_{ij}\, 2\pi r\, dr, \qquad (2.3)$$

where σ_{ij} is the stress tensor. Substituting for the stress and the strain into the above integral and integrating over the cylindrical volume of radius r surrounding the dislocation line, an expression for the self-energy of a screw dislocation is obtained:

$$\zeta = \mu b^2/4\pi \ln r/r_0, \qquad (2.4)$$

in which again r_0 is the cut-off radius within which the formulation of linear elasticity fails.

The determination of the state of deformation of an edge dislocation is more involved due to the lack of radial symmetry. The strain field of an edge dislocation which lies along the z_3 axis needs two co-ordinates for its description

since $u_3 = 0$ and the derivatives $u_{1,3} = u_{2,3} = 0$. Hence the solution to be sought here is one of plane deformation in which the spherical components of the stress and the shear component σ_{12} do not vanish. Thus all solutions of the equilibrium equation $\sigma_{ij,j} = 0$, satisfying the conditions of the deformation field around an edge dislocation are obtained from solutions of the Airy bi-potential equation for plane strain:

$$\nabla^4 \chi = 0, \tag{2.5}$$

in such a way that the Airy stress function satisfies the following expression:

$$\begin{aligned} \sigma_{11} &= \chi_{,22}, \\ \sigma_{22} &= \chi_{,11}, \\ \sigma_{12} &= -\chi_{,12}. \end{aligned} \tag{2.6}$$

For plane strain, the component σ_{33} is:

$$\sigma_{33} = \nu(\sigma_{11}+\sigma_{22}), \tag{2.7}$$

where ν is the Poisson's ratio. The Airy-stress function which satisfies the above condition is of the form:

$$\chi = \kappa z_2 \ln r \qquad (2.8)$$

where the value of κ is given by:

$$\kappa = \mu b/2\pi(1-\nu) \qquad (2.9)$$

A straight-forward substitution of Equation (2.8) into Equation (2.6) yields the stress field around the edge dislocation. The latter when substituted into the equations of the generalized Hooke's law yield the strain field relations.

From the derivation of the stress and the strain fields, indicated above, and making use of Equation (2.3), the self-energy of an edge dislocation is given by:

$$\zeta = \mu b/4\pi(1-\nu) \ln r/r_0. \qquad (2.10)$$

The above form differs from that of a screw dislocation by the constant $1/(1-\nu)$.

A significant quantity in the present formulation is the force exerted by an external stress field on a dislocation. Equating the work done by the external stress σ_{32} in causing a dislocation of Burgers vector b to move a distance d in a crystal of unit width, i.e., $\sigma_{32}bd$, to the work done in moving

the dislocation force per unit length F, caused by σ_{32}, the same distance d, i.e., $|F|d$, it can be seen that the force on a dislocation is:

$$|F| = \sigma_{32} b. \qquad (2.11)$$

It has been assumed in the above relation (2.11) that the non-linear contribution from the core can be neglected.

The force F is equally the force exerted by the stress field of one dislocation on another dislocation in its neighborhood. Accordingly, the force between two parallel screw dislocations has radial symmetry whilst that between two parallel edge dislocations has no radial symmetry since the condition of plane deformation implies dependence on z_1 and z_2.

In conclusion, the present chapter has dealt with the basic definitions and has given a brief exposition of the main characteristics of dislocations. It has been shown that in spite of the discreet atomic structure of dislocations, they strongly interact with each other and with external mechanical fields because of their long range effects, thereby allowing the use of linear elasticity in the description of their behaviour. A synthesis of these effects is believed to be at the foundation of most nonlinearities observed in the response of

solids. Certain of these nonlinearities will be explained in terms of the Frank-Read source in the following chapter.

CHAPTER III

THE FRANK-READ SOURCE

In polycrystalline solids, dislocations form three-dimensional networks randomly distributed within each crystal. Segments of each network are anchored to impurity atoms by the Cottrell force A. H. *Cottrell (1964)*. Since impurity atoms act as centers of dilatation, they only interact with edge dislocations which contain spherical components in their stress fields. When an external stress field is applied to a crystal containing such a three-dimensional network, a dislocation of length ℓ lying in a slip plane will deform according to the sequence 1, 2, 3, 4, 5, with an increase in the applied stress. See Figure 3.1. This topology was first proposed by F. C. *Frank and W. T. Read (1951)* and is now known as the *Frank-Read source*. It was later observed under the electron microscope.

The Frank-Read mechanism becomes very significant in the theory of plasticity since it can act as a source from which an infinite number of dislocations can be generated. Its importance lies in the fact that its activation as a dislocation multiplier is already possible at low stress levels. Previous to its introduction, the magnitude of plastic deformation at such low levels of stress estimated by considering the motion of existing dislocations could not be recon-

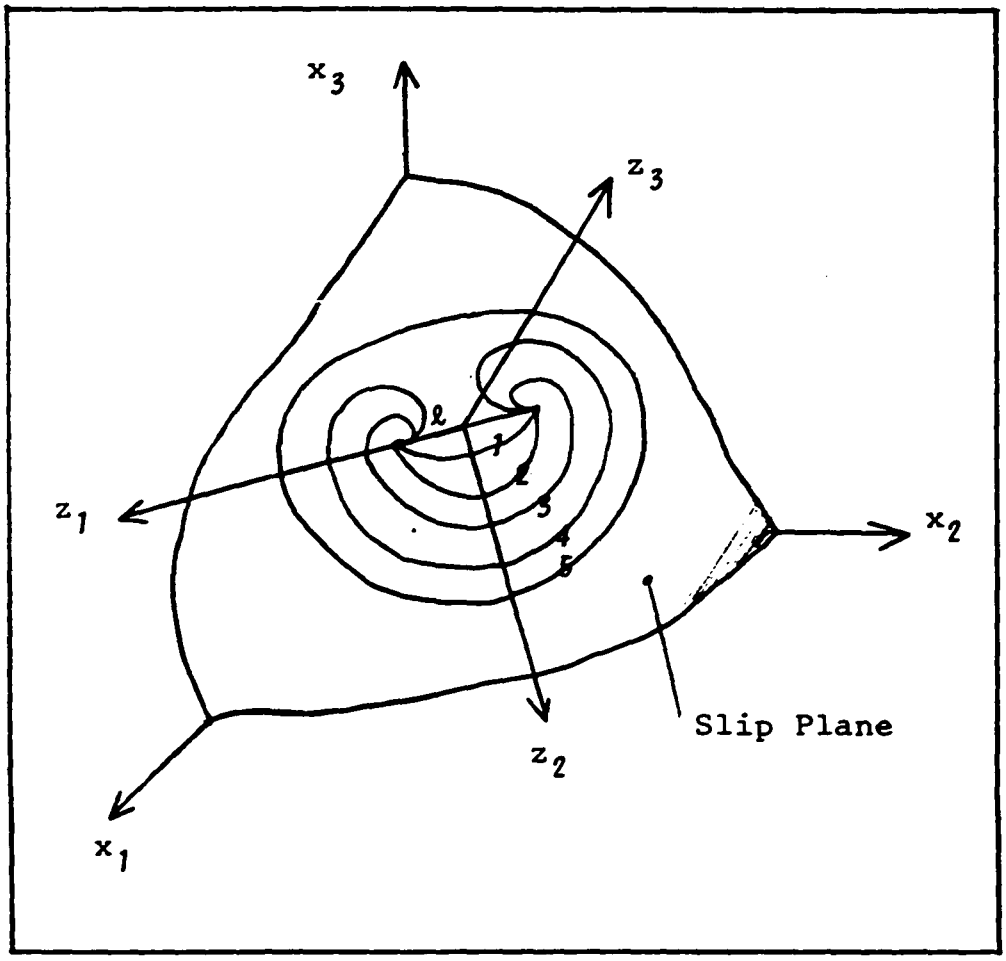

Figure 3.1

The Frank-Read Source

piled with experimentally observed values. Prior to this mechanism, a model was considered in which multiplication occured by reflection from a boundary and would necessitate that the dislocations move at sonic speeds. However, it is not possible to reach such speeds because of the retardation force a dislocation encounters when it moves through a crystal's lattice. *J. Weertman (1961)*. In order to accomplish this, stresses higher than the actual yield stress of the crystal would be required. Moreover, facts deduced from experimental observations show that the dislocations begin to multiply at speeds of the order of 1/10th of the sonic values. *W. G. Johnston and J. J. Gilman (1959)*.

If a number of equal, anchored dislocation segments having the same orientation are uniformly distributed in a slip plane, each of them will expand according to the sequence indicated in Figure 3.1, thus acting like sources for the multiplication of dislocation. Assuming that the slip plane is free from defects, which would have otherwise caused the dislocations to pile up, the head of a loop, which is a positive edge, upon meeting the tail of the one just ahead of it, which is a negative edge, will annihilate each other. Similarly, the right hand side of the loop, which is a positive screw, and the left hand side, which is a negative screw, of the neighboring dislocation will annihilate each other when

they meet. The locations where two dislocations of the same type, but of different signs, meet can be considered as sinks in which dislocations are annihilated.

Frequently, several slip planes having the same normal are operative simultaneously. When the spacing between two such planes is small, dipoles form (*K. Yazu (1968)*) between the positive dislocations at the head of one loop and the negative ones at the tail of another. This dipole formation may give rise to micro-cracks. *H. G. van Bueren (1960)*. The latter may also form when the dislocations emitted from a Frank-Read source pile up against the crystal boundary or against a sessile dislocation. Microcracks induced by these two mechanisms act to relieve the local stress concentration.

After the removal of the applied stress causing a pile-up of dislocations, all loops would collapse back to the source if no opposing forces resist to their motion. However, due to the existence of Peierls barriers (*R. Peierls (1940)*), the collapse would only be partial, i.e., the loops would move just enough to balance the repulsive forces between the dislocations and the opposing forces. The loops would totally collapse upon the application of a reverse stress. The reverse stress is smaller than the forward stress which caused the pile-up by an amount equal to the stress produced by the latter. Accordingly, the reverse strain is larger than the forward

strain and a hysteresis loop developes in the plot of the stress-strain curve. This phenomena is the well-known *Bauschinger effect* and constitutes one of the main dissipative mechanisms in solids.

Closely related to the Bauschinger effect is the friction in solids due to rapid reversal of loads at stress levels smaller than those required to cause the dislocations to multiply. *J. S. Koehler (1952) and A. V. Granato (1968).* The anchored segments of the mobile dislocations oscillate back and forth on their slip planes, causing part of the input mechanical energy to be dissipated in the form of heat. These oscillations leave the solid's structure intact as long as heat is allowed to be conducted away from the slip planes. On the other hand, if adiabatic conditions predominate, diffusion of the pinning points occurs, causing permanent changes in the solid's structure. *R. Bullough and R. C. Newman (1970).*

The very important phenomena of fatigue failure is due to all of the above mentioned effects. It involves, in general, slip bands, dipoles and dislocation pile-ups leading to the formation of micro-cracks. It also involves energy dissipation due to the Bauschinger effect or to internal friction. These effects lead to permanent changes in the crystalline structure resulting in eventual failure, inspite of the fact that the

applied external stress is macroscopically still within the domain of linear elasticity. *W. J. Plumbridge and D. A. Ryder (1969)*.

In deriving the quantitative equations pertaining to the activation of the Frank-Read source, it has been observed that the magnitude of the Burgers vector of a dislocation loop remains constant throughout the expansion of the anchored segments in the slip plane.

There exists therefore a line tension tending to decrease the total self-energy of the dislocation. *N. F. Mott (1952)*. Accordingly, in the first phase of deformation, a dislocation segment behaves like a string fixed at two ends. The string tension is obtained by dividing the increase in the dislocation self-energy by the corresponding increase in its length. See Figure 3.2.

Approximating the curve in the bowed out configuration by two straight segments pulled at the mid-span to an angle ϕ measured from the base line, it is seen that the line tension is to a first approximation equal to the self-energy per unit length of the dislocation. Substituting $r = 10^5 b$, corresponding to the radius of a typical crystal and choosing the cut-off radius $r_o = 5b$ into Equation (2.10), the line tension T is:

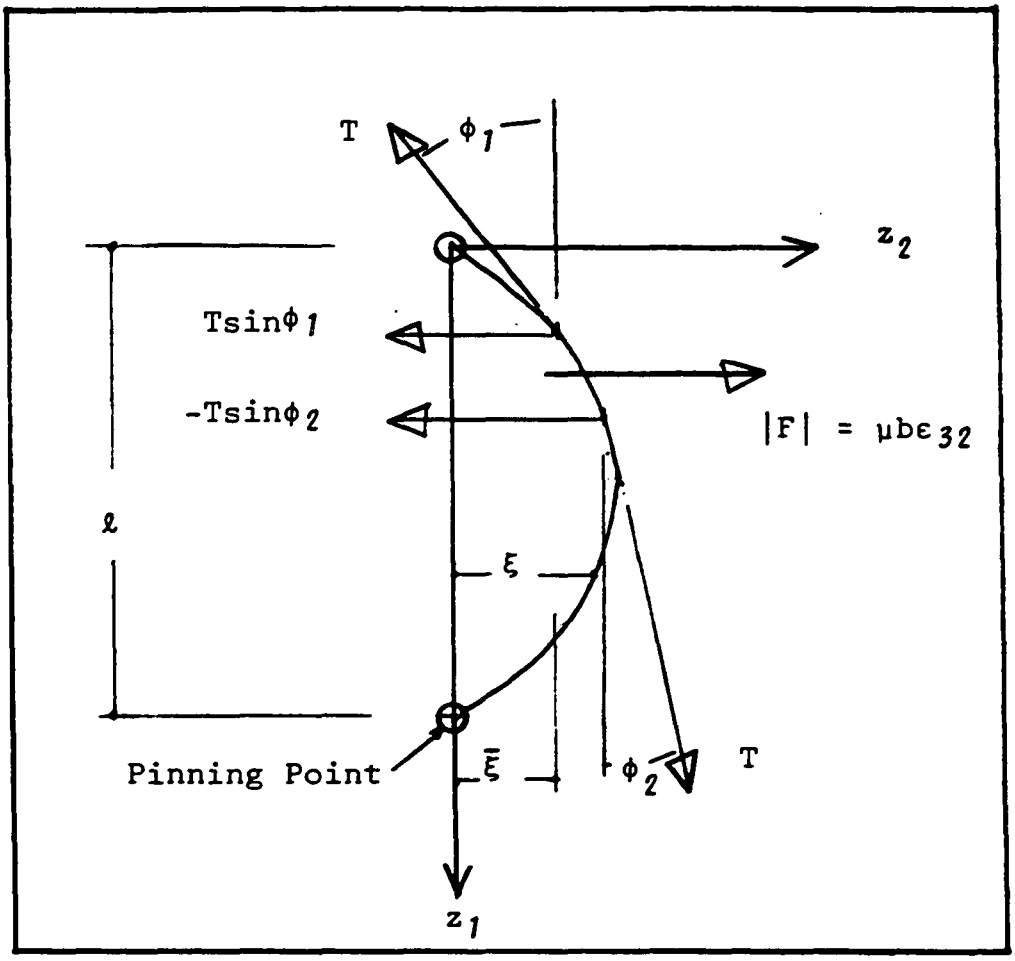

Figure 3.2

Dislocation String

$$T = \pi\mu b^2/4(1-\nu) \qquad (3.1)$$

where $\ln 2.10^4$ has been approximated by π^2. From this line tension the minimum value of the applied stress required to activate a Frank-Read source can be obtained by considering the equilibrium of forces acting on a semi-circular dislocation loop. Hence:

$$|F|\ell = \sigma_{32} b\ell = 2T. \qquad (3.2)$$

Substituting for T from Equation (3.1), it is observed that for linear elastic response, no stresses within the polycrystalline solid may exceed the value:

$$\sigma_{32} = \mu b/2(1-\nu)\ell \qquad (3.3)$$

Configuration 2 shown in Figure 3.1 corresponds to this stress. The reason for this limitation is that by neglecting the dependence of the line tension on the radius of curvature, the area swept by the dislocation line is proportional to the applied stress. This is shown by solving the differential equation expressing the balance between the line tension and the force exerted by the external stress, neglecting the Peierls stress. The resulting equilibrium equation can be written as follows:

$$T\, d^2\xi/dz_1^2 = -\sigma_{32} b = -\mu b \varepsilon_{32} \qquad (3.4)$$

where ξ is the displacement of the string in the z_2 direction, measured from the equilibrium position. Solving for ξ from (3.4), the average displacement $\bar{\xi}$ expressed in terms of the strain component ε_{32} is as follows:

$$\bar{\xi} = 1/\ell \int_0^{\ell} \xi dz_1 = 2(1-\nu)\ell^2/3\pi b\, \varepsilon_{32} \qquad (3.5)$$

where use has been made of Equation (3.1).

Although the effects of activating the Frank-Read sources and of the damping induced by the retardation forces encountered by moving dislocations are beyond the scope of the present thesis, they have been discussed in this chapter in order to indicate possible extensions of the above linear response into nonlinear domains. Hence, in what follows, only the linear relation between the dislocations displacement and the applied shear stress, given by Equation (3.5), will be used in the derivation of the equilibrium equations describing the quasi-static linear elastic response of polycrystalline metals.

CHAPTER IV

PROPOSED ANALYTICAL MODEL

The mechanical response of a polycrystalline aggregate is different from, although dependent on the response of its individual crystals. This behaviour of the aggregate is mainly due to the presence of defects whose mobilities are impeded either by grain boundaries or by restricted directions of motion. It is essential to correlate the mechanical response of the aggregate to the response of the individual crystals so that the important modes of deformation on the crystalline level can be identified. An approach of this kind can then lead either to a refinement of the phenomenological laws describing the microscopic response of the aggregate, hence leading to reliable predictions of its physical characteristics, or to the elimination of undesirable modes through the design of new materials. However, without certain assumptions it is inconceivable that these modes can be identified due to the seemingly incoherent structure of real polycrystalline solids.

Before enumerating the basic assumptions which are necessary to bring some order into the description of the aggregate's structure so that an analytical approach may be considered,

the three scales of crystalline structure introduced by *D. R. Axelrad (1971)* for the description of the deformation of heterogeneous media are incorporated. See Figure 4.1.

The *microscopic region*, which in Axelrad's notation corresponds to the smallest or micro-element to be dealt with in the heterogeneous medium, is taken to represent the individual crystal. The crystal has a volume υ^{α}, a dislocation density ρ^{α}, and slip direction $\Omega_{ij}^{k\alpha}$, where α designates the crystal and the superscript k identifies the particular slip direction interior to α. In the undeformed configuration, the center of mass of each microelement υ^{α} is denoted by a position vector $\underset{\sim}{x}^{\alpha}$, referred to a fixed Euclidean frame of reference.

The *mesoscopic region* contains a large number of close packed crystals so that a formulation similar to that of statistical mechanics can be employed. The number of crystals or micro-systems is n and hence $\alpha = 1, .., n$. The mesoscopic domain may be considered in the same sense as the *Gibbsian representative ensemble* of statistical mechanics.

The *macroscopic region* corresponds to the total solid of volume V. On the boundary of the macroscopic region, the tractions and deformations are considered specified for a par-

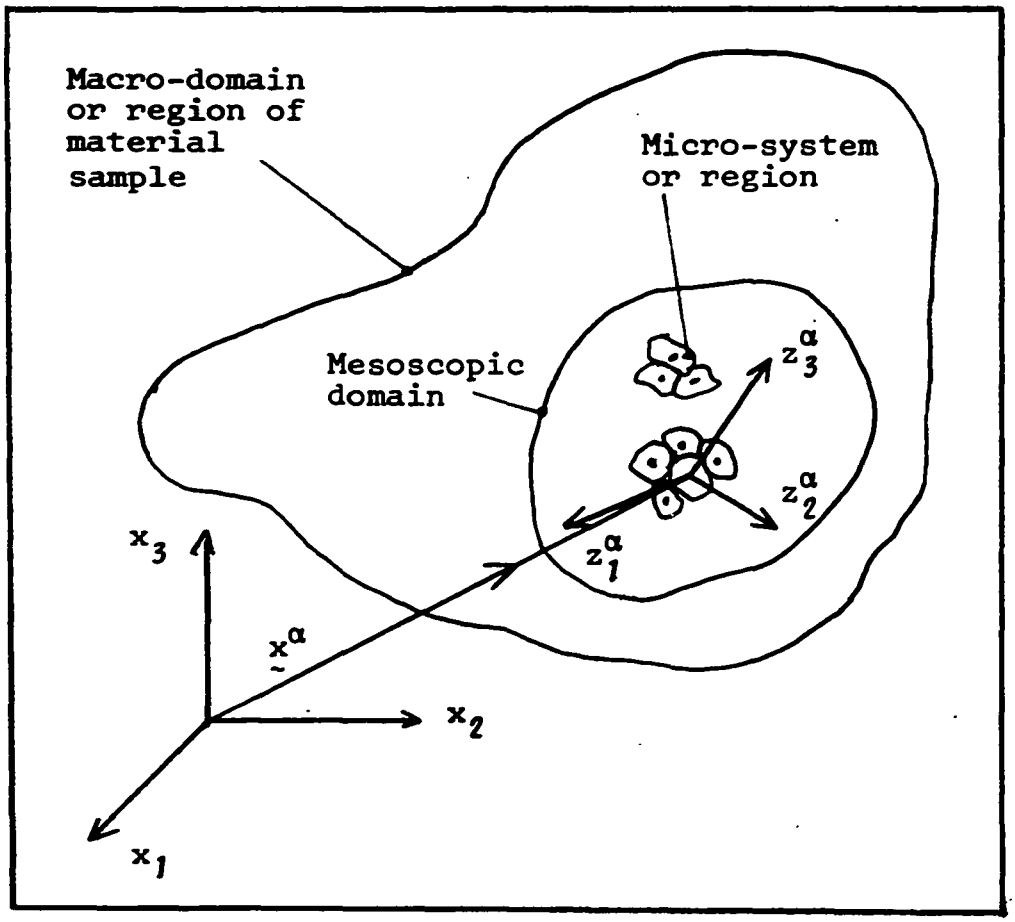

Figure 4.1

Axelrad's Size Scales

ticular boundary value problem.

Using this type of ordering of the polycrystalline aggregate the following assumptions are made pertaining to the microscopic element:

i) The crystal matrix whether free from or containing defects such as impurity atoms or sessile dislocations, responds to an applied stress according to the constitutive equations of a linear isotropic elastic material. These relations contain only two independent constants, i.e., the Lamé coefficients λ and μ.

ii) Since in the case of metals, a crystal has a preference to grow in the form of a close-packed structure tending to reduce its surface potential to a minimum, it follows that for an isotropic solid, crystals will grow spherically around nucleation points in the melt. Hence in the growth stage of a crystal around its nucleation point from a radius r to a radius r + dr, the difference $\Delta S = 8\pi r dr$, called the *misfit area*, is filled up with additional rows of atoms corresponding to dislocation lines. See Figure 4.2. From such geometrical consideration, the total misfit area S^{α} of an individual crystal of average radius r^{α} will be to

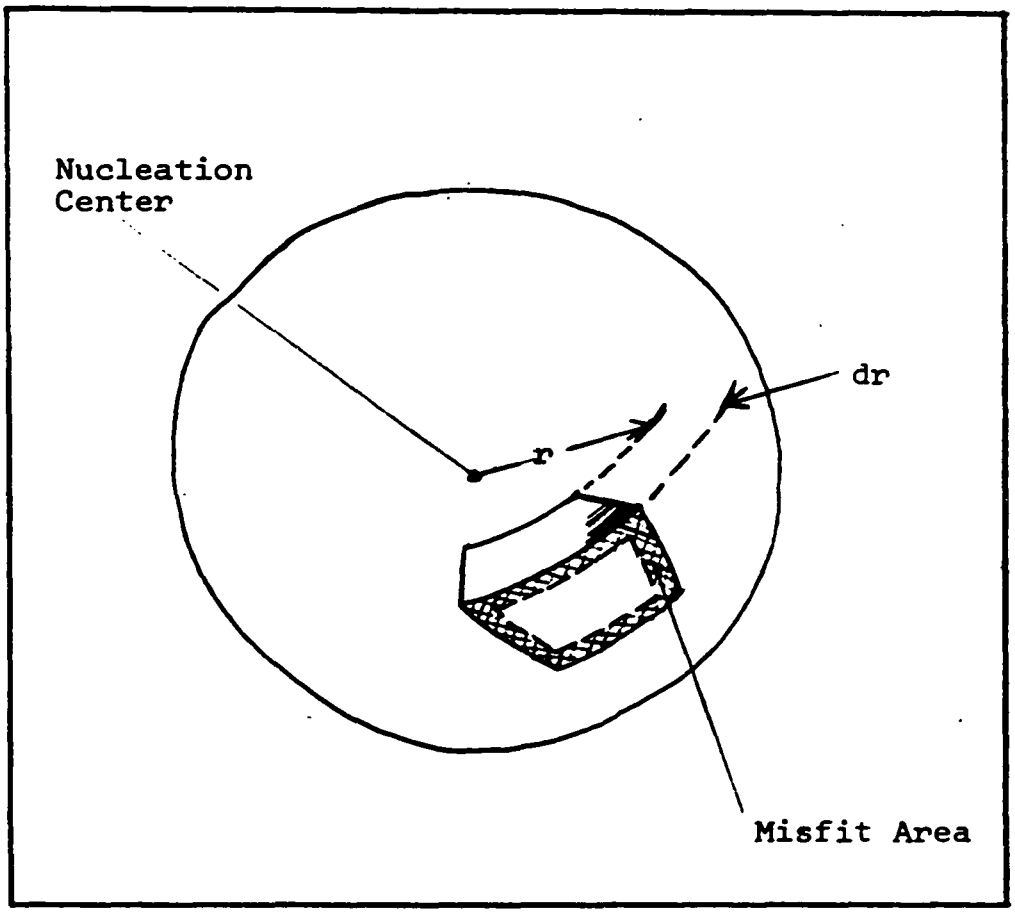

Figure 4.2

Misfit Area

a first approximation $4\pi(r^{\alpha})^2$. The density of dislocations ρ^{α} per unit volume of the crystal is then equal to the total length $\Lambda^{\alpha} = 2S^{\alpha}/b$ of the dislocation line divided by the crystal's volume, i.e.:

$$\rho^{\alpha} = 6/br^{\alpha}. \qquad (4.1)$$

Thus the density of the dislocations ρ^{α} in the α-th crystal can be expressed in terms of its volume υ^{α}.

iii) The dislocation density ρ^{α} does not vary from crystal to crystal, i.e., $\rho^{\alpha} = \rho$. This implies, in conjunction with ii), that the micro-element's radius r^{α} and its volume υ^{α} are constant, i.e., $r^{\alpha} = r$ and $\upsilon^{\alpha} = \upsilon$. By introducing this assumption, the effect of the density fluctuation on the solid's response is neglected and the individual crystal is considered as the unit element.

iv) A certain ratio τ of the dislocations within the crystal lie anchored to impurity atoms on crystallographic planes. A typical crystal of radius $r = 10^5 b$ will have an average dislocation density ρ of the order of 10^{11} cm/cm^3 as estimated from expression (4.1) given in assumption ii). The density of mobile dislocations

estimated from internal friction experiments is of the order $10^7 cm/cm^3$. A. V. *Granato* (1968). Thus, the ratio of the density of mobile dislocations to the total density in the crystal will be of the order 10^{-4}.

v) Out of the numerous possible slip systems $\Omega_{ij}^{k\alpha}$, there is only one slip direction $\Omega_{ij}^{1\alpha} = \omega_{\beta i}^{\alpha}$ $\beta = 2,3$, for the motion of mobile dislocations. Furthermore, the anchored segments of the mobile dislocations lie parallel to the z_1^{α}-axis of the co-ordinate system z_i^{α} attached to the α-th crystal's center of mass. The z_3^{α}-axis of this system whose direction cosines with respect to the reference Euclidean frame x_i are ω_{3i}^{α}, is the normal to the slip plane, while the dislocation segments bow-out in the z_2 direction whose direction cosines are ω_{2i}^{α}.

vi) The direction cosines of the co-ordinate system z_i^{α} are randomly distributed.

vii) Finally, dislocations will only interact with an externally applied stress field, i.e., the second order contributions, caused by the bowed-out dislocation segments, to the force exerted by the external stress

field on a dislocation segment will be neglected.

In summary, the model proposed for the study of the linear response characteristics of a polycrystalline aggregate consists of a large number of close-packed micro-elements of equal volume. Each micro-element in turn contains the same density of anchored semi-mobile dislocation segments which can only bow-out in one prefered slip direction differing from one crystal to another in a random fashion. Nonlinear contributions due to the interaction between these dislocation segments are neglected.

The quantitative description of this model will be given in the following chapter.

CHAPTER V

THE EFFECT OF DISLOCATIONS ON THE LINEAR ELASTIC RESPONSE OF POLYCRYSTALLINE METALS

The mechanisms for dislocations and the proposed analytical model discussed in the previous chapters will now be used to study the effect of dislocations on the quasi-static linear elastic response of polycrystalline solids. The retardation forces are neglected so that the response of the aggregate can be deduced using the equilibrium equations of linear elasticity and the dislocation string model discussed in Chapter III, implying that the deformation is completely reversible.

Within the framework of the above assumption and those given in Chapter IV, the total free energy U^n stored in a mesoscopic region of the solid due to an applied external load is equal to the sum of the strain energy stored in the elastic matrix and the increase in the self-energy of the anchored dislocation segments in each crystal summed up over the total number n of crystals in the polycrystalline aggregate. This may be expressed as follows:

$$U^n = \tfrac{1}{2} \sum_{\alpha=1}^{n} \{C_{ijkl} + \eta\, \Gamma^{\alpha}_{ijkl}\}\, \varepsilon^{\alpha}_{ij} \varepsilon^{\alpha}_{kl}\, \upsilon \qquad (5.1)$$

where:

$$C_{ijkl} = \lambda\delta_{ij}\delta_{ki} + 2\mu\delta_{ik}\delta_{jl}, \qquad (5.2)$$

is the fourth order isotropic tensor, $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$ is the Kronecker delta, and:

$$\eta = 2/3\pi\ \mu(1-\nu)\ell^2\tau\rho, \qquad (5.3)$$

$$\Gamma^{\alpha}_{ijkl} = \omega^{\alpha}_{3i}\omega^{\alpha}_{2j}\omega^{\alpha}_{3k}\omega^{\alpha}_{2l}. \qquad (5.4)$$

It should be noted that the second term on the right hand side of Equation (5.1) describes the influence of the deformation of the anchored dislocations on the work done by an external field. It is the product of the work done by the force $|F|\ell = \mu b\ell\varepsilon^{\alpha}_{32}$ acting on a dislocation segment of length ℓ to displace it a distance $\bar{\xi}^{\alpha}$, defined by Equation (3.5), and the number of mobile dislocation segments $\upsilon\tau\rho/\ell$ in the crystal. The transformation of the strain components $\varepsilon^{\alpha}_{32}$ from the z^{α}_{i} to the x_i co-ordinate system introduces the fourth order orientation tensor Γ^{α}_{ijkl} of Equation (5.4).

When expression (5.1) is differentiated with respect to $\upsilon\varepsilon^{\alpha}_{ij}$ the stresses in the α-th crystal are obtained, i.e.:

$$\sigma^{\alpha}_{ij} = (C_{ijk\ell} + \eta\Gamma^{\alpha}_{ijk\ell})\varepsilon^{\alpha}_{k\ell}, \tag{5.5}$$

$$\sigma^{\alpha}_{mm} = \{(3\lambda+2\mu)\delta_{k\ell} + \eta\Gamma^{\alpha}_{mmk\ell}\}\varepsilon^{\alpha}_{k\ell}, \tag{5.6}$$

$$\sigma'^{\alpha}_{ij} = \{2\mu\delta_{ik}\delta_{j\ell} + \eta(\Gamma^{\alpha}_{ijk\ell} - \tfrac{1}{3}\Gamma^{\alpha}_{mmk\ell}\delta_{ij})\}\varepsilon^{\alpha}_{k\ell}, \tag{5.7}$$

where:

$$\sigma'^{\alpha}_{ij} = \sigma^{\alpha}_{ij} - \tfrac{1}{3}\sigma^{\alpha}_{mm}\delta_{ij}, \tag{5.8}$$

and use has been made of relation (5.2). It can be seen from Equation (5.5), that due to the presence of dislocations, both the spherical components σ^{α}_{mm} as well as the deviatoric components σ'^{α}_{ij} of the stress tensor σ^{α}_{ij} contain the spherical and the shear components of the isotropic strain tensor.

In the present formulation, the strains $\varepsilon^{\alpha}_{ij}$ and the σ^{α}_{ij} pertaining to the α-th microelement are assumed to be random variables dependent on the orientation tensor $\Gamma^{\alpha}_{ijk\ell}$. These random quantities can be expressed in terms of an average, denoted by $\langle\cdot\rangle$, taken over the mesoscopic region, and a fluctuating component, denoted by *, where by definition $\langle^*\rangle = 0$.

Accordingly, when

$$\Gamma^{\alpha}_{ijkl} = \langle\Gamma_{ijkl}\rangle + \overset{*}{\Gamma}{}^{\alpha}_{ijkl}, \tag{5.9}$$

$$\varepsilon^{\alpha}_{ij} = \langle\varepsilon_{ij}\rangle + \overset{*}{\varepsilon}{}^{\alpha}_{ij}, \tag{5.10}$$

and

$$\sigma^{\alpha}_{ij} = \langle\sigma_{ij}\rangle + \overset{*}{\sigma}{}^{\alpha}_{ij}, \tag{5.11}$$

are substituted into Equation (5.5), the expression for the average and the fluctuating components of the stress tensor σ^{α}_{ij} are given by:

$$\langle\sigma_{ij}\rangle = C_{ijkl}\langle\varepsilon_{kl}\rangle + \eta\langle\Gamma_{ijkl}\rangle\langle\varepsilon_{kl}\rangle + \eta\langle\overset{*}{\Gamma}{}^{\alpha}_{ijkl}\overset{*}{\varepsilon}{}^{\alpha}_{kl}\rangle \tag{5.12}$$

$$\overset{*}{\sigma}{}^{\alpha}_{ij} = C_{ijkl}\overset{*}{\varepsilon}{}^{\alpha}_{kl} + \eta\{\langle\Gamma_{ijkl}\rangle\overset{*}{\varepsilon}{}^{\alpha}_{kl} + \overset{*}{\Gamma}{}^{\alpha}_{ijkl}\langle\varepsilon_{kl}\rangle + \overset{*}{\Gamma}{}^{\alpha}_{ijkl}\overset{*}{\varepsilon}{}^{\alpha}_{kl} - \langle\overset{*}{\Gamma}{}^{\alpha}_{ijkl}\overset{*}{\varepsilon}{}^{\alpha}_{kl}\rangle\} \tag{5.13}$$

It is important to note the dependence of $\langle\sigma_{ij}\rangle$ and $\overset{*}{\sigma}{}^{\alpha}_{ij}$ on the dislocation density, when $\eta = 0$, the stresses and the strains are only related through the isotropic material con-

stant tensor C_{ijkl}. On the other hand, when the fluctuating components of Γ^{α}_{ijkl} vanish, the average stresses depend in addition on the only preferred macroscopic direction of slip. The third term shows that due to the assumption made, there exists a correlation between the possible orientations and the strains defined as follows:

$$\langle \overset{*\alpha}{\Gamma}_{ijkl} \overset{*\alpha}{\epsilon}_{kl} \rangle = \lim_{N\to\infty} \sum_{\alpha=1}^{N} \overset{*\alpha}{\Gamma}_{ijkl} \overset{*\alpha}{\epsilon}_{kl} \quad /N+1. \qquad (5.14)$$

Similar remarks can be made concerning the fluctuating components $\overset{*\alpha}{\sigma}_{ij}$, given by Equation (5.13).

At this stage of the formulation, Axelrad's probabilistic concepts concerning the existence of a stress correlation function, i.e., a second order moment for the distribution, between two crystals in different stages of deformation is introduced. *D. R. Axelrad and L. G. Jaeger (1970).* The correlation theory, following Yaglom, hypothesises that for the description of a random process, its mean and correlation function have to be estimated. *A. M. Yaglom (1962).* However, it turns out that for a random function to be uniquely specified by the first and second moments, it is necessary as well as sufficient that its distribution be *Gaussian.* Thus, due to the lack of evidence to the contrary, and since

Random processes occuring in nature are often observed to be Gaussian, the independent variable $\Gamma^{\alpha}_{ijk\ell}$, as well as the dependent variables $\varepsilon^{\alpha}_{ij}$ and σ^{α}_{ij}, will be assumed normally distributed. *J. W. Provan (1971)*.

In a manner similar to the definition of the correlation given by Equation (5.14), the stress correlation may be approximated since the number n of crystals is finite in a mesoscopic region, as follows:

$$R_{ijk\ell}(\underset{\sim}{\sigma}^2:0;\underset{\sim}{\Psi}) = 1/n \sum_{\alpha=1}^{n} \overset{*}{\sigma}_{ij}(\underset{\sim}{x}^{\alpha})\overset{*}{\sigma}_{k\ell}(\underset{\sim}{x}^{\alpha}+\underset{\sim}{\Psi})$$

$$= \langle \overset{*}{\sigma}_{ij}(\underset{\sim}{x}^{\alpha})\overset{*}{\sigma}_{k\ell}(\underset{\sim}{x}^{\alpha}+\underset{\sim}{\Psi}) \rangle , \qquad (5.15)$$

where $\underset{\sim}{\Psi}$ is the vectorial distance between the centers of mass of the α-th crystal and the crystal at $\underset{\sim}{x}^{\alpha} + \underset{\sim}{\Psi}$. By analogy to the definition of the stress correlation tensor given in Equation (5.15), the correlation functions between the fluctuation components of the strain and orientation tensors are defined in the following manner:

$$R_{ijk\ell}(\underset{\sim}{\varepsilon}^2:0;\underset{\sim}{\Psi}) = \langle \overset{*}{\varepsilon}_{ij}(\underset{\sim}{x}^\alpha)\overset{*}{\varepsilon}_{ij}(\underset{\sim}{x}^\alpha+\underset{\sim}{\Psi})\rangle,$$

$$R_{ijk\ell mnpq}(0:\underset{\sim}{\Gamma}^2;\underset{\sim}{\Psi}) = \langle \overset{*}{\Gamma}_{ijk\ell}(\underset{\sim}{x}^\alpha)\overset{*}{\Gamma}_{mnpq}(\underset{\sim}{x}^\alpha+\underset{\sim}{\Psi})\rangle,$$

$$R_{ijk\ell mn}(\underset{\sim}{\varepsilon}:\underset{\sim}{\Gamma};\underset{\sim}{\Psi}) = \langle \overset{*}{\varepsilon}_{ij}(\underset{\sim}{x}^\alpha)\overset{*}{\Gamma}_{k\ell mn}(\underset{\sim}{x}^\alpha+\underset{\sim}{\Psi})\rangle, \tag{5.16}$$

$$R_{ijk\ell}(\underset{\sim}{\varepsilon}^2:\underset{\sim}{\Gamma};\underset{\sim}{\Psi}) = \langle \overset{*}{\varepsilon}_{ij}(\underset{\sim}{x}^\alpha)\overset{*}{\varepsilon}_{mn}(\underset{\sim}{x}^\alpha+\underset{\sim}{\Psi})\overset{*}{\Gamma}_{k\ell mn}(\underset{\sim}{x}^\alpha)\rangle,$$

$$R_{ijk\ell mn}(\underset{\sim}{\varepsilon}:\underset{\sim}{\Gamma}^2;\underset{\sim}{\Psi}) = \langle \overset{*}{\varepsilon}_{pq}(\underset{\sim}{x}^\alpha)\overset{*}{\Gamma}_{ijpq}(\underset{\sim}{x}^\alpha)\overset{*}{\Gamma}_{k\ell mn}(\underset{\sim}{x}^\alpha+\underset{\sim}{\Psi})\rangle,$$

$$R_{ijk\ell}(\underset{\sim}{\varepsilon}^2:\underset{\sim}{\Gamma}^2;\underset{\sim}{\Psi}) = \langle \overset{*}{\varepsilon}_{pq}(\underset{\sim}{x}^\alpha)\overset{*}{\varepsilon}_{mn}(\underset{\sim}{x}^\alpha+\underset{\sim}{\Psi})\overset{*}{\Gamma}_{ijpq}(\underset{\sim}{x}^\alpha)\overset{*}{\Gamma}_{k\ell mn}(\underset{\sim}{x}^\alpha+\underset{\sim}{\Psi})\rangle,$$

Using, for instance, Equation (5.13) the stress correlation tensor given by Equation (5.15) can be expressed in terms of the orientation and the strain correlations and their product moments given by Equations (5.16) in the following way:

$$
\begin{aligned}
R_{ijk\ell}(\underset{\sim}{\sigma}^2:0;\underset{\sim}{\Psi}) &= A_{ijk\ell pqmn}R_{pqmn}(\underset{\sim}{\varepsilon}^2:0;\underset{\sim}{\Psi}) \\
&+ B_{pqmn}R_{ijk\ell pqmn}(0:\underset{\sim}{\Gamma}^2;\underset{\sim}{\Psi}) \\
&+ C_{ijpqmn}R_{pqk\ell mn}(\underset{\sim}{\varepsilon}:\underset{\sim}{\Gamma};\underset{\sim}{\Psi}) \\
&- \eta^2 R_{pqijpq}(\underset{\sim}{\varepsilon}:\underset{\sim}{\Gamma};\underset{\sim}{\Psi})R_{mnk\ell mn}(\underset{\sim}{\varepsilon}:\underset{\sim}{\Gamma};\underset{\sim}{\Psi}) \\
&+ D_{ijpq}R_{pqk\ell}(\underset{\sim}{\varepsilon}^2:\underset{\sim}{\Gamma};\underset{\sim}{\Psi}) \\
&+ E_{mn}R_{ijk\ell mn}(\underset{\sim}{\varepsilon}:\underset{\sim}{\Gamma}^2;\underset{\sim}{\Psi}) \\
&+ \eta^2 R_{ijk\ell}(\underset{\sim}{\varepsilon}^2:\underset{\sim}{\Gamma}^2;\underset{\sim}{\Psi}) \qquad (5.17)
\end{aligned}
$$

where:

$$A_{ijklpqmn} = (C_{ijkl}+\eta\langle\Gamma_{ijpq}\rangle)(C_{klmn}+\eta\langle\Gamma_{klmn}\rangle),$$

$$B_{ijkl} = \eta^2\langle\varepsilon_{ij}\rangle\langle\varepsilon_{kl}\rangle,$$

$$C_{ijklmn} = 2\eta(C_{ijkl}+\eta\langle\Gamma_{ijkl}\rangle)\langle\varepsilon_{mn}\rangle, \qquad (5.18)$$

$$D_{ijkl} = 2\eta C_{ijkl},$$

$$E_{ij} = 2\eta^2\langle\varepsilon_{ij}\rangle.$$

Implicit in the above derivation is the assumption of *statistical homogeneity*, i.e., independence of the specific position $\underset{\sim}{x}^{\alpha}$, according to which the following relations were substituted:

$$\langle\overset{*}{\sigma}_{ij}(\underset{\sim}{x}^{\alpha})\overset{*}{\Gamma}_{klmn}(\underset{\sim}{x}^{\alpha})\rangle = \langle\overset{*}{\sigma}_{ij}(\underset{\sim}{x}^{\alpha}+\underset{\sim}{\psi})\overset{*}{\Gamma}_{klmn}(\underset{\sim}{x}^{\alpha}+\underset{\sim}{\psi})\rangle$$

$$\langle\{\overset{*}{\sigma}_{ij}(\underset{\sim}{x}^{\alpha})\overset{*}{\sigma}_{kl}(\underset{\sim}{x}^{\alpha}+\underset{\sim}{\psi})\}\overset{*}{\Gamma}_{pqmn}(\underset{\sim}{x}^{\alpha})\rangle =$$

$$\langle\{\overset{*}{\sigma}_{ij}(\underset{\sim}{x}^{\alpha})\overset{*}{\sigma}_{kl}(\underset{\sim}{x}^{\alpha}+\underset{\sim}{\psi})\}\overset{*}{\Gamma}_{pqmn}(\underset{\sim}{x}^{\alpha}+\underset{\sim}{\psi})\rangle \qquad (5.19)$$

$$\langle\{\overset{*}{\Gamma}_{ijkl}(\underset{\sim}{x}^{\alpha})\overset{*}{\Gamma}_{pqmn}(\underset{\sim}{x}^{\alpha}+\underset{\sim}{\psi})\}\overset{*}{\sigma}_{rs}(\underset{\sim}{x}^{\alpha})\rangle =$$

$$\langle\{\overset{*}{\Gamma}_{ijkl}(\underset{\sim}{x}^{\alpha})\overset{*}{\Gamma}_{pqmn}(\underset{\sim}{x}^{\alpha}+\underset{\sim}{\psi})\}\overset{*}{\sigma}_{rs}(\underset{\sim}{x}^{\alpha}+\underset{\sim}{\psi})\rangle$$

Thus, Equation (5.17) represents the general expression for the stress correlations, for the case where the stresses and the strains are dependent on the orientations. In this context it is important to note that once the strain and the orientation correlation tensors as well as their product moments have been experimentally determined, the stress correlation tensor can be obtained from expression (5.17).,which in addition to the mean value, given by Equation (5.12), will uniquely specify the probability distribution of the stresses in the polycrystalline aggregate. An experimental determination of the displacement of crystals in a model of a two phase structure has been shown to be possible using stress holographic interferometry. *J. Kalousek (1971).*

In discussing the general expression for the stress correlation tensor given in Equation (5.17) four cases that demonstrate the implications of some of the underlying assumptions concerning the linear response characteristics of solids may be discerned:

i) The crystal orientations have a uniform random distribution, thus implying statistical isotropy in addition to the statistical homogeneity. The case of isotropic homoeneity has been dealt with by Barenblatt and Gorodtsov in their discussion of the

random field of microstresses in the steady plastic flow of polycrystalline solids, *G. I. Barenblatt and V. A. Gorodtsov (1963)*. However, these authors did not include in their formulation the dependence of the stresses on either the crystals orientation or the dislocation density. In the present analysis so that the condition of statistical isotropy of the stress correlation tensor holds, the correlations and the product moments given in Equations (5.15) and (5.16) are redefined, for example, as follows:

$$R_{ijk\ell}(\underset{\sim}{\varepsilon}^2:0;\Psi) = 1/n+1 \sum_{\alpha=1}^{n} \{1/p \sum_{\gamma=1}^{p} \overset{*}{\varepsilon}_{ij}(\underset{\sim}{x}^{\alpha})\overset{*}{\varepsilon}^{\gamma}_{k\ell}(\underset{\sim}{x}^{\alpha}+\Psi)\}, \tag{5.20}$$

where the scalar $\Psi = |\underset{\sim}{\Psi}|$ has replaced the vector $\underset{\sim}{\Psi}$. Ψ may be visualized as representing the radius of a sphere centered at $\underset{\sim}{x}^{\alpha}$ on the surface of which lie the centers of mass of p crystals. Since the influence on the α-th crystal's state of stress by that of the neighboring crystals decreases with increasing Ψ, it may further be conjectured that p is the number of crystals in direct contact with the α-th crystal. It should be noted that the assump-

tion of isotropic homogeneity is frequently made in the analysis of turbulence in fluids.

ii) Under the assumption that the strains are independent of the orientations, the terms on the right hand side of Equation (5.17) which contain second and third order product moments will vanish, *V. S. Pugachev (1965)*. Moreover, the last term in this equation will be expressed as the product of the orientation and the strain correlation tensors. Hence, the expression for the stress correlation tensor will become:

$$R_{ijk\ell}(\underset{\sim}{\sigma}^2 : 0; \underset{\sim}{\Psi}) = A_{ijk\ell pqmn} R_{pqmn}(\underset{\sim}{\varepsilon}^2 : 0; \underset{\sim}{\Psi}) + B_{pqmn} R_{ijk\ell pqmn}(0 : \underset{\sim}{\Gamma}^2; \underset{\sim}{\Psi}) + R_{pqmn}(\underset{\sim}{\varepsilon}^2 : 0; \underset{\sim}{\Psi}) R_{ijpqk\ell mn}(0 : \underset{\sim}{\Gamma}^2; \underset{\sim}{\Psi}) \tag{5.21}$$

It follows therefore that the strain and orientation correlations represent the only quantities required to be experimentally determined for the unique specification of the stress state.

iii) In the work by *J. S. Koehler (1952) and A. V. Granato (1968)*, dealing with the internal friction in solids; it is implied in the derivation of the equations of motion that the distribution of the orientation tensor is a delta-function, i.e., that all mobile dislocations in a mesocopic region are constrained to move in slip planes having the same normal. Furthermore, this is equally the same assumption made by *H. Zorski (1968)* in his derivation of the equations of motion of a compound medium made up of an elastic matrix and a dislocation fluid. If this assumption is adopted, the stress correlation tensor can be written as follows:

$$R_{ijk\ell}(\underset{\sim}{\sigma}^2:0;\underset{\sim}{\Psi}) = A_{ijk\ell pqmn}{}^{R}{}_{pqmn}(\underset{\sim}{\varepsilon}^2:0;\underset{\sim}{\Psi}), \qquad (5.22)$$

i.e., the stress correlation is expressed in terms of the dislocation density, the average orientation and the strain correlation tensors. In the absence of dislocations, $A_{ijk\ell pqmn}$ will only depend on the isotropic tensor $C_{ijk\ell}$ defined in Equation (5.2)

iv) For completeness and although not directly related to the present analysis, an assumption is frequently encountered in literature dealing with the

plastic deformation of a polycrystalline metal, according to which the strain in each crystal corresponds to macroscopic strain, i.e., if, for instance, a uni-axial load is applied to a metal, each crystal will deform as if it were under uni-axial loading. *J. F. W. Bishop and R. Hill (1951a) and (1951b).* Assuming that this is the case, the fluctuating components of the strain will vanish and the stress correlation tensor can be expressed as follows:

$$R_{ijkl}(\underset{\sim}{\sigma}^2:0;\underset{\sim}{\Psi}) = B_{pqmn}R_{ijklpqmn}(0:\underset{\sim}{\Gamma}^2;\underset{\sim}{\Psi}) \qquad (5.23)$$

i.e., it is only dependent on the dislocation density, the average strains and the orientation correlation tensor. If the dislocation density vanishes, the stress correlation tensor vanishes, too.

Finally, a similar relation expressing the strain correlation tensor in terms of the stresses and the orientation correlation functions can be obtained in an analogous manner to the derivation of Equation (5.17). However, such an expression would not be of practical significance due to the conceptual difficulties encountered in evaluating the stress distribution. On the other hand, Equation (5.17), at least

in principle, yields ideally to experimental techniques.

CHAPTER VI

SUMMARY AND CONCLUSIONS

In studying the effect of dislocations on the linear elastic response of polycrystalline metals an ordering, indispensable for any analytic approach to be successful, has been incorporated making use of the three size scales introduced by Axelrad. It has been assumed that the close-packed crystals forming the heterogeneous aggregate are of equal volume each containing the same density of mobile dislocations anchored on their respective slip planes by impurity atoms. It has been further assumed that within a particular crystal the mobile dislocation segments have the same length and orientation and lie in slip planes having the same normal. On the other hand the slip directions vary from crystal to crystal in a random fashion.

The derivation of the equations pertaining to the equilibrium of stresses using an energy argument in which the dissipation has been neglected, introduces a fourth order orientation tensor appearing in conjunction with a term containing the dislocation density. Due to this orientation tensor the spherical as well as the deviatoric components of the stresses within a crystal were shown to depend on both the spherical

and shear components of the strain tensor. Furthermore, when the stresses and strains are assumed to be random variables, dependent on this orientation tensor, the average stresses have been found to depend on the averages of the strains and orientations throughout a mesoscopic region as well as the second order product moments of the strains and orientations. This is an extension over any continuum theory which, by definition, is totally incapable of including such a term.

A stress correlation tensor has been obtained in terms of correlations and product moments of the strain and orientation tensors assuming statistical homogeneity. Once the mean value and the stress correlation tensor are determined the distribution of stresses within a mesoscopic region of the polycrystalline aggregate can be uniquely determined, under the assumption that the strains and orientations throughout the mesodomain are normally distributed. Tests are being conducted in the Micromechanics Laboratory of McGill University to test the validity of this assumption when applied to displacements in a two-phase material.

Four cases pertaining to the evaluation of the stress correlation tensor have been discussed and, by indicating their connection to the general expression for the stress

correlation tensor, the implications of certain assumptions frequently encountered in the literature have been underlined. In the case where statistical isotropy is assumed it was shown that the dependence of the correlations on a vectorial geometric quantity could be relaxed to the dependence on a scalar representing the location of the centers of mass of crystals directly in contact with the one under consideration. The second dealt with the assumption concerning the independence of the strain and orientation tensors, in which it was shown that the orientation correlations are the only necessary functions required for the estimation of the stress correlation tensor. The third case concerned the assumption of one common slip direction for all crystals in a mesoscopic region. It followed that the stress correlations only depend upon the strain correlation functions. Finally, corresponding to the assumption made in the study of plastic deformation in polycrystalline solids, the effect of assuming that the fluctuating components of the strains vanish was examined.

By estimating the stress correlations in accordance to the general expression or to any of the four cases previously discussed it is possible quantitatively to estimate the number of crystals in which the shear stresses will exceed the value required for the activation of the Frank-Read mechanism. Accordingly the study which has been presented here may be

considered as an important step in the redefinition of certain basic concepts pertaining to the proper use of materials, since it leads to a specification of the limitations on the linear elastic response of polycrystalline metals containing dislocations.

Now, since the model proposed in the present work is only related to linear effects, several extensions naturally present themselves. The most obvious is to include dissipative effects by taking into consideration the activation of the Frank-Read mechanism. This will automatically extend the range of study into irreversible response characteristics of polycrystalline materials as proposed in Chapter III. Furthermore, since no feasible extension can justifiably ignore the interaction between two or more activated Frank-Read sources, a possible technique which includes such influences is at present under review. Briefly, it involves concepts similar to those leading to the Boltzmann equation for rarified gases where the dislocation interaction is analogous to the collision terms in the Boltzmann equation.

It is hoped by investigating this phenomenon to eventually arrive at a formulation which quantitatively describes fatigue failure in polycrystalline aggregates.

LIST OF REFERENCES

Axelrad, D. R., "Rheology of Structured Media," Archwm. Mech. stosow., in Press, *(1971)*.

Axelrad, D. R. and Jaeger, J. G., "Random Theory of Deformation in Heterogeneous Media," Pub. John Wiley and Sons, Ltd., London *(1970)*.

Barenblatt, G. J., and Gorodstov, V. A., "On the structure of the Field of Microstresses of Steady Plastic Flow," P.M.M., *(1964)*.

Bishop, J. F. W., and Hill, R., "A Theory of the Plastic Distortion of a Polycrystalline Aggregate under Combined Stresses," Phil. Mag., 42, pp. 414-427, *(1951a)*.

Bishop, J. F. W., and Hill, R., "A Theoretical Derivation of the Plastic Properties of a Polycrystalline Face-Centered Metal," Phil. Mag., 42, pp. 1298-1307, *(1951b)*.

Bullough, R., and Newman, R. C., "The Kinetics of Migration of Point Defects to Dislocations," Rep. Prog. Phys., 33, pp. 101-148, *(1970)*.

Cottrell, A. H., "Dislocations and Plastic Flow in Crystals," Clarendon Press, Oxford, *(1953)*.

Cottrell, A. H. "Theory of Crystal Dislocations," Gordon and Breach, New York, London, *(1964)*.

Frank, F. C., and Read, W. T., " Mechanism for the Multiplication of dislocations," Phys. Rev., 79, pp. 722-723, *(1951)*.

Granato, A. V., "Internal Friction Studies of Dislocation Motion," Dislocation Dynamics, Pub. McGraw-Hill, New York, pp. 117-157, (1968).

Johnston, W. G., and Gilman, J. J., "Dislocation Velocities, Dislocation Densities, and Plastic Flow in Lithium Fluoride Crystals," J. Applied Physics, 30, pp. 129-144, (1959).

Kalousek, J., "Stress Holographic Interferometry," Micromechanics of Solids Laboratory, Dept. of Mech. Eng., McGill Univ., Montreal, (to be published) (1971).

Koehler, J. S., "The Influence of Dislocations and Impurities on the Damping and the Elastic Constants of Metal Single Crystals,""Imperfections in Nearly Perfect Crystals," Shockley, Holloman, Maurer, Seitz, (Eds.), John Wiley and Chapman Hall, (1952).

Mott, N. F., "Mechanical Strength and Creep in Metals," in "Imperfections in Nearly Perfect Crystals," Shockley, Holloman, Maurer, Seitz, (Eds.), John Wiley and Chapman Hall, (1952).

Peierls, R. "The Size of a Dislocation," Proc. Phys. Soc., 52, pp. 34, (1940).

Plumbridge, W. J., and Ryder, D. A., "The Metallography of Fatigue," Metals and Materials and Metallurgical Reviews, 3, pp. 119-142, (1969).

Provan, J. W., "Deformation of Randomly Oriented Media," Archwm. Mech. stosow., in Press, (1971).

Pugachev, V. S., "Theory of Random Functions," Addison-Wesley Pub., Mass., (1965).

van Bueren, H. G., "Imperfections in Crystals," North Holland Pub. Co., Amsterdam, (1960).

Weertman, J., "Response of Metals to High Velocity Deformation," Metallurgical Society Conferences, Sheroman, P. G. and Zackary, V. P., (Eds.), Interscience, New York, pp. 205-247, (1961).

Yaglom, A. M., "Theory of Stationary Random Functions, Transl. by R. A. Silverman, Prentice-Hall, Inc., (1962).

Yazu, K., "Dislocation Pile-Up in the Primary System," Trans. JIM, Vol. 9, Supplement, pp. 10-20, (1968).

Zorski, H. "Statistical Theory of Dislocations," Int. J. Solids Structure, Vol. 4, pp. 959-974, Pergamon Press, G.B., (1968).