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Rice University, Ph.D., 1973
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PROBLEMS IN THE DEFORMATION OF METALS:
(1) VACANCY FORMATION FREE ENERGY;
(2) DISLOCATION ATTACK FREQUENCY;
(3) MICROSTRAIN IN STAGE I-EASY GLIDE REGION

by

William Joseph Arnoult III

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF

DOCTOR OF PHILOSOPHY

Thesis Director's signature:

Houston, Texas

May, 1973
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(2) DISLOCATION ATTACK FREQUENCY;
(3) MICROSTRAIN IN STAGE I—EASY GLIDE REGION

William Joseph Arnoult III

ABSTRACT

Specific problems associated with establishing an understanding of the defect structure and mechanical behavior of metals were treated. Analytical and experimental approaches to the problems were taken and the results contribute to the present knowledge and state of the field.

In Chapter I a new insight was given to the isotropic elastic continuum approach for the energy of vacancy formation. The misfitting sphere model of Friedel was employed under the assumption that the vacancy core is not a void region but contains a Fermi gas created by the local electronic rearrangement. The electron gas or fluid has a definite volume and compressibility. Three criteria were set forth. First, the boundary conditions at the interface between the vacancy and lattice region are satisfied so as to render the defect free of external stresses. Second, the experimentally determined value of vacancy formation volume to atomic volume was employed. Third, Voight averaged elastic constants were used to assure consistency with the uniform strain condition. The model not only gave good agreement with the experimentally determined values of formation energy for a wide variety of metals, but can predict the percentage of total energy contributed by the core region.
In Chapter II a complete non-quantum mechanical study of the stress dependence of dislocation attack frequency was made by considering all the physical parameters of a wide variety of dislocation-obstacle configurations. First the local, one dimensional fundamental attack frequency of the dislocation segment in front of the obstacle was found for the Mott-Nabarro cosine interaction law, the Cottrell-Bilby continuously pinned dislocation interaction relation, the Seeger large obstacle rigid barrier dislocation interaction, the Fleischer and Modified Fleischer tetragonal distortion interaction, the quasi-parabolic Peierl's mechanism for kink formation, the Saada forest dislocation interaction, and for the constriction and jog formation intersection mechanism in a dissociated glide dislocation. This local frequency was found over a continuous range of stress up to the maximum internal stress of the configuration. Second, the natural frequency of vibration of the dislocation line between obstacles was found taking into account the change in length as the dislocation bows out and encounters other obstacles over the same continuous range of stress. Third, in each configuration the randomly, discretely and continuously pinned cases were considered. Also, the effect of the longer dislocation segment on the frequency of the shorter was taken into account by employing an appropriate harmonic averaging technique. Coupling and correlation effects of the segments of dislocation next to and remote from the barrier were neglected. The stress dependence of the dislocation attack frequency thus evaluated is significant and should be considered and included in dislocation dynamic problems.

In Chapter III, the macroscopic work hardening theories of Seeger et al., Van Bueren, Hirsch and Lally,
and Hazzledine have all been extended to the microstrain region after easy glide prestrain according to the assumptions of Salama and Roberts in this region. By combining microstrain data taken on single crystal magnesium samples with optical and electron microscopic studies of slip line length and separation distance, the suitability of each theory was evaluated. The analysis demonstrated that only the Salama–Roberts modification of the Van Bueren macroscopic work hardening relation semi-quantitatively and qualitatively predicts the static and dynamic aspects of the microscopic and macroscopic parameters of the stage one work hardening in single crystal magnesium. The one-quarter power relation of microstrain related to stress appears to be the dominant stress-microstrain law for magnesium after Stage I prestrain.
CHAPTER I

ON THE ELASTIC APPROXIMATION TO THE
VACANCY FORMATION ENERGY IN METALS

1.1 INTRODUCTION

There exists in the literature many models for estimating the energy of formation of vacancies in metals. These models represent either the isotropic or anisotropic homogenous elastic strain approximation [1.1-1.5] or the discrete atomic lattice model, and sometimes a combination of the two approaches is employed [1.1, 1.6-1.14]. Hall [1.1] and Gibbs [1.4] made a qualitative comparison between the two model types and showed how the discrete and elastic continuum models are basically related. The elastic model can represent the smoothing out of a discrete atomic displacement model without serious loss of quantitative stored energy value estimates. The results derived from the discrete atomistic approach are usually very sensitive to the assumed interaction potential. The present paper attempts to place new insight into the elastic continuum model. This is accomplished by assuming the vacancy core is not a void region but one containing a Fermi gas which can be assigned isotropic elastic constants. Under this assumption, the model predicts half the energy of vacancy formation is contributed by the core region.
To apply the isotropic elastic continuum model to the calculation of the energy of vacancy formation, three basic criteria must be satisfied. Firstly, the boundary conditions at the interface between the vacancy and the lattice region should be satisfied so as to render the defect free of external stresses [1.15]. Secondly, the ratio of the vacancy formation volume to the atomic volume should be equal to the experimentally determined value which is found to be approximately 0.5 for metals with cubic symmetry [1.16-1.20]. Thirdly, a Voigt [1.21] average over the single crystal elastic constants should be used in order to assure the solution is for the uniform strain condition [1.22].

The present work modifies the misfitting sphere model of Friedel [1.23-1.25], so that self-consistent elastic continuum relationships are obtained. In these calculations the three criteria for the model are satisfied. The thermodynamic parameters related to vacancy formation are developed and the calculated values are compared with known experimental results.
1.2 THE FRIEDEL MODEL

In the elastic model due to Friedel [1.23-1.25] a spherically symmetric isotropic material I is assumed having radius \( R \), atomic radius \( a \), and compressibility and shear modulus \( \chi \) and \( \mu \) respectively. A spherical cavity of volume \( \Omega = 4\pi a^3 / 3 \) is removed from the interior of the bulk and replaced by a material II with atomic radius \( a' \), and compressibility and shear modulus \( \chi' \) and \( \mu' \) respectively. The two materials are then allowed to adjust under the influence of unbalanced surface stresses across their respective interfaces until the latter become one and the same interface. Continuity of the two media exists at a radius \( b \). At this point, the surface traction on the two interfaces cancel to leave the resultant interface stress free. The displacements in materials I and II have the respective functional forms

\[
U_I (\vec{r}) = Br + Cr/|r|^3 \quad (1.1)
\]

\[
U_{II} (\vec{r}) = Ar \quad (1.2)
\]

where \( A \), \( B \) and \( C \) are constants to be determined from the boundary conditions. Balancing the stresses in medium I and II at \( r = b \) and imposing continuity of media yields:
A = -\eta \chi' / x \chi \beta \\
B = \eta b^3 / x \kappa^3 \beta \\
C = \eta b^3 / \beta 

where \ \eta = (a'-a)/b , \ x = 3/4 \mu \chi \ and \ \beta = 1 + \chi' / x \chi .

1.3 APPLICATION TO VACANCIES

1.3.1 The Elastic Model

To apply this model to vacancies, material II is assumed to be a compressible and perturbed Fermi electron gas originating from the local electron charge redistribution when a vacancy is formed and the local lattice relaxes. The effective electron gas pressure in the vacancy cavity is balanced with the negative pressure of the relaxing elastic material across the interface at \ r = b , so that

\[-4 \mu \eta / \beta = 3/5 \chi' \]

The expression for the bulk modulus of a free electron gas has been employed [1.26] in the above relation. This expression is consistent with vacancy formation because when the ion core is removed, the surrounding lattice
relaxes and, although the electron density is initially low, the screening radius, \( r_s \) \([1.27]\), decreases from its initial value of 3 to 5 to \( r_s \approx 1 \). The electrons in the vacancy core region should then be approximately non-interacting.

The elastic model described above defines the displacement at \( r = b \) as radial and equal to \((b - a)\), so that the local vacancy dilatation is \(3(b - a)/a\). We define the local vacancy dilatation as \((f - 1)\) where \( f \) is the experimentally evaluated vacancy formation volume ratio. The local and atomic vacancy dilatations being assumed equal, it follows that:

\[
3(b - a)/b = f - 1
\]  

(1.7)

where the approximation \((b - a)b \approx (b - a)a\) has been made and an error of less than 10\% introduced. The reported experimental values of \( f \) appear to be in agreement only to within 20\%. Also, the volume change at the external surface \((\Delta V)_{r=R} = 4\pi R^2 U_1(R)\) is found to be \((f - 1)\Omega\) within 20\% accuracy for all metals considered in this paper except Cd, Zn and Sn. In most cases the accuracy was within 10\% which makes the preceding approximation a self-consistent model. The exact expression for \((\Delta V)_{r=R}\) is given by \((\Delta V)_{r=R} = (f - 1)\Omega 27(1 + 4\mu\chi/3)/(4 - f)^3\).
The continuity of media criterion of the elastic model shows:
\[ \mathcal{B}_b = a' + a'\chi'/\chi \]  \hspace{1cm} (1.8)

Solution of Eq. (1.6), (1.7) and (1.8) shows that:
\[ b = \frac{3a}{(4 - f)} \]  \hspace{1cm} (1.9)
\[ a' = \frac{[3a + a(f-1)\chi'/\chi]}{(4 - f)} \]  \hspace{1cm} (1.10)
and \[ \chi' = \frac{9}{20} \mu(1 - f) \]  \hspace{1cm} (1.11)

The elastic stored energy of the vacancy is found by evaluating the work done on the internal surface of medium I and the external surface of medium II, each surface undergoing determined displacements under known forces. Combining the two contributions to the total energy, one finds the elastic stored energy per vacancy to be:
\[ E_0 = \frac{8\pi\mu\eta^2b^3}{(1 + 4\mu\chi'/3)} \]  \hspace{1cm} (1.12)

Use of Eq. (1.9), (1.10) and (1.11) reduces Eq. (1.12) to:
\[ E_0 = \frac{18(1 - f)^2}{(4 - f)^3} \left[ 1 + \frac{3}{5(1 - f)} \right] \mu\Omega \]  \hspace{1cm} (1.13)
1.3.2 Thermodynamics of the Model

The elastic stored energy $E_0$ is a Gibbs free energy associated with forming a vacancy. Following a development given by Friedel [1.23,1.24], the total free energy change per vacancy in the crystal can be considered as the sum of two terms:

$$\Delta G = \Delta G_1 + \Delta G_2$$  \hfill (1.14)

where $\Delta G_1$ is the configurational free energy change associated with placing a vacancy in the crystal so that:

$$\Delta G_1 = kT \left\{ c_v \ln c_v + (1 - c_v) \ln (1 - c_v) \right\}$$  \hfill (1.15)

where $c_v$ is the atomic concentration of vacancies and $k$ and $T$ have their usual meaning. $\Delta G_2$ is the Gibbs free energy change per vacancy due to other contributing terms and may be written as

$$\Delta G_2 = \Delta H_2 - T \Delta S_2$$  \hfill (1.16)

where $\Delta H_2$ is the enthalpy of formation of the defect and $\Delta S_2$ is an entropy change due to the change in vibrational frequency of the atoms locally associated with the crystal defect. Knowing $E_0$ to be the Gibbs free energy change evaluated at low temperature ($0^\circ K$ in the present paper), one obtains the vacancy formation enthalpy at any
temperature $T$, as

$$\Delta H_2 = E_O + T\left(\frac{dE_O}{dT}\right)_{P,c_v}$$  \hspace{1cm} (1.17)

The total free energy change of the crystal is therefore

$$\Delta G = c_v\left[E_O + T\left(\frac{dE}{dT}\right)_{P,c_v} - TS_2\right] + kT\left[c_v\ln c_v + (1-c_v)\ln(1-c_v)\right]$$  \hspace{1cm} (1.18)

The size effect refinement is neglected in this type of calculation [1.28] since the radius of the sample is assumed to be in the macroscopic size range of 1 cm. Upon minimizing $\Delta G$ with respect to $c_v$, one finds the equilibrium concentration of vacancies, $c_v^0$, to be

$$c_v^0 = \exp\left\{\frac{-E_O - T\left(\frac{dE}{dT}\right)_{P,c_v} + T\Delta S_2}{kT}\right\}$$  \hspace{1cm} (1.19)

Differentiation of Eq. (1.12) with respect to $T$ yields

$$\left(\frac{dE_O}{dT}\right)_{P,c_v} = E_O(3\alpha + \frac{\delta\mu}{\mu dT})$$  \hspace{1cm} (1.20)

where $\alpha$ is the coefficient of linear expansion.

To evaluate $\Delta S_2$, it is assumed that each atom can be approximated as a simple harmonic oscillator vibrating with a frequency $\nu$. Applying a high temperature approximation to a quantum statistical average vibrational energy, the free energy per oscillator per degree of freedom is
found to be $kT \ln(h\nu/kT)$ [1.29]. Differentiating this expression with respect to temperature, one finds the change in atomic vibrational entropy to be

$$\Delta S_2 = -k \ln(\nu'/\nu)$$

(1.21)

where $\nu'$ is a reduced vibration frequency per atom associated with the relaxed lattice neighboring the vacancy. Because $\nu'$ is very close to $\nu$, $\ln(\nu'/\nu)$ can be expanded in a Taylor series around $\nu$. Multiplying and dividing by the local lattice dilatation, $\Delta V/\Omega$, it is found per $Z$ nearest neighbor oscillators per degree of freedom that:

$$\Delta S_2/\Delta V = -Zk \frac{d(\ln \nu)}{\Omega} \frac{d(\ln \nu)}{d(\ln \nu)}$$

(1.22)

The negative of the differential is the Grüneisen's constant, $\gamma$, which is relatively independent of the temperature and the Einstein frequency. Since the local atomic dilatation per oscillator surrounding the vacancy is given by $(1 - f)/Z$ and we assume, as did Cottrell [1.30] for the atoms near the core of a dislocation, that only one degree of freedom has its frequency perturbed, Eq. (1.22) becomes:

$$\Delta S_2 = k\gamma(1 - f)$$

(1.23)
Applying relations (1.20) and (1.23) to (1.19), one obtains:

\[ c_v^0 = \exp\left[ \frac{-E_o}{kT} \right] \exp\left[ \frac{-E_o(3\alpha + \delta \mu/\mu dT) + k\gamma(1-f)}{k} \right] \]

(1.24)

1.3.3 Application of the Model to Experiment

The concentration of vacancies is determined experimentally usually by either resistivity measurements on quenched wires or by the simultaneous measurement of length and lattice parameter change. When \( \ln c_v^0 \) or some property proportional to \( c_v^0 \) is plotted vs \( 1/kT \), the slope of the resultant straight line is designated \( E_v^f \) and the intercept at \( 1/T \to 0 \) is designated \( S_v^f \). From Eq. (1.24) then, it appears:

\[ E_o = E_v^f \]

(1.25)

and

\[ S_v^f = k\gamma(1-f) - E_o(3\alpha + \delta \mu/\mu dT) \]

(1.26)
1.3.4 Prediction and Results of the Model

The present model has been solved, i.e., Eqs. (1.13) and (1.26) evaluated for a variety of metals with cubic symmetry using the experimentally determined value of 0.5 for $f$. Low temperature values (near $0^\circ K$) of the elastic constants published by Simmons [1.31] were used in the calculations. The Voigt elastic constants $\mu_v$ and $\chi_v$ were evaluated and $d\mu/dT$ was calculated at room temperature from the selected single crystal data published by Simmons. Values of $\Omega$ and $\alpha$ were taken from the Metals Handbook [1.32] and values of $\gamma$ were taken from Mott and Jones [1.29]. Table 1.1 lists the values of the actual physical constants employed. The temperature for which the elastic constants were determined was $0^\circ K$ unless stated otherwise.

A wide range of experimental values of $E_v^f$ and $S_v^f$ were found to exist in the literature. Friedel's published values, being averages of many experimental observations, were used in conjunction with the latest review articles [1.33,1.34] to yield the experimental values cited in Tables 1.2 and 1.3. There now appears to be unanimity of many investigators for the $E_v^f$ values, but we have favored the more recent and slightly higher experimental values for $S_v^f$ reported in the review book due to Seeger et al. [1.33].
Table 1.2 suggests that the present model with the value of 0.5 for $f$ yields good agreement with the experimentally determined values of vacancy formation energy for a variety of cubic metals. Agreement was also found in the case of the almost ideally close-packed hcp metals, Mg and Co ($c/a = 1.623$). This agreement can be expected since the value of $f = 0.5$ used in calculating $E_f$ is that determined experimentally on gold and copper. Co undergoes a phase change to fcc at $703^\circ K$ and it is not known over what temperature range the referenced experimental value of formation energy was determined. It is interesting that agreement is obtained in this case where the elastic constant undergoes a change. Using the same value of $f$ in the case of bct Sn and hcp Zn and Cd ($c/a = 1.856, 1.886$ respectively), the agreement was poor. Knowing the experimentally determined values of the vacancy formation energy for these metals, $f$ was adjusted in Eq. (1.13) until agreement was obtained. For Cd and Zn a value of $f = 0.78$ and for Sn a value of $f = 0.75$ was obtained. These $f$ values are in fair agreement with the value of 0.67 for $f$ assumed by Wallmark and Gilder [1.35] in their work on Zn. Higher values of $f$ than 0.5 suggest that there is less lattice relaxation in the non-cubic lattices than the fcc lattices.

The ratio $E_{core}/E_{total}$, the fraction of core energy to total energy of vacancy formation, is found from
the theory to be $E_{\text{core}}/E_{\text{total}} = 3/[5(1 - f) + 3]$. Table 1.2 shows this ratio varies from 0.55 for cubic crystals to 0.72 for the hcp, indicating that the largest portion of the total defect formation energy is contributed by the core region. One minus this ratio clearly yields the fraction of the total energy of formation stored as elastic energy in the lattice surrounding the vacancy, i.e., medium I.

In addition to the results reported in Table 1.2, the energy of vacancy formation was calculated using the arithmetic average [1.36] of the Voigt and Reuss [1.22] appropriate elastic constants for each element. The energies thus evaluated were found to be consistently smaller in value by 30% than those shown in Table 1.2. This result indicates that the Voigt average forms an upper bound to the various averaging techniques and the uniform strain elastic constant appears to be correct for this type of calculation.
1.4 DISCUSSION

Table 1.2 shows that the present model predicts rather well the energy of vacancy formation in many metals with the exception of some of the bcc metals. This agreement is rather surprising when one considers the approximations involved in the present model which might alter the true representation of the displacement field. The linear 2nd order anisotropic elastic solution to this problem for crystals of cubic symmetry has been recently published by Masumura and Sines [1.39]. These authors normalized the anisotropic radial displacement to the isotropic case. The present authors find this normalizing constant to be the same as that used in the current calculations, i.e., C in Eq. (1.1). Therefore, it is expected that the displacement strengths in the current study are comparable to those of the anisotropic solution even though the direction and senses are different. Energy calculations are not sensitive to the anisotropy or azimuthal variation of the radial displacements but depend strongly on their magnitude. The present model treats the electronic charge redistribution near the vacancy in a phenomenological manner and does not take into consideration the nonlinearity in the stress-strain behavior. However, it would be possible to extend the present calculations to include third order effects in a similar manner.
as described by Holder and Granato [1.40].

There are, however, distinct advantages to the current type of calculation. The local ion core rearrangement due to their mutual repulsion [1.1] and the electron charge density redistribution at the vacancy site have, in fact, been qualitatively considered through the estimated core distortion as a medium of different compressibility and shear modulus from the host lattice. Secondly, the model predicts that more than one-half of the energy of vacancy formation is local core energy and the remaining amount originates from the elastic distortion of the surrounding medium. This result is in good agreement with the work of Hall [1.1], who also quantitatively compared the core to surrounding lattice stored energy. In the latter work, the comparison is made from a discrete lattice type calculation and the average value of the ratio of core energy to the total energy of vacancy formation was 0.5 for cubic crystals. Thirdly, this method produces a continuous stress and strain field associated with the vacancy everywhere in the body. Therefore, the model could be extended to predict the interaction effects of vacancies with either interstitials or substitutional impurities in metals.
Table 1.2 shows that the predicted formation energies are lower than the experimental values for the bcc metals Li, Nb and Ta. Adjusting the $f$ value to give agreement between experiment and theory shows $f = 0.27$ for Li, and practically zero for Nb and Ta. It seems difficult to justify such a large local vacancy dilatation. It is possible vacancy formation in the bcc metals may be accompanied by atomic rearrangements in the $<111>$ direction such that the configuration appears more like two split half vacancies. In this case, the present model would not be applicable and agreement between theory and experiment not expected.

Table 1.3 shows the order of magnitude agreement between the experimental values of entropy of vacancy formation and those predicted by the current model. Analytically, the calculated values of the entropy of vacancy formation are quite sensitive to the values of $du/\nu_v dT$ employed. This coefficient can vary considerably with temperature and in the present work was evaluated at room temperature from the elastic constant data of single crystals. These data exhibit appreciable scatter between differing experimenters studying the same metal.

The data points taken for monovacancy concentrations representative of relatively high temperatures with respect to the melting point are extrapolated several orders of
magnitude to infinite temperature, $T^{-1} \to 0$, in order to find the intercept of the $\ln c_v$ vs $T^{-1}$ curve. This intercept is related to the experimental value of $S_v^f$ and due to the above extrapolation procedure, is very sensitive to the accuracy of the data points. For these reasons, the agreement we find between experiment and theory for $S_v^f$ is considered satisfactory.

In summary, it appears the advantages enumerated above for the current model favor a reliable calculation of the energy and entropy of monovacency formation in metals. This agreement results even though the actual displacement field surrounding the defect may in some cases be quite different from that predicted by the model.
| Element | \( u_{\text{Voigt}} \times 10^{-12} \text{ d/cm}^2 \) & \( \Omega \times 10^2 \text{ cm}^3 \) & \( \alpha \times 10^6 \text{ (°K)}^{-1} \) & \( \gamma \times 10^3 \text{ (°K)}^{-1} \) & \(- (\text{d}u/\text{d}T) \) |
|---------|----------------|----------------|----------------|----------------|----------------|
| Cu      | 0.593          | 11.77          | 16.5           | 1.96           | 0.266          |
| Ag      | 0.375          | 17.07          | 19.7           | 2.4            | 0.373          |
| Au      | 0.337          | 16.94          | 14.2           | 3.03           | 0.24           |
| Pt      | 0.665          | 15.11          | 8.9            | 2.54           | 0.13           |
| Ni      | 1.011          | 10.94          | 13.3           | 1.88           | 0.329          |
| Al      | 0.29           | 16.59          | 23.9           | 2.17           | 0.536          |
| W       | 1.753          | 15.82          | 4.3            | 1.62           | 0.099          |
| Pb      | 0.137          | 30.34          | 29.3           | 2.73           | 0.735          |
| Na      | 0.044          | 39.85          | 71             | 1.25           | 1.2            |
| Li      | 0.071          | 21.5           | 56             | 1.17           | 0.412          |
| K       | 0.017          | 75.3           | 83             | 1.34           | ---            |
| Mo      | 1.277          | 15.6           | 4.9            | 1.57           | 0.13           |
| Nb      | 0.396          | 17.98          | 7.1            | ---            | ---            |
| Ta      | 0.706          | 18.01          | 6.5            | 1.75           | ---            |
| Co      | 0.8            | 11.13          | 12.4           | 1.87           | 0.24           |
| Mg      | 0.194          | 23.23          | 25.0           | 1.51           | 0.40           |
| Cd      | 0.319          | 21.6           | 29.8           | 2.19           | 1.09           |
| Zn      | 0.51           | 15.24          | 39.7           | 2.01           | 0.42           |
| Sn      | 0.26           | 27.3           | 23.0           | 2.14           | 1.21           |

a: extrapolated from 300°K
b: extrapolated from 90°K
c: extrapolated from 78°K
d: value at 83°K
e: extrapolated from 77°K
f: extrapolated from 300°K
### TABLE 1.2

Theoretical Predictions of the Model and Experimentally Determined Values of the Energy of Vacancy Formation

<table>
<thead>
<tr>
<th>Element</th>
<th>$\chi'$ x10^{12} (d/cm²)^{-1}</th>
<th>$E_{\text{core}}/E_{\text{total}}$</th>
<th>$E_{\nu}^f$ (ev)</th>
<th>$E_{\nu}^e$ (ev)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>1.52</td>
<td>0.55</td>
<td>1.0</td>
<td>1.0</td>
<td>1.24,1.33,1.34</td>
</tr>
<tr>
<td>Ag</td>
<td>2.4</td>
<td>0.55</td>
<td>0.92</td>
<td>0.96</td>
<td>1.24,1.33,1.34</td>
</tr>
<tr>
<td>Au</td>
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*a f = .78 ,  b f = .78 ,  c f = .75*
TABLE 1.3

Theoretical and Experimental Values of the Entropy of Vacancy Formation

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CHAPTER II
DISLOCATION ATTACK FREQUENCY

2.1 INTRODUCTION

Many mechanical metallurgical phenomenon such as yield point, creep, and damping are known to be controlled by the microscopic action of dislocations overcoming obstacles to their movement. The obstacles are widely varied, including such barriers as forest dislocations, point defects and Peierl's barriers. The barrier may be on or off the glide plane of the dislocation, large or small with respect to atomic dimensions, and rigid or flexible. Whatever type obstacle exists, the important factors working to aid the dislocation to surmount the barrier are: 1) externally applied stress, 2) thermally supplied energy, and 3) the frequency with which the dislocation attacks the barrier.

Thermally activated phenomenae, for example a dislocation surmounting an obstacle barrier, can in general be described by an Arrhenius type of relation describing the number of successful thermal activations, \( \Gamma \), per unit time. The general form is \( \Gamma = \nu_0 e^{-\Delta G/kT} \) where \( \Delta G \) is the Gibbs free energy change associated with surmounting the barrier and the exponential form means back fluctuations are neglected. The pre-exponential factor, \( \nu_0 \), is an
effective attack frequency of the process which contains the natural attack frequency. The temperature dependence of the effective attack frequency has been thoroughly studied for a limited number of configurations [2.1]. The stress dependence of the attack frequency is always considered to be negligible and the local segment of dislocations in front of the obstacle is never taken into account. A complete study of the stress dependence of dislocation attack frequency was therefore made by considering three effects:

First, the local one dimensional fundamental attack frequency of the dislocation segment in front of the obstacle was found for a wide variety of dislocation-obstacle configurations and cases.

Second, the natural frequency of vibration of the dislocation line between obstacles was found taking into account the change in length as the dislocation bows out and encounters other obstacles.

Third, in each configuration the randomly, discretely and continuously pinned cases were considered. Also, the effect of the longer dislocation segment on the frequency of the shorter was taken into account by employing an appropriate harmonic averaging technique.

There exists in the literature many dislocation-obstacle interaction relations from which the obstacle's energy profile can be determined. These relations were
reviewed and those describing the more important varied interactions were employed. The general model employed in the investigation of the localized, one dimensional, athermal, non-quantum mechanical fundamental attack frequency of the dislocation segment in front of the obstacle is shown pictorially in Fig. 2.1. It is assumed that a dislocation line, acting under the influence of an external stress, $\sigma_a$, encounters rigid obstacles of physical width $\Lambda$ to its motion at some distance $l$ along its length. In general, these obstacles may all be repulsive or both repulsive and attractive. Further, they may be randomly distributed or ordered in which case they would constitute discrete pinning points. The obstacles exert a localized one-dimensional force on the dislocation line causing the dislocation to bow out between them. For an applied force $\sigma_{ab^l}$ less than the maximum repulsive force, $\sigma_m b\Lambda$, a local dislocation segment is located at an equilibrium position of $x_{eq}$ in front of the obstacle determined by the condition that the sum of forces on the dislocation segment equal zero. Given the force-displacement relation for the particular obstacle under investigation, the restoring force acting on the segment under a slight displacement $\delta$ from $x_{eq}$ can be found by expanding around the equilibrium position.
a) Pinning of dislocation line

\[ F_{\text{int}} = \sigma_m b \Lambda \]
\[ F_{\text{ext}} = \sigma_{\text{app}} b \ell \]

b) Typical force-displacement relation

\[ \frac{F_{\text{ext}}}{F_{\text{int}}} \]
\[ \frac{F_{\text{eq}}}{F_{\text{int}}} \]

\[ (x_{\text{eq}} - \delta), (x_{\text{eq}} + \delta), x_{\text{eq}} \]

(c) Dislocation breakaway

Fig. 2.1. Dislocation Pinning
\[ F(x_{eq} + \delta) = F(x) \bigg|_{x=x_{eq}} + \frac{\delta F}{\delta x} \bigg|_{x=x_{eq}} \cdot \delta \quad (2.1) \]

But the net force evaluated at \( x = x_{eq} \) is identically zero. Therefore,

\[ F(x_{eq} + \delta) \approx \frac{\delta F}{\delta x} \bigg|_{x=x_{eq}} \cdot \delta \quad (2.2) \]

Because the net force is proportionate to the displacement, the fundamental attack frequency can be found by employing the expression for a simple harmonic oscillator, assuming no quantum effects.

\[ \nu = \left[ \frac{\delta F}{\delta x} \bigg|_{x=x_{eq}} / 4\pi^2 m_{\text{eff}} \right]^{1/2} \quad (2.3) \]

Because the \( x_{eq} \) term was found by setting the sum of forces acting on the dislocation segment equal to zero, it contains a term of the form \( \sigma_{\text{app}} \ell / \sigma_{\text{max}} \Lambda \) which acts as an effective multiplying factor for the applied stress and points out that locally the attack frequency is dependent on the height, \( \sigma_m \), and width, \( \Lambda \), of the obstacle barrier.

For each dislocation-obstacle interaction relation employed, two cases were considered -- the discretely pinned dislocation and the randomly pinned dislocation. In the discretely pinned or square array case, the
dislocation is pinned at localized points an average distance $l$ along the straight dislocation. In the randomly pinned case the pinning points rather than being localized are dispersed throughout the lattice. Two random cases were considered. First, the case where the dislocation is given a zig-zag configuration in a state of minimum energy due to the interplay between an increase in line energy and a decrease in interaction energy with attractive obstacles. Secondly, the case where the dislocation bows out between strongly attractive or repulsive obstacles and encounters other obstacles along its length. Friedel [2.2] has derived expressions for the average distance between obstacles along the dislocation line for these random cases. Under an applied stress $\sigma_a$, line tension $\tau$, atomic concentration of solute atoms $C$, and average distance between obstacles $l$, the stress dependent distance between fixed obstacles along the bowed out dislocation line is

$$D_f = \left[\frac{2\tau l^2}{\sigma_a b}\right]^{1/3}$$

(2.4)

where the line tension, $\tau$, is usually taken to equal $\frac{\mu b^2}{2}$. The average distance between random attractive obstacles along the dislocation is given by

$$D_s = \frac{2l}{C\left(\frac{U}{\tau_b}\right)^{1/3}}$$

(2.5)
The interaction energy, $U$, is given as \( \frac{\mu b^3 \eta}{2} \), where $\eta$ is a misfit parameter which takes into account size effects associated with the inclusions. Assuming $\ell = \Lambda c^{-1/2}$, $D_s$ then reduces to the form

$$D_s = \left[ \frac{8}{\eta} \frac{\ell^4 - 1}{\Lambda} \right]^{1/3}$$  \hspace{1cm} (2.6)

Throughout the analysis the values of $\ell$ were varied from a large value of $10^4 b$ to the continuously pinned case of $\ell = \Lambda$. The maximum internal stress, $\sigma_m$, was kept below the critical stress necessary to activate a Frank-Reed source.

$$\sigma_a \leq \frac{\sigma_m b}{\ell} < \sigma_{\text{critical}} = \frac{\mu b}{\ell}$$

$$\therefore \quad \sigma_m \leq \mu \quad \text{where } \mu = \text{shear modulus}$$

This assured that the maximum stress attained was not adequate for mechanical breakaway by the dislocations pinching off around the obstacles. Breakaway is accomplished by the mechanism as shown in Fig. 2.1C. Under an externally applied stress the dislocation bows-out between the obstacles and takes up an $x_{eq}$ in front of the obstacle. If one of the obstacles along the line of the dislocation is suddenly surmounted, then locally the dislocation
segment goes from \( l \) to \( 2l \). By the ratio of force term 
\( \sigma_a \Delta l / \sigma_m \Delta l \) in the \( x_{eq} \) expression, the local average length
is now twice as large. Under the same applied stress \( \sigma_a \),
the dislocation takes on an \( x_{eq} \) closer to the peak of the
obstacle barriers which are pinning the segment of length
\( 2l \). It is therefore successively easier for the dislo-
cation to surmount the obstacles pinning the larger segments
as the segments get larger. This progression continues,
with the result that the dislocation zips down the line of
obstacles in both directions from the initial one to be
surmounted until breakaway is complete provided \( kT \ll \sigma_a 
\text{bdl} \), i.e., thermal energy is negligible.

In analysing the force displacement relations, the
dislocation is assumed to have an average effective rest
mass defined by

\[
m_{\text{eff}} C_t^2 = E_o
\]  
(2.7)

where \( C_t \) is the transverse velocity of sound in a crystal
and \( E_o \) is the rest energy of the dislocation line given
by \( E_o = \frac{\mu b^2}{4\pi} \ln \frac{r_1}{r_o} \). The term \( \frac{1}{4\pi} \ln \frac{r_1}{r_o} \) is approxi-
mately equal to unity. Applying the relation \( C_t^2 = \mu / \rho \)
where \( \rho \) is the density of the material, the mass per unit
length is

\[
m_o = \rho b^2
\]  
(2.8)
An order of magnitude estimate of the average velocity of the dislocation indicates that a relativistic correction to the rest mass is negligible.

2.2 INTERACTION RELATIONS - LOCAL ANALYSIS

2.2.1 Cosine Law

N. F. Mott and F.R.N. Nabarro [2.3] proposed a cosine relation to describe a dislocation located in an energy well between strain hills created by a concentration of inclusions. The dislocation-imperfection force per unit length has the form

$$F = \sigma_m b \cos \left( \frac{2\pi x}{\lambda} \right)$$

(2.9)

where $\lambda$ is a measure of the interaction distance along the $x$ direction. The cosine relation is general in that it is not restricted to a particular dislocation-obstacle configuration. Therefore the analysis was carried out by employing the cosine relation in the three separate cases of 1) random pinning points, 2) forest dislocations, and 3) discrete pinning points along the dislocation line. These three cases were studied as a function of the range of interaction, $\lambda$, as well as $\ell$, the average distance between points on the glide plane.
Fig. 2.2 shows pictorially the force displacement relation for the Mott-Nabarro relation as well as the three specific cases studied.

By balancing forces at equilibrium under an applied stress, $\sigma_a$, there results the relations:

$$\sigma_m b\Lambda \cos[2\pi x/\lambda] = \sigma_a b D_s$$ for random pins

$$\sigma_m b\Lambda \cos[2\pi x/\lambda] = \sigma_a b D_f$$ for forest dislocations

$$\sigma_m b\Lambda \cos[2\pi x/\lambda] = \sigma_a b \lambda$$ for discrete pinning

(2.10)

where the Friedel correction to the length between pinning points along the dislocation has been employed. Solving for the equilibrium position $x_{eq}$, there results:

$$x_{eq} = \frac{\lambda}{2\pi} \cos^{-1}\left(\frac{\sigma_a D_s}{\sigma_m \Lambda}\right)$$ random

$$x_{eq} = \frac{\lambda}{2\pi} \cos^{-1}\left(\frac{\sigma_a D_f}{\sigma_m \Lambda}\right)$$ forest

$$x_{eq} = \frac{\lambda}{2\pi} \cos^{-1}\left(\frac{\sigma_a \lambda}{\sigma_m \Lambda}\right)$$ discrete

(2.11)
a) Mott and Nabarro Cosine Relation.

b) Dislocation given a zig zag configuration by randomly distributed pinning points.

c) Dislocation encountering obstacles as it bows-out under an applied stress.

d) Discretely pinned dislocation line.

Fig. 2.2. Cosine Relation and Various Cases of Interest
The restoring force is found to be

\[ F(x_{eq} + \delta) = \frac{2\pi \sigma_m b \lambda}{\lambda} \left[ 1 - \left( \frac{\sigma_a D_i}{\sigma_m \lambda} \right)^2 \right]^{1/2} \delta \quad (2.12) \]

where \( i = \{ 1 \text{ random}, 2 \text{ forest}, 3 \text{ discrete} \). The fundamental frequency is then found to be

\[ \nu = \left[ \sigma_m b \sqrt{2 \pi m_{\text{eff}}} \lambda \right]^{1/2} \left[ 1 - \left( \frac{\sigma_a D_i}{\sigma_m \lambda} \right)^2 \right]^{1/4} \quad (2.13) \]

It is suggested that this result constitutes an improvement over the original Mott and Nabarro attack frequency calculation. The original calculation was performed by expanding the cosine function twice about the value \( x = 0 \) which makes the results appropriate only for small displacements from the stress peak. The present calculation makes only one expansion of the force law about the equilibrium position of the dislocation \( x_{eq} \) which varies with the applied stress. Further, since the amplitude of vibration \( \delta \) is small, the expansion is a good approximation. The results of the Mott-Nabarro calculation yielded:

\[ \nu = \left[ \sigma_m b \sqrt{2 \pi m_{\text{eff}}} \right]^{1/2} \left[ 1 - \left( \frac{\sigma_a}{\sigma_m} \right)^2 \right]^{1/4} \quad (2.14) \]
**Random Solutes**

In applying the cosine relation to the case of random solutes, Friedel has estimated from energy considerations that the average distance from the random solute to the straight dislocation line is given by \( x = \left( \frac{\eta}{8C} \right)^{1/3} b \) when the barrier width, \( \Lambda \), is of the order of 1b.

Letting \( x = \lambda \) and putting the concentration \( C \) in terms of \( \ell \), there results \( \lambda = \left( \frac{\eta b}{8} \right)^{1/3} \). \( \eta \) is a size factor of the inclusion which has usual values between 0.01 to 0.3.

The value of \( b \) is assumed to be constant at 3 \times 10^{-8} \text{cm}. The distance between inclusions, \( D_s \), enters into the expansion for the localized attack frequency only in the ratio of stresses term \( \left( \frac{\sigma_a D_s}{\sigma_m \Lambda} \right) \). The values of \( \ell \) were allowed to vary from 10 \( \text{b} \) to the continuously pinned case of 10 \( \text{b} \). The maximum internal stress of the inclusion \( \sigma_m \) was assigned the values 10\( ^7 \), 10\( ^9 \) and 10\( ^{11} \) dy/cm\( ^2 \).

According to Eq. (2.8), the mass of the dislocation segment located in front of the barrier is \( \rho b^2 \Lambda \), which reduces to \( \rho b^3 \) for this analysis. The density, \( \rho \), was assigned the value 10 gm/cm\( ^3 \). Under these assumptions, Eq. (2.13) for the localized attack frequency takes the form

\[
\nu = \left[ \frac{\sigma_m}{10\pi(\eta b^4 \ell^2)^{1/3}} \right]^{1/2} \left[ 1 - \left( \frac{\sigma_a D_s}{\sigma_m \Lambda} \right)^2 \right]^{1/4}
\]

Eq. (2.15)

Fig. 2.3 shows the results of the analysis for the random solute according to the cosine relation.
Fig. 2.3 - Cosine Relation - Random Solute Case

\[ \frac{\sigma_a D_s}{\sigma_m \Lambda} \]

- \( \ell = 10^4 \text{b} \)
- \( \ell = 10^2 \text{b} \)
- \( \ell = 10^0 \text{b} \)

Attack Frequency (sec\(^{-1}\))

* \( \sigma_m \) in g/(cm\(^2\))
Forest Dislocations

For the case of forest dislocations it is known that the range of elastic interaction varies widely from a maximum obtainable value down to practically zero, depending on both the crystal structure and relative orientation of the gliding dislocation loop and "tree". The analysis was therefore carried out by allowing the interaction length, \( \lambda \), to vary from a maximum length between Frank-Read sources of \( 10^4 b \) down to the short range length of \( 1b \). This range of values includes the magnitude of the length along the gliding dislocation between "trees", \( D_f \). The maximum internal stress was allowed to vary from \( 10^7 \) to \( 10^{11} \) dy/cm². Eq. (2.13) reduces for this analysis to

\[
\nu = \left[ \frac{\sigma_m}{\sigma_0} \right]^{1/2} \left[ 1 - \left( \frac{\sigma_a D_f}{\sigma_m \lambda} \right)^2 \right]^{1/4} \tag{2.16.1}
\]

In addition, the analysis was performed by allowing the interaction distance, \( \lambda \), to equal the distance between "trees" along the dislocation line, \( D_f \). By defining the normalized applied stress as \( N \), Eq. (2.13) reduces for this analysis to

\[
\nu = \left[ \frac{\sigma_m}{\sigma_0} \right]^{3/2} \left[ N^{1/2} \frac{1}{2 \pi b \mu} \right]^{1/2} \left[ 1 - \left( \frac{\sigma_a D_f}{\sigma_m \lambda} \right)^2 \right]^{1/4} \tag{2.16.2}
\]
Fig. 2.4 shows the results of both analyses. The attack frequency employing $D_f$ for the value of $\lambda$ is shown only for the extreme cases of $\sigma_m = 10^{11}$ and $\sigma_m = 10^7$ dy/cm$^2$.

**Discretely Pinned Dislocations**

As shown in Fig. 2.2, the discretely pinned dislocation is held in place by inclusions spaced an average distance $\lambda$ apart. By assuming the physical width of the inclusion, $\Lambda$, is equal to $b$, Eq. (2.13) for the localized attack frequency becomes:

$$
\nu = \left[ \frac{\sigma_m}{2 \pi b \lambda} \right]^{1/2} \left[ 1 - \left( \frac{\sigma_a \lambda}{\sigma_m b} \right)^2 \right]^{1/4}
$$

(2.17)

The interaction distance, $\lambda$, was assigned the range of values from $10^4 b$ down to the short range continuously pinned case of $10^0 b$. It is seen that this analysis is the same as that carried out for the forest dislocation case and the results should then be the same. The distinction in the two cases comes from the difference between $D_f$ and $\lambda$ in the normalized stress term. In general $D_f \leq \lambda$ which should have the effect of slightly reducing the applied stress, $\sigma_a$, for the discretely pinned case to produce the same attack frequency as the forest dislocation case.

Fig. 2.5 shows the attack frequency dependence on applied stress as a function of $\sigma_m$ and $\lambda$ for discretely pinned dislocations.
\[ \nu = \left( \frac{\sigma_m}{20\pi L} \right)^{1/2} \left\{ 1 - \left( \frac{a_D}{\sigma_m} \right)^2 \right\}^{1/4} \]

For the Cosine Relation in the Forest Dislocation Case, the expression is:

\[ \sigma_m = 10^{11} \text{dy/cm}^2 \]

\[ \sigma_m = 10^7 \text{dy/cm}^2 \]
Fig. 2.5 - Cosine Relation - Discretely Pinned Case
2.2.2 Cottrell-Bilby

A. H. Cottrell and B. A. Bilby [2.4] in studying yielding in iron have looked at the configuration of a dislocation pinned along its length by an "atmosphere" of attractive solute atoms. The solute atoms take up low energy positions in the highly dilated region surrounding the dislocation at a distance \( \rho \) from the core of the dislocation. The distance \( \rho \) is specified to be greater than \( r_o \), the core radius of the dislocation. At shorter distances than \( r_o \), second order elasticity theory does not hold. The dislocation is assumed to lie along the \( z \) axis and move in the positive \( x \) direction under an applied stress. The force per atomic plane was found to be

\[
F = \frac{2A\rho x}{(x^2 + \rho^2)^2} \tag{2.18}
\]

where \( A = \frac{4\pi bG}{3\pi} \left( \frac{1+v}{1-v} \right) \). As shown in Fig. 2.6 the force reaches a maximum value at a displacement \( x = \frac{\rho}{\sqrt{3}} \) equal to \( F_o = \frac{3\sqrt{3}}{8\rho^2} A \). The balance of force equation which holds at equilibrium is

\[
\frac{2AX}{\rho^2 (x^2 + 1)^2} = \sigma_a b \tau_i \tag{2.19}
\]
a) Configuration of solute atoms and pinned dislocation

\[
\frac{F}{F_m}
\]

\[
0 \leq \frac{\rho}{\sqrt{3}} \leq 1
\]

b) Cottrell-Bilby force-displacement relation

Fig. 2.6 - Configuration and Force-displacement Relation for Cottrell-Bilby Pinned Dislocation
where \( i = 1 \) Random Solute
\( i = 2 \) Forest
\( i = 3 \) Discrete

and where \( X \) is the normalized displacement \( X = \frac{X}{\rho} \).

In order to get the equilibrium displacement in a closed form solution, the \( X^4 \) term was neglected at this point and a 6\% maximum error was encountered. As is seen from Fig. 2.6, \( 0 \leq X \leq \frac{1}{\sqrt{3}} \); therefore \( 0 \leq X^4 \leq 0.11 \).

This approximation gives an equilibrium displacement term given by

\[
x_{eq} = \frac{4\rho}{3\sqrt{3}} \frac{\sigma_m b}{\sigma_a D_i} - \rho \left[ \frac{4}{3\sqrt{3}} \left( \frac{\sigma_m b}{\sigma_a D_i} \right)^2 - \frac{1}{2} \right]^{1/2} \quad (2.20)
\]

where \( \sigma_m \) is defined from the maximum force expression to be

\[
\sigma_m = \frac{\sqrt{3}}{8\pi} \frac{G \Delta v}{\rho^2 b} \frac{1+v}{1-v}, \quad \text{where } v \text{ is Poisson's ration and}
\]

\( \Delta v \) is the local volume change caused by the introduction of a solute atom, equal to \( 4\pi r_s^3 \eta \).

The restoring force about the equilibrium position is found to be:

\[
F(x_{eq} + \delta) = \frac{2A}{\rho^3} \left[ \frac{1 - 3\left( \frac{x}{\rho} \right)^2}{\left( 1 + \left( \frac{x}{\rho} \right) \right)^3} \right] \bigg|_{x=x_{eq}} \cdot \delta \quad (2.21)
\]
The attack frequency is then found to be:

\[
\nu = \left[ \frac{4}{3 \sqrt{3}} \frac{\sigma_m b^2}{\pi^2 m_{\text{eff}} \rho} \right]^{1/2} \left[ \frac{1 - 3 \left( \frac{x}{\rho} \right)^2}{\left( 1 + \left( \frac{x}{\rho} \right)^2 \right)^3} \right]^{1/2} \quad \text{for } x = x_{\text{eq}} \tag{2.22}
\]

It is seen that the attack frequency is dependent on the dislocation-inclusion separation distance, \( \rho \), which can also be taken as the interaction distance.

Fig. 2.7 shows the results of the analysis as the attack frequency plotted against normalized applied stress. The separation distance, \( \rho \), was held fixed at 2b where b is a burger's vector approximately 3 x 10^{-8} \text{cm}. \( \sigma_m \) was varied from a low of 10^{7} \text{ dy/cm}^2 to the critical value of 10^{11} \text{ dy/cm}^2. The results show a maximum attack frequency close to zero applied stress which reflects the linearity of the force-displacement law of Fig. 2.6 about \( x = 0 \). The frequency then decreases steadily with increasing applied stress and drops sharply to zero close to the maximum internal stress.
Fig. 2.7 - Cottrell-Bilby

\[ \rho = 2b \]
2.2.3 Seeger

Seeger [2.5] has studied the rigid barrier dislocation interaction of the large obstacles produced by irradiation such as Frenkel defects, vacancy clusters and crowdions. On the assumption of a normally distributed energy per obstacle, a generalized energy function was proposed of the form

$$U = U_o \left[1 - \frac{1}{1 + \exp\left(\frac{x}{x_o}\right)}\right]$$  \hspace{1cm} (2.23)

$U_o$ is the maximum value of the energy hill and $x_o$ is 1/8 the diameter of the obstacle or defect "zone". By appropriate differentiation the force relation is found to be

$$F = \frac{U_o \exp\left(\frac{x}{x_o}\right)}{x_o \left(1 + \exp\left(\frac{x}{x_o}\right)\right)^2}$$  \hspace{1cm} (2.24)

As shown in Fig. 2.8, a maximum value occurs in the force at $x = 0$ given by $F_{\text{max}} = \frac{U_o}{4x_o}$ which defines a maximum stress $\sigma_m$. This stress acts over a length equal to the diameter of the zone, $8x_o$, to prevent the dislocation from moving. By balancing forces at equilibrium, the equilibrium equation is
Fig. 2.8 - Seeger's Rigid Barrier Force-Displacement Law
\[
\frac{U_o}{x_o} \frac{\exp\left(\frac{x}{x_o}\right)}{(1 + \exp\left(\frac{x}{x_o}\right))^2} = \sigma_a b D_i
\] (2.25)

From the equilibrium equation, the expression for the equilibrium displacement of the dislocation under the influence of an external applied stress, \(\sigma_a\), is found to be

\[
x_{eq} = x_o \ln\left\{\frac{2\sigma_m 8x_o}{\sigma_a D_i} - 1 + 2\left[\frac{\sigma_m 8x_o}{\sigma_a D_i}\right]^2 - \frac{\sigma_m 8x_o}{\sigma_a D_i}\right\}^{1/2}
\]

(2.26)

The restoring force which the dislocation feels at a displacement \(\delta\) from \(x_{eq}\) is found to be

\[
P(x_{eq} + \delta) = \frac{U_o}{x_o^2} \left[ \frac{x}{x_o} - \frac{2x}{x_o} e^{-\frac{x}{x_o}} \right] \left(1 + \frac{x}{x_o}\right) \delta 
\]

(2.27)

The normal vibrational mode is then found to be

\[
v = \left[ \frac{8\sigma_m}{10\pi^2 b 8x_o} \right]^{1/2} \left[ \frac{x}{x_o} - \frac{2x}{x_o} e^{-\frac{x}{x_o}} \right]^{1/2} 
\]

(2.28)
Fig. 2.9 shows the results of the analysis for various values of $\sigma_m$ and inclusion diameter $8 x_o$. The internal stress, $\sigma_m$, is varied from $10^7$ dy/cm$^2$ to a maximum of $10^{11}$ dy/cm$^2$. The diameter of the inclusion is varied from the maximum of $10^2 b$ to a point defect of $10^0 b$. The outstanding feature of the results is the definite peak in the attack frequency curve. This shows that for the particular configuration under discussion, the attack frequency is not a slowly varying function of stress.

### 2.2.4 Fleischer and Modified Fleischer

In his study of the effects of tetragonal distortions on "rapid hardening" in lithium fluoride, Fleischer [2.6] has looked at the large rigid barrier of an impurity ion-solvent vacancy pair in an ionic lattice. The strain field of these tetragonal distortions produces large interactions with the stress field of glissile dislocations. Fleischer has calculated the interaction energy per atomic volume between a dislocation and tetragonal distortions of different crystallographic orientation.

Fig. 2.10 shows the assumed orientation of Fleischer's model. With the tetragonal distortion of value $\Delta \varepsilon$ at the origin, the dislocation lies along the $z$ axis and glides on the plane given by $y = a$ constant, $\varphi$. 
Fig. 2.9 - Seeger Relation -
diameter of inclusion is $8x_o$
Fig. 2.10 - Energy Contours for the Interaction of a \langle 110 \rangle
Distortion with a \langle 101 \rangle Screw Dislocation
after Fleischer
With this configuration, the interaction energy per atomic volume was found to be:

\[
E_{\langle 111 \rangle} = \frac{Gb^4 \Delta \varepsilon}{3\sqrt{3} \pi \rho} \left[ \frac{\sqrt{2} - \frac{X}{\rho}}{1 + \left( \frac{X}{\rho} \right)^2} \right]
\]

\[
E_{\langle 100 \rangle} = \frac{Gb^4 \Delta \varepsilon}{2\sqrt{6} \pi \rho} \left[ \frac{1 + \sqrt{2} \frac{X}{\rho}}{1 + \left( \frac{X}{\rho} \right)^2} \right]
\]

\[
E_{\langle 110 \rangle} = \frac{Gb^4 \Delta \varepsilon}{4\sqrt{3} \pi \rho} \left[ \frac{2\sqrt{2} + \frac{X}{\rho}}{1 + \left( \frac{X}{\rho} \right)^2} \right]
\]

(2.29)

The \( \langle 111 \rangle \) means a tetragonal distortion in this direction, all interactions pertain to screw dislocations gliding in a (111) [101] system. This is the normal slip system for ionic crystals.
By appropriate differentiation, the force per atomic volume is found to be

\[ F_{\langle 111 \rangle} = \frac{F_o}{3} \left[ \frac{x^2 - 2\sqrt{2} x - 1}{(x^2 + 1)^2} \right] \]

\[ F_{\langle 100 \rangle} = \frac{F_o}{2} \left[ \frac{x^2 + \sqrt{2} x - 1}{(x^2 + 1)^2} \right] \]

\[ F_{\langle 110 \rangle} = \frac{F_o}{4} \left[ \frac{x^2 + 4\sqrt{2} x - 1}{(x^2 + 1)^2} \right] \tag{2.30} \]

where \( x \) is the normalized displacement \( x = \frac{X}{\rho} \) and \( F_o = \frac{G b^4 \Delta \varepsilon}{\sqrt{3} \pi \rho^2} \). Fig. 2.11 shows the functional relation of \( F \) for the above three orientations as well as a "modified Fleischer" force law. This modified form was proposed by Fleischer as an approximation to the energy of the \( \langle 110 \rangle \) type distortion. As can be seen from Fig. 2.11 the approximate modified form is indeed a good approximation to the exact form of the \( \langle 110 \rangle \) distortion force from large values of \( x \) down to \( x = 1 \) or \( x = \rho \). Therefore, for energy consideration in which Fleischer was interested, the modified form could greatly simplify the calculations. However, because attack frequency
(1) \langle 111 \rangle \text{ tetragonal distortion} \quad F_0 = \frac{1}{3} \left[ \frac{x^2}{x^2 + 1} \right] \quad (x+1) \\
(2) \langle 100 \rangle \text{ tetragonal distortion} \quad F_0 = \frac{1}{2} \left[ \frac{x^2}{x^2 + 1} \right] \quad (x+1) \\
(3) \langle 110 \rangle \text{ tetragonal distortion} \quad F_0 = \frac{1}{4} \left[ \frac{x^2}{x^2 + 1} \right] \quad (x+1) \\
(4) \text{ Modified Fleisher} \quad F_0 = \frac{\mu b^4 \Delta \varepsilon}{\beta v y} \left[ \frac{1}{(x+1)^2} \right] \\
\begin{align*}
\text{Fig. 2.11 – Fleisher Force Relations} \\
\end{align*}
calculations are very sensitive to the shape of the force-displacement curve, and because the approximate modified form differs greatly from the exact form in the region of interest about the force peak $0.7 \leq X \leq 1.0$, the modified form is not a good approximation for attack frequency calculations. In the following analysis of the attack frequency both the modified Fleischer form and the relatively weak interaction of the $\langle 100 \rangle$ tetragonal distortion were omitted from consideration. Only the strong interactions of the $\langle 111 \rangle$ and $\langle 110 \rangle$ configurations were used.

Interaction of a screw dislocation with a $\langle 111 \rangle$ tetragonal distortion

By using the above force equation for the interaction of a screw dislocation with a $\langle 111 \rangle$ tetragonal distortion, we have at equilibrium the balance of force condition:

$$\frac{F_o}{3} \left[ \frac{X^2 - 2\sqrt{2} X - 1}{(X^2 + 1)^2} \right] = \sigma_{ab}D_i$$

(2.31)

This relation gives for the equilibrium displacement $X_{eq}$ the $X$ which satisfies the equation
\[ x_{eq}^4 + \left(2 + \frac{F_0}{3\sigma_a b D_i}\right)x_{eq}^2 - \left(\frac{2\sqrt{2} F_0}{3\sigma_a b D_i}\right)x_{eq} + \left(1 - \frac{F_0}{3\sigma_a b D_i}\right) = 0 \]

(2.32)

Because the values of \( X \) in the Fleischer model get relatively large, \( X \approx 2.5 \), the \( x_{eq}^4 \) term cannot be neglected without encountering a large percent error at distances away from the peak in the force-displacement curve. Therefore, the equilibrium values of displacement as well as the location of the maximum force and the attack frequencies were solved numerically.

Because the force equations are not normalized, the displacement which maximizes \( F \) was found numerically and resubstituted to find the \( F_{\text{max}} \) in terms of \( F_0 \). \( F_{\text{max}} \) is then set equal to \( \sigma_m b^2 \) where the diameter of one atomic volume is assumed to be \( b \). The expression for \( \sigma_m^{(111)} \) is then found to be

\[ \sigma_m^{(111)} = \frac{F_0 (1.484)}{3b^2} \]  

The equilibrium equation can then be put in the form

\[ x_{eq}^4 + \left(2 + \frac{\sigma_m b}{1.484 \sigma_a D_i}\right)x_{eq}^2 - \left(\frac{2\sqrt{2} \sigma_m b}{1.484 \sigma_a D_i}\right)x_{eq} + \left(1 - \frac{\sigma_m b}{1.484 \sigma_a D_i}\right) = 0 \]

(2.33)

Values of \( x_{eq} \) were then found numerically for various discrete values of \( \frac{\sigma_m b}{\sigma_a D_i} \) and are shown in Table 2.1.
TABLE 2.1

Numerically Determined Values of $X_{eq}$ for (111) Tetragonal Distortion

<table>
<thead>
<tr>
<th>$\frac{\sigma_{aD_i}}{\sigma_{mB}}$</th>
<th>$\frac{\sigma_{mb}}{\sigma_{aD_i}}$</th>
<th>$X_{eq}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.001</td>
<td>1000</td>
<td>3.097447</td>
</tr>
<tr>
<td>0.01</td>
<td>100</td>
<td>2.781030</td>
</tr>
<tr>
<td>0.05</td>
<td>20</td>
<td>2.170838</td>
</tr>
<tr>
<td>0.1</td>
<td>10</td>
<td>1.8361175</td>
</tr>
<tr>
<td>0.2</td>
<td>5</td>
<td>1.475537</td>
</tr>
<tr>
<td>0.3</td>
<td>3.33</td>
<td>1.258641</td>
</tr>
<tr>
<td>0.4</td>
<td>2.5</td>
<td>1.099896</td>
</tr>
<tr>
<td>0.5</td>
<td>2.0</td>
<td>0.9713212</td>
</tr>
<tr>
<td>0.6</td>
<td>1.667</td>
<td>0.878399</td>
</tr>
<tr>
<td>0.7</td>
<td>1.429</td>
<td>0.7514258</td>
</tr>
<tr>
<td>0.8</td>
<td>1.25</td>
<td>0.6535371</td>
</tr>
<tr>
<td>0.9</td>
<td>1.11</td>
<td>0.54416179</td>
</tr>
<tr>
<td>0.95</td>
<td>1.05</td>
<td>0.47572582</td>
</tr>
<tr>
<td>0.99</td>
<td>1.0101</td>
<td>0.389969</td>
</tr>
</tbody>
</table>
By comparing the results of Fig. 2.11 and Table 2.1 we see that the $X_{eq}$ for high stress corresponds to the peak in the force curve and therefore the equations are self consistent.

The restoring force which the dislocation feels at a small displacement, $\delta$, from the equilibrium displacement is found by employing the force equation for the $\langle 111 \rangle$ distortion and is

$$F(x_{eq} + \delta) = \frac{F_0 \delta}{3 \rho} \left[ \frac{2X^3 - 6\sqrt{2} X^2 - 6X + 2\sqrt{2}}{(X^2 + 1)^3} \right]_{X=X_{eq}}$$  \hspace{1cm} (2.34)

The attack frequency is then given in terms of $\sigma_m$ as

$$\nu(111) = \left[ \frac{2\sigma_m b^2}{4\pi^2 (1.484) \rho \text{eff}} \right]^{1/2} \left[ \frac{X^3 - 3\sqrt{2} X^2 - 3X + \sqrt{2}}{(X^2 + 1)^3} \right]^{1/2} \bigg|_{X=X_{eq}}$$  \hspace{1cm} (2.35)

Interaction of a screw dislocation with a $\langle 110 \rangle$ tetragonal distortion

In a manner similar to that used in analyzing the $\langle 111 \rangle$ distortion, the balance of force condition is

$$\frac{F_0}{4} \left[ \frac{X^2 + 4\sqrt{2} X - 1}{(X^2 + 1)^2} \right] = \sigma_a b D_i$$  \hspace{1cm} (2.36)
where \( X \) is the normalized displacement \( X = \frac{x}{\rho} \). The equilibrium displacement is the \( X \) which satisfies the equation

\[
x_{eq}^4 + \left( 2 - \frac{F_o}{4\sigma_a b D_i} \right) x_{eq}^2 - \left( 4\sqrt{2} \frac{F_o}{4\sigma_a b D_i} \right) x_{eq} + \left( 1 + \frac{F_o}{4\sigma_a b D_i} \right) = 0
\]

(2.37)

By numerical methods similar to those used in the \( \langle 111 \rangle \) distortion, the maximum internal stress is found to be

\[
\sigma_m^{(110)} = \frac{F_o (1.559)}{4b^2}
\]

which puts the equilibrium equation in the form

\[
x_{eq}^4 + \left( 2 - \frac{1}{1.559} \frac{\sigma_m b}{\sigma_a D_i} \right) x_{eq}^2 - \left( 4\sqrt{2} \frac{\sigma_m b}{1.559 \sigma_a D_i} \right) x_{eq} + \left( 1 + \frac{1}{1.559} \frac{\sigma_m b}{\sigma_a D_i} \right) = 0
\]

(2.38)

The restoring force which the dislocation feels at a small displacement, \( \delta \), from the equilibrium displacement is found to be

\[
F(x_{eq} + \delta) = \frac{F_o}{2\rho} \delta \left[ \frac{-x^3 - 6\sqrt{2} x^2 + 3x + 2\sqrt{2}}{(x^2 + 1)^3} \right] \bigg|_{x = x_{eq}}
\]

(2.39)
The attack frequency is then given in terms of $\sigma_m$ as

$$\nu\langle 110 \rangle = \left[ \frac{\sigma_m 2b^2}{4\pi^2 (1.559)m_{\text{eff}}^2} \right]^{1/2} \left[ \frac{-x^3 - 6\sqrt{2}x^2 + 3x + 2\sqrt{2}}{(x^2 + 1)^3} \right]^{1/2} \left|_{x=x_{\text{eq}}} \right.$$ 

(2.40)

Figs. 2.12 and 2.13 show the results of the attack frequency calculation for the $\langle 111 \rangle$ and $\langle 110 \rangle$ tetragonal distortions respectively. The analysis was made with $\rho$ set equal to $2b$. This is the closest distance of approach of the dislocation-defect pair under the assumption of linear elasticity. For values of $\rho$ greater than $2b$, the frequency will be reduced by $\left[ \frac{2b}{\rho} \right]^{1/2}$.

2.2.5 Quasi-Parabolic Peierl's Mechanism for Kink Formation

As was noted by Peierls [2.7], under zero applied stress, dislocations lie in the low energy positions between the close packed rows of atoms on their slip planes. Under the influence of an applied stress the dislocations move closer to the adjacent row of atoms which act as a continuous pinning obstacle to the movement of the dislocation. A double kink is pictured as forming when a local
Fig. 2.12 - Fleischer (111) tetragonal distortion
Fig. 2.13 - Fleischer (110) tetragonal distortion
dislocation segment suddenly surmounts the atomic barrier. After this segment is nucleated, the two kinks move apart in the manner describing mechanical breakaway and the dislocation is advanced to the next energy valley an atomic distance, a, away. Many energy profiles proposed to describe this process exist in the literature [2.8]. Of the empirical type the quasi-parabolic Peierls hill affords a closed form solution to the problem of nucleation of pairs of kinks.

Fig. 2.14 shows the quasi-parabolic dislocation line energy profile as a function of displacement. Neglecting the projections of edge and screw orientations, the variation of line energy with curvature according to the quasi-parabolic relation is given by

$$\Gamma(x) = \Gamma_o \left( \Gamma_o + \frac{ab}{2} \frac{\tau_p}{(1 - \frac{4x^2}{a^2})} \right)^{1/2}$$  (2.41)

where a is the lattice spacing, b the dislocation strength, $\Gamma_o$ the line energy of a straight dislocation, and $\tau_p$ the Peierls' stress. By differentiating, a force per unit length acting to prevent the dislocation motion is found. Assuming continuous pinning of the dislocation, the local equilibrium condition is given by
\[ \Gamma(x) = \Gamma_o \frac{1}{2} \left[ \Gamma_o + \frac{ab}{2} \tau_p \left(1 - \frac{4x^2}{a^2}\right)\right]^{1/2} \]

\begin{align*}
a & = \text{lattice spacing} \\
b & = \text{Burger's distance} \\
\Gamma_o & = \text{line energy of straight dislocation} \\
\tau_p & = \text{Peierl's stress}
\end{align*}

Fig. 2.14 - Quasi Parabolic Line Energy Profile
\[
\left( \frac{2b^2 \tau_p}{a} \right) x \left[ 1 + \frac{ab \tau_p}{2 \Gamma_o} \left(1 - \frac{4x^2}{a^2}\right) \right]^{1/2} = \sigma_{ab} b^2 
\]

(2.42)

Solving for the equilibrium displacement \( x_{eq} \) gives

\[
x_{eq} = \frac{a}{2} \left[ \frac{1 + \frac{ab \tau_p}{2 \Gamma_o}}{\left( \frac{\tau_p b}{\sigma_{ab}} \right)^2 + \frac{ab \tau_p}{2 \Gamma_o}} \right]^{1/2}
\]

(2.43)

The restoring force acting on the segment of dislocation when it is displaced a distance \( \delta \) from equilibrium is given by

\[
F(x_{eq} + \delta) = \frac{2b^2 \tau_p \delta}{a} \left[ 1 + \frac{ab \tau_p}{2 \Gamma_o} \left(1 - \frac{4x^2}{a^2}\right) \right]^{1/2} + \frac{4 \left( \frac{ab \tau_p}{2 \Gamma_o} \right) x^2}{a^2} \left[ 1 + \frac{ab \tau_p}{2 \Gamma_o} \left(1 - \frac{4x^2}{a^2}\right) \right]^{1/2}
\]

(2.44)
From this expression, the attack frequency is found to be

\[
\nu = \left[ \frac{2 \tau_p b^2}{4\pi^2 m_{\text{eff}}^a} \right]^{1/2} \left[ \frac{1}{\left[ 1 + \frac{ab\tau_p}{2\Gamma_0} \left( 1 - \frac{4x^2}{a^2} \right) \right]^{1/2}} + \frac{4}{a^2} \left( \frac{ab\tau_p}{2\Gamma_0} \right)^{x^2} \left[ 1 + \frac{ab\tau_p}{2\Gamma_0} \left( 1 - \frac{4x^2}{a^2} \right) \right]^{3/2} \right]
\]

(2.45)

The results of the analysis as represented by Fig. 2.15 show that under the assumed form of the quasi-parabolic energy-hill, the attack frequency is independent of applied stress. Fig. 2.15 shows the attack frequency magnitude for various values of \( \tau_p \). \( \Gamma_0 \) was given the value of \( \frac{ub^2}{2} \).

2.2.6 Saada Dislocation-Dislocation Interaction

A forest dislocation is one which is inclined to the glide plane of the primary slip system. It exists as part of the dislocation network or is formed by glide or secondary slip systems. A forest dislocation or "tree" forms a high, and broad obstacle barrier to the movement of glissile dislocations prior to dislocation intersection.
Fig. 2.15 - Quasi Parabolic Peierl's Hill

\[ a = b \]
Saada [2.9] has studied this dislocation-dislocation interaction and has derived the following stress-displacement relation describing the force needed for a glissile dislocation to cut through a repulsive tree.

\[ \sigma = \frac{\sigma_m}{1 - \frac{p}{\ell} x} \]  

(2.46)

\(\rho\) is a negative constant \(\approx -\frac{5}{8}\) and \(x\) is the separation between the glissile dislocation and the tree. Fig. 2.16 shows the shape of the stress curve.

By balancing forces at equilibrium we have the condition

\[ \frac{\sigma_m b^2}{1 - \frac{p}{D_f} x} = \sigma_a b D_f \]  

(2.47)

where Friedel's correction to the length of dislocation between "trees" has been employed. This leads to the equilibrium displacement

\[ x_{eq} = \frac{D_f}{p} \left[ 1 - \frac{\sigma_m b}{\sigma_a D_f} \right] \]  

(2.48)

The restoring force on the glissile dislocation at a small displacement, \(\delta\), from equilibrium is found to be
Fig. 2.16 - Stress-Displacement Relation of Saada for a Dislocation Cutting through a Forest Dislocation

\[ \sigma = \frac{\sigma_m}{1 - \frac{P}{\ell} x} \]
\[ F(x_{eq} + \delta) = \frac{\sigma_m b^2 p \delta}{D_f \left(1 - \frac{D}{D_f} x\right)^2} \bigg|_{x=x_{eq}} \] (2.49)

The above restoring force predicts a frequency of vibration given by

\[ \nu = \left[ \frac{\sigma_m b^2}{4\pi^2 m_{\text{eff}} D_f} \right]^{1/2} \left[ \frac{\sigma_a D_f}{\sigma_m b}\right] \] (2.50)

By applying Friedel's expression for \( D_f \), Eq. (2.50) reduces to

\[ \nu = \left[ \frac{\sigma_m^{3/2} b^2}{4\pi^2 m_{\text{eff}} u^{1/2} \ell} \right]^{1/2} \left[ \frac{\sigma_a D_f}{\sigma_m b}\right]^{5/4} \] (2.51)

Fig. 2.17 shows the derived attack frequency plotted as a function of the normalized applied stress for various values of \( \sigma_m \) and \( \ell \). It is seen that according to Saada's relation, the attack frequency is a monotonically increasing function of applied stress and does not reach an absolute maximum value as did most of the other interaction relations. There is, however, an additional restriction placed on the system. Because linear elasticity theory
Fig. 2.17 - Saada Forest Dislocation Relation

\[ \frac{\sigma_{a-D}}{\sigma_{m-b}} \]

\[ \text{Attack Frequency (sec)}^{-1} \]

\[ \sigma_m = 10^7 \quad \sigma_b = 10^6 \]
\[ \sigma_m = 10^8 \quad \sigma_b = 10^7 \]
\[ \sigma_m = 10^9 \quad \sigma_b = 10^8 \]
\[ \sigma_m = 10^{10} \quad \sigma_b = 10^9 \]
\[ \sigma_m = 10^{11} \quad \sigma_b = 10^{10} \]
does not hold in the core region of the dislocation, the value of $x_{eq}$ must be restricted to be greater than a separation of roughly 2b. This puts a corresponding restriction on the value of $\frac{\sigma_a^D}{\sigma_m^b}$ for which the theory holds.

$$\frac{\sigma_a}{\sigma_m^b} \leq \frac{1}{1 + \frac{b}{\ell}}$$ (2.52)

On Fig. 2.17 are shown the cut-off values of normalized applied stress for various values of $\ell$. For a particular $\ell$ the theory holds for all values of $\frac{\sigma_a}{\sigma_m^b}$ to the left of that indicated by the appropriate vertical line and for all values $\frac{\sigma_a}{\sigma_m^b}$ to the right the predicted attack frequency values are extrapolations of the theory. A new model of two cutting dislocations would have to be worked out for this larger $\frac{\sigma_a}{\sigma_m^b}$ domain. This is done in the next section.
2.2.7 Constriction and Jog Formation

One interesting case of the dislocation-non rigid barrier type interaction is the cutting of a non-interacting undissociated forest dislocation with a dissociated glide dislocation in forming a pair of jogs. Before the pair of jogs are formed, the dissociated glide dislocation must be constricted or pinched-off by the combined action of the externally applied stress and the relatively rigid forest dislocation. Dorn [2.10], using a line-energy model, has given a force-displacement relation for modestly dissociated dislocations as

\[
\frac{2}{3} \Gamma \left\{ 1 - \left[ 1 - .18 \left( -\frac{x}{x_0} + \ln \frac{x_0}{x_0 - x} \right) \right]^2 \right\}^{1/2}, \quad (x_0 - x) \geq b
\]

\[
F \approx \frac{2}{3} \Gamma \left\{ 1 - \left[ 1 - .18 \left( -\frac{x}{x_0} + 1 - \frac{x_0 - x}{b} + \ln \frac{x_0}{b} \right) \right]^2 \right\}^{1/2}, \quad (x_0 - x) \leq b
\]

(2.53)

Fig. 2.18 shows the model of a dissociated dislocation ribbon of width \( x_0 \) being constricted by a non-interacting forest dislocation. In the analysis of the attack frequency,
\[ F = \begin{cases} \frac{2\tau}{3} \left[ 1 - \left[ 1 - 0.18 \left( -\frac{x}{x_0} + \ln \frac{x_0}{x_0-x} \right) \right]^2 \right]^{1/2} & (x_0-x) > b \\ \frac{2\tau}{3} \left[ 1 - \left[ 1 - 0.18 \left( -\frac{x}{x_0} + 1 - \frac{x_0-x}{b} + \ln \frac{x_0}{b} \right) \right]^2 \right]^{1/2} & (x_0-x) \leq b \end{cases} \]

Fig. 2.18 - Constriction and Job in a Dissociated Glide Dislocation by an Undissociated Forest Dislocation - after Dorn
the line energy, \( \Gamma \), is taken to equal \( \frac{\mu b^2}{2} \) and following Dorn's analysis the width of the dissociated dislocation, \( x_o \), is taken to be \( 5b \). The force necessary to produce two jogs is taken to be

\[
F_{2j} = \frac{\Gamma}{\pi}
\]

which defines a maximum internal stress

\[
\sigma_m = \frac{\Gamma}{b^2 \pi} = \frac{\mu}{2\pi}
\]

By equating forces at equilibrium, we have for the equilibrium displacement

\[
x_{eq} = \frac{x_o b}{b - x_o} \left[ \frac{1 - (3\sigma_a D_f / 2\pi \sigma_m b)^2}{.18} \right]^{1/2} + \left( 1 - \frac{1}{.18} \right) + \ln \frac{x_o}{b} - \frac{x_o - x}{b}
\]

\[(x_o - x) \leq b\]

By the method of analysis outlined previously, the attack frequency was found to be given by
\[ \nu = \frac{\sigma_m b^2}{6\pi m_{\text{eff}}} \left[ \frac{\ln \frac{x_0}{x_0-x}}{\left(1 - \frac{x_0}{x_0-x}\right)^{1/2}} \right]^{1/2} \]

\[ \nu = \frac{\sigma_m b^2}{6\pi m_{\text{eff}}} \left[ \frac{\ln \frac{x_0}{x_0-x}}{\left(1 - \frac{x_0}{x_0-x} - \frac{\ln \frac{x_0}{x_0-x}}{2} \right)^{1/2}} \right]^{1/2} \]

\( x = x_{\text{eq}} \)

\( (x_0-x) \geq b \)

\( (x_0-x) \leq b \)

(2.56)
Fig. 2.19 shows the results of the analysis as attack frequency plotted against normalized applied stress. The continuous curve shown is a result of requiring that the two functional forms of the force-displacement relation are equal at \( x = b \). The curve shows the reasonable result of constant attack frequency during constriction and a peak in the frequency during the cutting of the more rigid forest dislocation.

It should be mentioned that although the attack frequency is plotted for a range of values for \( \sigma_m \), by definition \( \sigma_m \) should be of the order of magnitude of \( 10^{11} \) dy/cm\(^2\) which predicts an attack frequency of \( 10^{11} \text{(sec) }^{-1} \).

2.3 LINE ANALYSIS

Friedel [2.2], using a line tension approach, has calculated the natural frequency of vibration of a dislocation of length \( l \) pinned between two obstacles to be

\[
\nu_{\text{line}} = \nu_{\text{atomic}} \left( \frac{b}{l} \right)
\]  

(2.57)

This expression is appropriate for the idealized discretely pinned case. For a consistent attack frequency calculation, the corrections, Eqs. (2.4) and (2.5), to
Fig. 2.19 - Constriction and Job Formation
the distance between obstacles along the dislocation line were employed for the random obstacle cases. Figs. 2.20
and 2.21 show the applied corrections as well as the
stress dependence in the two random cases. In the case
of $D_s$ which is appropriate for size-effect obstacle
interactions, the natural frequency is shown also as a
function of $\eta$.

2.4 INTERACTION RELATIONS - EFFECTIVE ATTACK FREQUENCIES

It is reasonable to define an effective attack
frequency as the average number of times per second both
the line segment and local segment of the dislocation are
simultaneously travelling towards the peak of the obstacle
barrier. This effectively defines the average number of
times per second in which there is the greatest possibility
of the local dislocation segment surmounting the barrier.
The idea of an effective attack frequency is most pro-
nounced when the local and line frequencies are widely
different. In this case it is evident that the cooperative
efforts of the two dislocation segments should be governed
by the lower of the two frequencies.
Fig. 2.20 - Friedel's Natural Frequency of Oscillation of the Dislocation Line - Random Solute Case

- $\nu = 15.2 \times 10^6$, $\Lambda = b$, $\eta = 0.3$, $\ell = 10^4b$
- $\nu = 13.3 \times 10^6$, $\Lambda = b$, $\eta = 0.2$, $\ell = 10^4b$
- $\nu = 10.6 \times 10^6$, $\Lambda = b$, $\eta = 0.1$, $\ell = 10^4b$
- $\nu = 7.1 \times 10^9$, $\Lambda = b$, $\eta = 0.3$, $\ell = 10^2b$
- $\nu = 6.2 \times 10^9$, $\Lambda = b$, $\eta = 0.2$, $\ell = 10^4b$
- $\nu = 4.9 \times 10^9$, $\Lambda = b$, $\eta = 0.1$, $\ell = 10^4b$
- $\nu = 3.3 \times 10^{12}$, $\Lambda = b$, $\eta = 0.3$, $\ell = 10^6b$
- $\nu = 2.29 \times 10^{12}$, $\Lambda = b$, $\eta = 0.1$, $\ell = 10^6b$
Fig. 2.21 - Friedel's Natural Frequency of Oscillation of the Dislocation Line - Forest Dislocation Case

\[ \frac{\sigma_{\text{Df}}}{\sigma_{\text{mb}}} \]

\[ \times 10^6 \quad \sigma_m = 10^7, \quad \lambda = 10^{-4} \]
\[ \times 10^8 \quad \sigma_m = 10^7, \quad \lambda = 10^{-2} \]
\[ \times 10^{10} \quad \sigma_m = 10^7, \quad \lambda = 10^{-2} \]
\[ \times 10^8 \quad \sigma_m = 10^{11}, \quad \lambda = 10^{-4} \]
\[ \times 10^{10} \quad \sigma_m = 10^{11}, \quad \lambda = 10^{-2} \]
\[ \times 10^{12} \quad \sigma_m = 10^{11}, \quad \lambda = 10^{-2} \]
To accomplish this result, an appropriate harmonic average was applied to the frequency of the two dislocation segments. The harmonic average has the form

\[ \nu_{\text{eff}} = \frac{2}{\frac{1}{\nu_{\text{local}}} + \frac{1}{\nu_{\text{line}}}} \]  \hspace{1cm} (2.58)

and has the effect of weighting the lower of the two frequencies.

The frequency of the local dislocation segment is dependent strongly on the interaction relation under consideration, the maximum internal stress of the barrier, \( \sigma_m \), the width of the barrier, \( \Lambda \), and the physical constants of the obstacle. On the other hand, the frequency of the line dislocation segment is dependent strongly on the length of the dislocation segment between pinning points and the way the length changes as a function of applied stress and the physical array of obstacles in the lattice, \( D_f \) and \( D_s \). Appropriately averaging these two frequencies then produces a consistent and complete attack frequency analysis in that all variables of the system are consistently taken into account.

Figs. 2.22-2.38 show the results of the effective attack frequency calculation for all interaction relations and cases considered. The results are shown as a function of normalized applied stress and various values of the system parameters.
Fig. 2.22 - Effective Attack Frequency -
Cosine Relation - Random Solute Case
Fig. 2.23 - Effective Attack Frequency -
Cosine Relation - Forest Dislocation Case
Fig. 2.24 - Effective Attack Frequency -
Cosine Relation - Discretely Pinned Case
Fig. 2.26 - Effective Attack Frequency - Cottrell Bilby Relation - Discrete Pin Case
Fig. 2.27 - Effective Attack Frequency -
Cottrell Bilby Relation -
Forest Dislocation Case
Fig. 2.28 - Effective Attack Frequency - Seeger Relation - Random Solute Case
Fig. 2.30 - Effective Attack Frequency - Seeger Relation - Random Forest Case
Fig. 2.31 - Effective Attack Frequency - Fleischer (111) Distortion - Random Solute Case
Fig. 2.32 - Effective Attack Frequency -
Fleischer (111) Distortion -
Forest Dislocation Case
Fig. 2.33 - Effective Attack Frequency - Fleischer ⟨111⟩ Distortion - Discrete Pin Case
Fig. 2.34 - Effective Attack Frequency -
Quasi Parabolic Peierl's Relation -
Discrete Pin Case
Fig. 2.35 - Effective Attack Frequency - Saada Relation - Random Forest Case

$\sigma_{\bar{d}} = \frac{D_{\bar{d}}}{\sigma_{d}}$
Fig. 2.37 - Effective Attack Frequency -
Constriction and Jog Formation -
Forest Dislocation Case
Fig. 2.38 - Effective Attack Frequency - Constriction and Jog Formation - Discrete Pin Case
2.5 RESULTS

The preceding section shows the results of taking into account both the local and line segments of the dislocation when calculating the average effective attack frequency. Some interaction relations by their nature are restricted to a particular case of loop lengths. For example, the Peierl's relation is appropriate for only the continuously pinned discrete case, and the Saada and jog formation relations are appropriate for the random forest dislocation case. In all relations, the discretely pinned case was included in the analysis to compare to the current procedure for attack frequency calculations. As was already stated, this case, also called the "square array" configuration, is an idealized first order approximation to the actual pinning configuration and does not explicitly take into account the stress dependence.

The magnitude of the average effective attack frequency was found to have the same dependence on the maximum value of internal stress, $\sigma_m$, as on the length $\ell$ of dislocation between pinning points. It was found over all the configurations studied that the average effective attack frequency is in the range $10^9$ to $10^{11}(\text{sec})^{-1}$ assuming the moderate values of $10^9 \, \text{dy/cm}^2$ and $10^2 \, \text{b}$ for $\sigma_m$ and $\ell$ respectively. This is two to four orders of magnitude
different from the Debye frequency of $10^{13} \text{(sec)}^{-1}$.

Friedel's expression for the natural frequency of vibration of a dislocation line of the same length would be $10^{11}$ or $10^9 \text{(sec)}^{-1}$ depending on whether $l$, or $D_s$, $D_f$ are used.

Although this refined estimate of the line attack frequency gives the correct range of magnitudes in these cases, it does not take into account the $\sigma_m$ of the system and therefore would not be appropriate for configurations with internal stress maximum amplitudes much different from $10^9 \text{dy/cm}^2$.

The results of the analysis also show that for all the interaction relations studied, generally there is strong stress dependence for the continuously pinned case of $l = b$. Of the non-continuously pinned cases, $l > b$, generally the random forest case showed the highest degree of stress dependence. After the random forest case, both the random solute and square array cases showed about equal amounts of stress dependence ranging from slowly varying to zero stress dependence. This result is reasonable and consistent with the fact that $D_f$ was explicitly stress dependent and therefore should enhance the inherent stress dependence of the obstacle configuration.

Therefore, it is felt that the present analysis has significance in that it is complete and consistent in
taking into account all the physical parameters of a wide variety of dislocation-obstacle configurations. Also, by showing that the discretely pinned case is not realistic as a general approach and that the Friedel line frequency can predict the correct order of magnitude of the attack frequency for a $\sigma_m$ of the order of $10^9 \text{ dy/cm}^2$, the present analysis places these approximations in prospective. It is now possible to place the correct $v_{\text{eff}}$ for a particular model in the basic rate equation

$$
\dot{\varepsilon} = \dot{\varepsilon}_0 \exp\left(\frac{-\Delta G}{kT}\right)
$$

(2.59)

where $\dot{\varepsilon}_0 = N\bar{A}v_0$ and the other terms are as described by Schoeck [2.11]. The stress dependence of $\dot{\varepsilon}_0$ shows that it is highly unlikely any real mechanical property data will satisfy the appropriate thermodynamic treatment presented by Schoeck.
CHAPTER III
MICRODEFORMATION

3.1 INTRODUCTION

3.1.1 Anelasticity

As an externally applied tensile stress is applied to a metal sample, it passes consecutively from the short, almost non-existent, initial elastic region through an anelastic region to finally the macroscopic work hardening region. The early anelastic region is characterized by dislocations moving reversibly through displacements in the order of the interdislocation separation distance. Upon unloading there is a net flux of dislocations moving in the reverse direction which is equal in magnitude to the flux moving forward during loading for closed anelastic damping loops. In the high amplitude anelastic region just before macroscopic plastic deformation this equality no longer holds. There is a net flux of dislocations moving in one direction over the total stress cycle which contributes to the establishment of an internal or bias stress. The low amplitude closed damping loop domain of strain is usually $< 10^{-4}$. This is a significant domain in that it may be possible to consider a microstrain model in the light of a macrostrain model under a stress independent,
constant dislocation density situation. Also, a microstrain study may reveal data which would establish knowledge related to the operative microscopic structural parameters. An understanding and quantitative description of the dislocation processes operating and causing the macroscopic feature of work hardening in the easy glide region could possibly be obtained through correlation with the microstrain study.

3.1.2 Macroscopic Theories of Easy Glide

An understanding of Stage I (Easy Glide) work hardening is necessary to get the foundation of knowledge of the stress-strain curve on sound ground. This understanding is being brought about largely by the increased amount of experimental data on fcc and hcp metals through three principal methods of study: measurement of surface slip lines [3.1, 3.2, 3.3], transmission electron microscopy [3.3, 3.4, 3.5, 3.6] and shape and size experiments [3.7].

This development of experimental data has had a varying degree of influence on the subsequent development of some of the theories proposed to explain work hardening in fcc and hcp metals in the easy glide region. The Hirsch
and Lally theory [3.3], for example, was developed mainly as an interpretation of the experimental results of their extensive electron microscopic investigation of magnesium single crystals. They propose that the dislocation loops emitted by sources present in the crystal glide through the crystal until they become blocked or annihilated by combining with dislocations (via cross slip or climb) of opposite sign on parallel slip planes created by other sources. The origin of the work hardening is proposed to be due to the enhanced stress fields produced by the increase in the number of clusters with excess dislocations of one sign. Their development predicts for the normalized work hardening coefficient a strain dependent function

$$\frac{\delta}{G} = \left( \frac{b}{L_s} \right)^{1/2} \frac{1}{4\pi(2n)^{1/4}} \left[ \rho_o L_s b (2n)^{1/4} + \epsilon \right]^{-1/2}$$

(3.1)

where $L_s$ is the average screw dislocation slip line length, $n$ is the average number of dislocation loops emitted per source, $\rho_o$ is the initial dislocation density, $\epsilon$ is the amount of prestrain, and $b$ is the dislocation strength.

Seeger [3.8] pictures the mechanism of easy glide work hardening as dislocations, after being generated by Frank-Reed sources, become blocked by ingrown obstacles in the crystal and spread-out behind these obstacles. A
nearby gliding dislocation on another glide plane will overcome the stress fields of the blocked dislocations individually with the help of the externally applied stress. By employing a probabilistic approach to each stage of the above process, Seeger et al. have developed a Stage I work hardening theory in terms of slip line parameters which has the form

\[
\frac{\theta}{G} = \frac{8}{9\pi} \left( \frac{x}{L_2} \right)^{3/4}
\]  

(3.2)

where \(x\) is the active slip plane separation distance and \(L_2\) is the average length a screw dislocation moves prior to blockage.

Using a development very similar to that employed by Hirsch and Lally, Hazzledine [3.9] has developed a macroscopic work hardening relation assuming dislocation multipole interaction across parallel slip planes. The resultant stress-strain relation has the form

\[
\tau = \tau_0 + \frac{Gb}{8\pi(1-\nu)} \left( \frac{18}{7bD^2} \right)^{1/3} \epsilon^{1/3}
\]

(3.3)

where \(D\) is related to the density of sources and all other terms are as defined by Hirsch and Lally.
Taking a theoretical approach, Van Bueren [3.10] has developed a Stage I work-hardening relation by simply considering the elastic interaction stress necessary for one dislocation bundle to glide past another dislocation bundle on a parallel slip plane. Assuming the edge and screw dislocation displacements delineating dislocation loop geometry are approximately equal, Van Bueren's resultant work hardening relation has the form

\[
\frac{\delta}{G} = \frac{\delta}{S^{1/2}A^{3/4}}
\]  

(3.4)

where \( S \) is the density of dislocation sources, \( A \) is the average area swept out per newly created dislocation loop, and \( \delta \) is a constant of the order of 0.10.

These relations will be explained more completely and investigated more fully in Section 3.3 where their modification will be considered.

3.1.3 Microstrain Work Hardening

Microstrain work by recent investigators [3.11, 3.12, 3.13] indicates that the fundamental difference between the microscopic anelastic region and the early stages of macroscopic work hardening is that the dislocation density increases with strain during macroscopic easy glide
deformation whereas the dislocation density is constant during microstrain. Salama and Roberts [3.14] in order to describe anelastic microstrain behavior during loading and unloading in the easy glide region have modified the Van Bueren easy glide macroscopic work hardening theory to the constant density of dislocation criterion. The modification consisted of assuming the elastic interaction of a constant density of mobile dislocation bundles with other bundles of constant density on parallel glide planes during loading and unloading in the easy glide prestrain region. Van Bueren's expression for the internal stress opposing dislocation generation and motion is

$$\tau = \alpha G b n ( S A^{1/2})^{1/2}$$

(3.5)

where \(n\) is the number of dislocation loops emitted per source and all other terms are as previously defined. If after prestraining the sample to a stress level \(\tau\), the stress is lowered by an amount \(d\tau\), the dislocation bundles will relax and sweep back an average incremental area \(dA\), given by

$$d\tau = \frac{\alpha}{4} G b n S^{1/2} A^{-3/4} dA$$

(3.6)

The recovered microstrain increment is given by

$$d\gamma = n S b dA$$

(3.7)
and for constant \( n \) and \( S \), the total recovered microstrain is given by

\[
\Delta \gamma_R = n S b a_R
\]

Upon substituting 3.7 and 3.8 into 3.6 and integrating these results the microstrain work hardening relation

\[
\tau = \left[ \alpha G S^{1/4} (nb)^{3/4} \right] \gamma_R^{1/4} + C
\]

where \( \tau \) is the amount the stress has been lowered below the flow stress in order to obtain the recovered microstrain, \( \gamma_R \). \( C \) is a constant of integration which takes into account all contributions to the net internal stress acting upon the anelastic mobile dislocations. A term \( K \) can be defined in terms of the microscopic dislocation arrangement parameters by

\[
K = \alpha G S^{1/4} (nb)^{3/4}
\]

A detailed study of unidirectional stress cycle damping loops carried out by Salama and Roberts on a pure magnesium single crystal indicated that the proposed stress-microstrain relation adequately described the microstrain behavior. The magnesium sample was 99.99% pure and both the loading and unloading curves of the
damping loops were analyzed at various amounts of applied stress at both 300°K and 77°K up to a total prestrain of 7.44%. It was also shown that the operative microscopic parameters appeared to be independent of strain rate and temperature. A strain rate change by a factor of 25 produced negligible effect in the slope, K, and over the above mentioned temperature range the value of K increased by only about 20%, when the temperature was decreased from R.T. to 77°K. A fractional change of this amount is the same as can be expected from the temperature dependence of the shear modulus alone. The data then indicated practically no temperature dependence of the microscopic parameters, verifying the athermal elastic interaction assumptions of the theory. Fig. 3.1 is representative data taken on magnesium by Salama and Roberts and reproduced by permission. These data show clearly the validity of the one quarter power relation at low temperature (77°K) as well as at 300°K.

3.1.4 Objective

Seeger [3.15] relates his work hardening theory to slip line studies and notes that the Seeger et al. theory adequately describes the data. Equation (3.2) shows the 3/4 power dependence of the Seeger et al. relation on
Fig. 3.1 - Microstrain Data of Salama and Roberts at both Room Temperature and 77°C. Reproduced by permission.
the parameters $x$ and $L_2$. By putting Van Bueren's macro-
scopic work hardening theory in terms of the same para-
meters, Salama and Roberts [3.16] found a $1/2$ power
dependence of the form

$$\frac{\theta}{G} = \frac{\alpha}{3^{1/4}} \left(\frac{x}{L_2}\right)^{1/2} \quad (3.11)$$

By applying the Salama-Roberts extension of the Van Bueren
relation to the same data as employed by Seeger et al.,
Salama and Roberts [3.15] point out that the macroscopic
data is equally well described by either the Seeger et al.
or their modified Van Bueren relation. Therefore, from
the point of view of agreement with macroscopic parameters,
Van Bueren's model appears no less successful than the
Seeger et al. relation in describing the Stage I work
hardening. Figure 3.2 shows a plot of Eq. (3.11) using
the data described by Seeger. The significance of this
comparison is that it illustrates that consistency of a
dislocation model with its attendant application to
macroscopic parameters is not unique in establishing the
validity of the model.

The agreement afforded by the Salama and Roberts
analysis on the equal relative merits of the Seeger et al.
and Van Bueren macroscopic work hardening relations demands
a new method to discriminate between the success of one
a. Analysis of Seeger, et. al.

b. Salama and Roberts interpretation of the Van Bueren Model

Fig. 3.2 - Analysis from macroscopic data
theory over another. The Salama-Roberts microstrain relation, which was developed by a modification of the Van Bueren relation, has lead to the idea that the adequacy of a work hardening theory may be determined by the consistency of interrelation of its macroscopic and microscopic predictions. Therefore, by employing a complete and integrated experimental approach, i.e., by taking microstrain data in many samples through large values of $\gamma_p$ and at various temperature in conjunction with electron microscopy techniques, three objectives were to be accomplished.

Firstly, it has been shown by Salama and Roberts [3.14] that the microstrain unloading curve after Stage I prestraining of Mg crystals is given by

$$ (\tau_m + \tau_{BU} - \tau_a) = K\gamma_r^{1/4} \quad (3.9) $$

where $\tau_m$ is the maximum stress prior to unloading, $\tau_{BU}$ is a constant bias stress acting upon dislocations which take part in strain recovery, $\tau_a$ is the instantaneous unloading applied stress and $\gamma_r$ is the recovered microstrain. $K$ is a constant given by:

$$ K = \alpha G b^{3/4} (Sn^3)^{1/4} \quad (3.10) $$
where $S$ is the number of active dislocation sources/cm$^3$, $n$ is the number of dislocation loops emitted per source, $\alpha$ a numerical factor of the order of 0.1 and $G$ and $b$ have their usual meaning. This model predicts a finite recovered microstrain during total unloading given by:

$$\gamma_{r_0} = nSB(A_r)_0$$ (3.8)

where $(A_r)_0$ is the average total area swept out during backward motion of the dislocations upon unloading. The anelastic microstrain relations (2) and (3) contain three unknowns, $S$, $n$ and $(A_r)_0$. However, the macroscopic stage I work hardening relation is given by

$$\theta = \alpha G(SA^{3/2})^{-1/2}$$ (3.4)

where $A$ is the average area swept out per dislocation loop at the macroscopic flow stress. Slip line length studies can yield a value for $A$, and hence, $S$ is evaluated from (3.4). Now relations (3.10) and (3.8) can be solved for $n$ and $(A_r)_0$, provided $S$ (macroscopic) is the same as $S$ (anelastic). The current study was undertaken to see if this combination of anelastic microstrain and macroscopic macrostrain data yields a reasonable correlation and interpretation to the phenomena.
Secondly, it is intended to develop the Seeger et al., Hirsch and Lally, and Hazzledine theories of easy glide in the manner described by Salama and Roberts to see what these theories predict with respect to microstrain data. In addition, each theory must be interpreted correctly so that the resulting equations which predict experimental results to dislocation structure parameters are established in terms of the same defined variables for each of the theories. The combination of electron microscopic results, macrostrain and microstrain should evaluate if one theory is self consistent in explaining all of the results. If no theory is adequate, it is intended to evaluate which one seems most reasonable. Therefore, thirdly, it is intended to evaluate how the most reasonable theory should be modified if it cannot explain consistently all of the results.

3.2 EXPERIMENTAL PROCEDURE

To carry out this investigation, single crystals of magnesium were used. Magnesium is a particularly appropriate metal to use for this investigation since there already existed some initial results on this metal. The primary slip system of magnesium is the basal slip
(0001)\langle 2\overline{1}10\rangle$. Secondary slip systems have been observed as \langle 10\overline{1}0\rangle\langle 2\overline{1}10\rangle and \langle 10\overline{1}1\rangle\langle 2\overline{1}10\rangle denoted as prismatic and pyramidal respectively. All three slip systems have the same slip direction. The stage I or easy glide work hardening region is characterized by a work hardening coefficient of the order of magnitude of \( \frac{\mu}{10^4} \) where \( \mu \) is the shear modulus. In magnesium, the stage I region extends as far as 100% shear strain and therefore affords a large region over which the easy glide microstrain theory of Salama and Roberts can be investigated. Table 3.1 lists the magnesium samples employed in the investigation as well as the physical properties of each. \( \theta \) is the angle between the basal plane normal and the cylinder axis, and \( \varphi \) is the angle between the \langle 1\overline{1}20\rangle slip direction and the cylinder axis. The spectrographic analysis for these specimens was reported by Hartman [3.13] in his Ph.D. thesis. Hartman is credited for growing the crystals. The values of Young's modulus were calculated from the most reliable sources of elastic constant data and incorporate the orientation dependence of the Young's modulus via the usual relation [3.13].

The stress-microstrain curves for the samples were taken using the capacitance gauge strain system [3.17] in conjunction with an Instron tensile machine. The capacitance gauge technique, which is fully described in the
TABLE 3.1

<table>
<thead>
<tr>
<th>Sample</th>
<th>θ</th>
<th>φ</th>
<th>(\cos \theta \cos \phi)</th>
<th>Initial Area (sq in)</th>
<th>ppm major impurity</th>
<th>Calculated Young's Modulus g/mm² x 10^6</th>
</tr>
</thead>
<tbody>
<tr>
<td>M1A2A</td>
<td>35°</td>
<td>59°</td>
<td>0.42</td>
<td>0.145</td>
<td>Al/81 Si/52 C/47</td>
<td>4.56</td>
</tr>
<tr>
<td>M1A2B</td>
<td>35°</td>
<td>59°</td>
<td>0.42</td>
<td>0.145</td>
<td>Al/81 Si/52 C/47</td>
<td>4.56</td>
</tr>
<tr>
<td>M4A</td>
<td>66°</td>
<td>32°</td>
<td>0.34</td>
<td>0.153</td>
<td>---</td>
<td>4.97</td>
</tr>
<tr>
<td>M1B</td>
<td>37°</td>
<td>56°</td>
<td>0.446</td>
<td>0.15</td>
<td>---</td>
<td>4.60</td>
</tr>
<tr>
<td>M10B</td>
<td>37°</td>
<td>56°</td>
<td>0.446</td>
<td>---</td>
<td>Al/45 Zn/37 Si/35</td>
<td>4.60</td>
</tr>
</tbody>
</table>
above reference, was essentially developed at the University of Pennsylvania and Rice University. This technique is easily capable of achieving a strain sensitivity of $10^{-6}$ with an accuracy of $\pm 5\%$.

It is basically a capacitance bridge circuit employing a Wayne-Kerr capacitance electronic micrometer and an x-y recorder. Prior to a macroscopic prestrain increment, the gap of the capacitance gauge is set at a small predetermined value by balancing the Wayne-Kerr capacitance electronic micrometer of the strain system. The initial gap spacing of the specimen capacitance gauge is determined by the amount of macroscopic pre-strain one wishes to put into the sample and the length of the strain gauge being used. The Wayne-Kerr micrometer is then set to a gap of approximately 0.025" for balance. At this gap it was found that the strain system has a strain sensitivity of about $10^{-6} \pm 5\%$. The sample was then strained until the predetermined amount of macroscopic strain had been introduced into the sample. The strain system was then again balanced. The sample was then unloaded and the details of the unloading curve were recorded on the x-y recorder. At strain levels below a few times $10^{-5}$, the sample can be recycled to obtain the details of the loading curves and the unidirectional closed damping loops.
Low temperature data was taken at 77°K employing the same techniques as cited above while both the sample and the strain gauge were immersed in a liquid nitrogen bath. The dielectric constant of liquid nitrogen is approximately 1.454, while that of air is approximately 1.000. This difference has the effect of shifting the balance point of the strain system by changing the capacitance of the strain gauge. By taking into account the difference in both the dielectric constants and the capacitor plate areas between the capacitance gauge and the Wayne-Kerr capacitance micrometer, it was calculated that for liquid nitrogen temperatures

\[ 0.9 \, g_{WK} = g_G \quad (3.12) \]

whereas for room temperature

\[ 0.61 \, g_{WK} = g_G \quad (3.13) \]

where \( g_{WK} \) is the micrometer capacitor gap read directly from the Wayne-Kerr micrometer and \( g_G \) is the actual gap of the capacitor strain gauge. From the work of Hartman, Bresie and Roberts [3.18]

\[ g_{WK}/g_G = \frac{\alpha_{WK}}{K_G} A_G \]
where \( \alpha \) is a temperature independent proportionality constant, \( A_{WK} \) and \( A_G \) are the plate areas for the Wayne-Kerr and gauge respectively, \( K_G \) is the dielectric constant of the gauge. Therefore, this result is consistent with \( (K_G)_{N_2} \) being greater than \( (K_G)_{AIR} \).

Figures 3.3 and 3.4 are representative stress-microstrain curves taken at 300°K and 77°K respectively. The curves were taken on crystal MIB after total pre-strain intervals of 0.174 and 0.274 respectively. Incorporated in the figures are the calculated elastic modulus lines which serve as an indication of the elastic microstrain and also delineate the anelastic microstrain region. The loading and unloading sequence is shown by the arrows along the curves.
Fig. 3.3

\[ \gamma_p = 0.174 \]
\[ T = 300^\circ K \]

Shear Stress

Shear Strain

\[ \tau_f \]

159.4 psi

119.4 psi

79.6

39.8

Elastic Modulus

12 \times 10^{-5}
$\gamma_p = 0.274$

$T = 77^\circ K$

Fig. 3.4

Shear Stress vs. Shear Strain diagram with:
- $258.7$ psi
- $159.2$ psi
- $79.6$ psi

$\tau_f$ and $\gamma_r$ indicate specific shear stress and shear strain levels.

$L x 10^{-5}$
3.3 MICROSTRAIN ANALYSIS

3.3.1 The $1/4$ Power Relation

From the stress-microstrain work of Argon and Brydges [3.11] on copper, Hartman [3.13] on magnesium, and Roberts and Brown [3.12] on zinc, empirical relations of the form $\tau = c\gamma^n$ are published that fit the stress-strain curve in the microstrain region. The value of $n$ reported by the above authors varies considerably. Hartman reports $n = 3/4$ while Argon and Brydges report $0.31 \rightarrow 0.37$. Roberts and Brown found $n = 0.12$ to .57 for zinc.

The stress-microstrain relation of Salama and Roberts ($\tau_m - \tau_a + \tau^* = K\gamma^{1/4}$) contains a bias stress term, $\tau^*$, whereas the above empirical relation does not. An analysis was made to determine the sensitivity of the one-fourth power dependence of stress on microstrain.

The presence of the $\tau^*$ term, which is an experimental variable in the Salama-Roberts relation, made finding the slope of a $\ln\ln$ plot of the appropriate experimental data points an improper procedure for obtaining the experimentally determined power of the microstrain. Therefore, stress was plotted against various powers of associated microstrain and the linearity and slope of the experimental points was compared to theory. Figure 3.5 shows the analysis carried out on unloading curves of crystal M1A2A at 300$^\circ$K.
Fig. 3.5.1

\[ \tau_m - \tau_a \quad \text{psi} \]

\[ \gamma^{1/n} \]

Points and lines indicating data with denominators 1/3, 1/2, 1/4, and 1/5.
after a total prestrain of 0.9%. The analysis shows that, within the limits of experimental error, the $1/3$, $1/4$ and $1/5$ powers of microstrain can adequately describe the observed behavior. In all three cases the experimental data deviates from a linear relation only at the extreme low or high values of stress, where the present theory is expected to not be completely valid. A similar variance in the powers of microstrain was noted when analyzing loading curves and unloading curves at different temperature and amounts of prestrain. Appendix I shows actual data taken on various crystals at various amounts of prestrain at both $300^\circ$K and $77^\circ$K. The stress is plotted against recovered strain to the one quarter power, $\gamma_{r}^{1/4}$, and the slope and intercept, $\tau^{*}$, is noted.

3.3.2 Other Microstrain Work Hardening Models

Having established the stress microstrain region as obeying a $1/4$ power relation and having an idea of the sensitivity of the data to this power, the other principal macroscopic relations were modified in a manner following that of Salama and Roberts in order to investigate their predictions in the anelastic region.
Seeger has given the macroscopic work hardening relation in the general form

\[ \tau = \tau_o + \frac{nbG}{2\pi} \left( R_0 L_2 \right)^{-1/2} \]  \hspace{1cm} (3.14)

where \( R_0 = \left( \frac{1}{NL_1^2} \right)^{1/2} \) where \( L_1 \) and \( L_2 \) are the lengths of edge and screw slip line lengths respectively, and \( N \) is the density of sources. Letting \( L_1 = \alpha L_2 \) where \( \alpha > 1 \) and using Seeger's expression for the macroscopic area swept out per dislocation loop \( A = \frac{9}{16} \alpha L_2^2 \), Eq. (3.14) in terms of \( A \) becomes

\[ \tau = \tau_o + \left( \frac{9}{16} \right)^{1/8} \left( \frac{nbS}{2\pi} \frac{1/4 G\alpha^{3/8}}{2\pi} \right) A^{-1/8} \]  \hspace{1cm} (3.15)

Following the Salama-Roberts assumption that the microstrain region is controlled by a constant active dislocation density, Eq. (3.7) can be applied to a differential form of Eq. (3.15) when \( n \) and \( S \) are assumed constant. After integration, there results the microstrain relation

\[ \tau = \left[ \frac{(nb)^{9/8}S^{3/8}G\alpha^{3/8}}{2\pi} \left( \frac{9}{16} \right)^{1/8} \right] \gamma_r^{-1/8} + c_1 \]  \hspace{1cm} (3.16.1)
where $C_1$ is an integration constant. If $\tau$ is taken to be the applied stress, $\tau_a$, plus a bias stress, $\tau_b$, the boundary condition that $\gamma_r$ should equal the total recovered microstrain $\gamma_{r_0}$ when $\tau_a = 0$, yields $C_1 = \tau_b - \beta \gamma_{r_0}^{-1/8}$ where $\beta$ is the above bracketed term. This then gives

$$\tau_a = \beta \left[ \gamma_r^{-1/8} - \gamma_{r_0}^{-1/8} \right] \quad (3.16.2)$$

$\gamma_r^{-1/8} \geq \gamma_{r_0}^{-1/8}$, therefore, as $\tau_a$ decreases $\gamma_r$ increases, which is a reasonable functional form.

However, from the preceding analysis, it is seen that the $1/8$ power dependence is beyond the experimental variance of data and does not appear adequate to describe the microstrain region of magnesium as observed experimentally.

A similar analysis is made on the macroscopic work hardening relation of Hirsch and Lally. They assume the total stress opposing dislocation motion is given by

$$\tau = \tau_0 + \frac{Gb}{\ell} + \frac{Gb}{2\pi(2n)} \frac{1}{\ell^{1/4}} \sqrt{\rho_s} \quad (3.17)$$

where the individual terms are the contributions from the frictional stresses, line tension and internal stresses respectively. $G$ and $b$ are as defined previously, $\ell$ is
the Frank-Read source length, \( n \) is the number of dislocation loops emitted per source, \( \sqrt{2n} \) is the number of excess dislocations of one sign on one slip line relative to that on another, and \( \rho_S \) is the total screw dislocation density. A unique feature of the Hirsch-Lally development is that it is assumed that only a certain number of dislocation sources, \( dN \), operate in a strain interval \( d\varepsilon \). Therefore

\[
d\varepsilon = (4L_S L_E bn) \, dN \tag{3.18}
\]

where \( L_S \) and \( L_E \) are the lengths of the screw and edge slip line traces respectively. The increase in dislocation density, \( d\rho_S \), is assumed to depend on the number of sources, \( dN \), operating in a strain interval \( d\varepsilon \) by

\[
d\rho_S = (4L_S n) \, dN \tag{3.19}
\]

The increase in dislocation density is then dependent on the strain increment and by integration an expression for the total dislocation density, \( \rho_S \), is

\[
\rho_S = \sqrt{2n} \rho_0 + \frac{\varepsilon}{L_S b} \tag{3.20}
\]

where \( \rho_0 \) is the initial dislocation density and \( \varepsilon \) is the total prestrain given to the sample. This \( \rho_S \) expression is then put into the total stress equation and the line
tension term is neglected to yield

$$\tau - \tau_0 = \frac{G}{2\pi(2n)^{1/4}} \left( \frac{b}{L_S} \right)^{1/2} \left[ \rho_o b (2n)^{1/2} + \epsilon \right]^{1/2}$$

(3.21)

Hirsch and Lally picture the area swept out per dislocation loop as having the dimensions $3L_S \times 2L_E$ and $L_E$ has a value anywhere from $L_S$ to $2L_S$. By letting $L_E = L_S$, the area is given by $A = 6L_S^2$ and Eq. (3.21) becomes in terms of the area

$$\tau - \tau_0 = \frac{Gb^{1/6}(2n)^{1/4}}{2\pi(2n)^{1/4}} \left[ \frac{\rho_o b (2n)^{1/2}}{\sqrt{6}} + \frac{\epsilon}{A^{1/2}} \right]^{1/2}$$

(3.22)

Differentiating with respect to $A$ and applying the Salama-Roberts assumption of constant density of sources and dislocations during microstrain recovery, which means $dY_r = nbN\delta A$ and $Y_r = nbNA$ there results the relation

$$d\tau = \frac{-Gb^{1/6}(2n)^{1/4} \epsilon (nbS)^{1/2}}{2\pi(2n)^{1/4} 4Y^{5/4} \left[ \frac{\rho_o b (2n)^{1/2}}{\sqrt{6}} + \gamma^{1/2} \right]^{1/2} (nbS)^{1/2}}$$

(3.23)

After integration, there results the present author's modification of the Hirsch-Lally macrostrain relation to describe microstrain recovery.
\[ \tau = \frac{G b (\rho_o)^{1/2}}{2\pi} \left[ 1 + \frac{\varepsilon^{1/3}}{b^{1/2} \rho_o \gamma_r^{1/2}} \right]^{1/2} + C \quad (3.24) \]

It can be seen by an order of magnitude estimate that the second term in the brackets is always much greater than one. For prestrain, \( \varepsilon \), as small as \( 1 \times 10^{-2} \), if 
\( S = 10^8 \text{ cm}^{-3}, b = 10^{-8} \text{ cm}, \rho_o = 10^6 \text{ cm}^{-2}, \gamma_r = 3 \times 10^{-5} \),
then the second term is approximately equal to \( 10^3 \).
Therefore, the above relation can be approximated by

\[ \tau = \left[ \frac{G b^{3/4} S^{1/4} \varepsilon^{1/2}}{2\pi} \right] \gamma_r^{-1/4} + C \quad (3.25.1) \]

The negative exponent is found in this case as well as in the Seeger relation. Applying the boundary condition that
\( \gamma_r \) must equal the total recovered microstrain, \( \gamma_{r_o} \), when
the applied stress, \( \tau_a \) equals zero, the constant of integration becomes
\( C = -\beta \gamma_{r_o}^{-1/4} \) where \( \beta \) is the above term in brackets. The above relation then becomes

\[ \tau_a = \beta \left[ \gamma_r^{-1/4} - \gamma_{r_o}^{-1/4} \right] \quad (3.25.2) \]

\( \gamma_r^{-1/4} \geq \gamma_{r_o}^{-1/4} \) therefore \( \gamma_r \) must decrease as \( \tau_a \) increases,
which is the proper functional form and apparently the
proper power dependence on $\gamma_r$. Eq. (3.25.2) was applied to experimental data taken on both crystal M1A2B and crystal M1B at various amounts of prestrain and at 77°K as well as 300°K. Figures 3.5.2 to 3.5.5 show the comparison of Eq. (3.25.2) to Eq. (3.9) after the same boundary conditions have been applied. It is noticed that the present modification of the Hirsch-Lally relation is more appropriate for large values of $\tau_m - \tau_a$ and deviates drastically at small values. The Salama-Roberts relation, however, holds over a much larger range and deviates only slightly at the two extreme ends of the microstrain region.

The macroscopic relation proposed by Haazledine [3.9] employs the concept of dislocation multipole interaction which is a concept different from those of the other macroscopic relations considered. The sources on one slip plane emit dislocation loops which are trapped by dislocations emitted by a source on a nearby slip plane and form multipoles. Because the interaction stress is proportional to $y^{-1}$ when $y$ is the separation distance between glide planes, for a given applied stress there is a maximum value of $y$ below which the dislocations are trapped. As the flow stress increases the value of $y$ decreases. Therefore, in a stress increment $d\tau$ a number of groups glide and form a multipole with another group in a closer slip
crystal M1A2B

\[ \gamma_p = 0.0003 \]

\[ T = 300^\circ K \]

Fig. 3.5.2
crystal MLB
\[ \gamma_p = 0.174 \]
\[ T = 300^\circ K \]

Fig. 3.5.3
\[ \frac{1}{4} \gamma_r - \frac{1}{4} \gamma_{r_0} \]

Crystal MLB
\[ \gamma_P = 0.274 \]
\[ T = 77^\circ K \]

\[ \tau_m - \tau_a \quad \text{psi} \]

H-L S-R

\[ \gamma_r^{-1/4} - \gamma_{r_0}^{-1/4} \]

\[ \frac{1}{4} \gamma_{r_0} - \gamma_r \]

Fig. 3.5.4
crystal MLA2B

\( \gamma_p = 0.81 \)

\( T = 300^\circ\text{K} \)

\( \gamma_r - \gamma_{r_0} \)

\( \frac{1}{4} \)

\( \frac{1}{4} \)

\( \tau_m - \tau_a \) psi

Fig. 3.5.5
plane. Assuming random sources, Hazzledine develops the relation

\[ L_E = \frac{D^2}{D^*} \]  

(3.26)

where \( L_E \) is the edge dislocation slip distance, \( D \) is the mean separation of sources when projected onto a plane normal to the slip plane and parallel to the Burger's vector, and \( D^* \) is a critical value of \( y \) for which two groups in a multipole will just pass. In the stress increment \( d\tau \), \( D^* \) will vary according to

\[ d\tau = \frac{-Gb}{8\pi(1-\nu)} \frac{dD^*}{D^{*2}} \]  

(3.27)

\( D^* \) is related to \( L_E \) by Eq. (3.26) and by assuming \( L_E = \alpha A^{1/2} \) where \( \alpha > 1 \), Eq. (3.27) can be put in the form

\[ d\tau = \frac{Gb}{8\pi(1-\nu)} \frac{\alpha}{2D^2} \frac{dA}{A^{1/2}} \]  

(3.28)

In the microscopic concept of Salama and Roberts, the dislocation source density is assumed to remain constant during unloading. In the Hazzledine relation, however, during loading or unloading the value of \( D^* \) decreases or increases respectively causing a corresponding respective decrease and increase in the density of active
sources due to blocking. This effect, although intuitively negligible, can be easily taken into account so that an inconsistency between the two regions does not develop. The total differential of the recovered microstrain is given as

\[ \text{d}v_r = nbS \text{d}A_r + nbA_r \text{d}S \]  \hspace{1cm} (3.29)

Hazzledine has defined an areal density of active sources, \( dN \), operating during the strain interval \( \text{d}\varepsilon \) as

\[ dN = \frac{\text{d}D^*}{D^* D^2} \]  \hspace{1cm} (3.30)

By assuming \( \text{d}S = \frac{dN}{D} \) and putting \( D^* \) in terms of \( \Lambda \) as was done previously, the change in the active source density during microscopic unloading is given by

\[ \text{d}S_r = -\frac{\text{d}A_r}{2A_r D^3} \]  \hspace{1cm} (3.31)

The recovered area is then given in terms of the recovered microstrain from Eq. (3.29) as

\[ \text{d}A_r = \frac{\text{d}v_r}{nb(S - \frac{1}{2D^3})} \]  \hspace{1cm} (3.32)
Eq. (3.32) can be put into Eq. (3.28) and immediately integrated to yield the present author's stress-microstrain modification of the Hazzledine relation

$$\tau = \left[ \frac{G b s^{1/2}}{8\pi(1-\nu)2d^2 nb^{1/2}} \left( s - \frac{1}{2d^3} \right) \right] \gamma_r^{1/2} + c \quad (3.33.1)$$

Evaluating the integration constant as was done in the previous relations we come to the relation

$$\tau_a = \beta \left[ \gamma_r^{1/2} - \gamma_{r0}^{1/2} \right] \quad (3.33.2)$$

The resultant 1/2 power relation, while corresponding more closely to experiment than the results of the other major macroscopic relations, still falls outside of the previously determined range of agreement with experiment.

It is apparent, then, that the assumptions of Salama and Roberts for the microscopic region coupled with the assumptions of Van Bueren's macroscopic relation forms the only consistent relation capable of adequately describing both the macroscopic and microscopic regions.

As an overview of the present analysis and to facilitate comparison of all relations considered, Table 3.2 summarizes concepts, terms and significant equations.
TABLE 3.2

Comparative Study of Major
Work Hardening Relations
<table>
<thead>
<tr>
<th>Macroscopic Easy Glide Model</th>
<th>Hirsch-Lally</th>
<th>Seegar et al.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proposed Operative Mechanism</td>
<td>Excess dislocations of one sign on one plane interacting elastically with excess dislocations on a neighboring plane of opposite sign forming multipoles</td>
<td>Single dislocations interacting elastically with other blocked single dislocations</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Density of Active Dislocation Sources</th>
<th>Variable</th>
<th>Constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Variable with Stress</td>
<td>( \tau = \frac{GB}{4\pi(1-\nu)d^2} )</td>
<td>( (\tau - \tau_0) \frac{d\tau}{dn} = \frac{GB^2}{2\pi R_0 L_2} )</td>
</tr>
<tr>
<td>Variable with Strain</td>
<td>( \sigma = (4 L_0 L_2 \eta) \frac{d\sigma}{d\eta} )</td>
<td>( \sigma = \frac{9}{16} \cdot \frac{b L_0 L_2 \eta}{d\eta} )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stress-Strain Relation Macroscopic</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Macroscopic</td>
<td>( \tau - \tau_0 = \frac{GB}{L_0^{1/2} 2\pi(2n)\epsilon^{1/2}} \left[ \frac{\tau}{\theta_{0}^{1/2} b(2n)^{1/2} + \epsilon} \right]^{1/2} )</td>
<td>( \tau - \tau_0 = \frac{G}{2\pi} \left( \frac{\sigma}{L_2} \right)^{3/4} \epsilon )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Area of Dislocation Loop</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>A = 6 ( L_0^2 )</td>
<td>when ( L_B = L_S )</td>
<td>A = ( \frac{9}{16} L_1 L_2 )</td>
</tr>
<tr>
<td>A = 12 ( L_0^2 )</td>
<td>when ( L_B = 2L_S )</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Present author's Microstrain Modification Salama-Roberts</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tau = \left( \frac{GB^{3/4} L_0^{1/4} \epsilon^{1/4}}{2\pi} \right) \sqrt{\frac{\tau}{\theta_{0}^{1/2} b(2n)^{1/2} + \epsilon}} )</td>
<td>( \tau = \left[ \frac{(nb)^{9/8} L_0^{3/8} \epsilon^{1/8}}{2\pi(1\epsilon^{1/8})} \right] \sqrt{\frac{\tau}{\theta_{0}^{1/2} b(2n)^{1/2} + \epsilon}} )</td>
<td>( \tau = \left[ \frac{(nb)^{9/8} L_0^{3/8} \epsilon^{1/8}}{2\pi(1\epsilon^{1/8})} \right] \sqrt{\frac{\tau}{\theta_{0}^{1/2} b(2n)^{1/2} + \epsilon}} )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stress-Recovered Area Relation in Microstrain</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tau - \tau_0 = \frac{Gb^{1/2} L_0^{1/4} \epsilon^{1/4}}{2\pi(2n)^{1/4}} \sqrt{\frac{\tau}{\theta_{0}^{1/2} b(2n)^{1/2} + \epsilon}} )</td>
<td>( \tau - \tau_0 = \left( \frac{9}{16} \left( \frac{gb^{1/2} L_0^{1/4} \epsilon^{1/4}}{2\pi(2n)^{1/4}} \right) \right) \sqrt{\frac{\tau}{\theta_{0}^{1/2} b(2n)^{1/2} + \epsilon}} )</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Definitions</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_e ) - distance between clusters and isolated edge dislocations</td>
<td>( R_0 = \sqrt{\frac{L_2}{\pi}} )</td>
<td>( D^* ) - the effective thickness of the material</td>
</tr>
<tr>
<td>( f ) - the excess number of dislocations of one sign, per cluster</td>
<td>( x ) - slip plane separation distance</td>
<td>( \mu ) - the proportionality between ( L_1 ) and ( L_2 )</td>
</tr>
<tr>
<td>( \eta ) - density of active sources</td>
<td>( \sigma ) - proportionality between</td>
<td></td>
</tr>
<tr>
<td>Seeger et al.</td>
<td>Hazzledine</td>
<td>Van Bueren</td>
</tr>
<tr>
<td>--------------</td>
<td>------------</td>
<td>-----------</td>
</tr>
<tr>
<td>Single dislocations interacting elastically with other blocked single dislocations</td>
<td>Edge dislocation multipoles interacting elastically across slip planes</td>
<td>Dislocation bundles interact elastically with other bundles on neighboring planes</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Constant</th>
<th>Variable</th>
<th>Constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>( (t-\tau_c) ) ( d\tau = \frac{GB^2 b}{2\pi R_0 L_s} ) ( dn )</td>
<td>( d\tau_a = \frac{GB}{8\pi(1-\nu)D^2} ) ( dD^* )</td>
<td>( d\tau = \sigma Gb (S \nu A)^{1/2} ) ( 1/2 ) ( dn )</td>
</tr>
<tr>
<td>( de = \frac{9}{16} b L_1 L_2 ) ( b ) ( dn )</td>
<td>( de = (n_1^2 L_2^0 - n_1 L_1 \nu) ) ( b ) ( dn )</td>
<td>( de = SbA ) ( dn )</td>
</tr>
</tbody>
</table>

\( 2^{1+\nu} \)

\( \tau - \tau_0 = \frac{G}{2\pi} \left( \frac{16}{9} \right)^{3/4} \) \( \epsilon \) \( \tau_a - \tau_f = \frac{GB}{8\pi(1-\nu)} \left( \frac{18\nu}{7bD^2} \right)^{1/3} \)

\( \epsilon = \frac{G(\nu A)^{3/2}}{1-\nu} \)

<table>
<thead>
<tr>
<th>Constant</th>
<th>Variable</th>
<th>Constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \nu L_1 ) ( 1/2 )</td>
<td>( \nu L_1 ) ( S ) ( A = \frac{9}{16} L_1 ) ( L_2 )</td>
<td>( \nu L_1 ) ( S ) ( A = 4 ) ( \nu L_1 ) ( S ) ( A = L_1 ) ( L_2 )</td>
</tr>
</tbody>
</table>

\( C \)

\( \tau = \left[ \frac{(nb)^9 A}{2\pi(1-\nu)S x^{1/3} b G^2} \right]^{1/8} \) \( \nu \) \( b \) \( + C \) \( \nu \) \( b \) \( + C \) \( \nu \) \( b \) \( + C \)

\( 2^{1/2} \)

\( \tau_a - \tau_0 = \left( \frac{1}{16} \right) \left( \frac{A x L_2^0}{2\pi} \right)^{1/3} \) \( \nu \) \( b \) \( + C \) \( \nu \) \( b \) \( + C \) \( \nu \) \( b \) \( + C \)

\( 2^{1/4} \)

\( \tau = \frac{GB}{8\pi(1-\nu)D^2} \) \( A_x \) \( \nu \) \( b \) \( + C \) \( \nu \) \( b \) \( + C \) \( \nu \) \( b \) \( + C \)

\( R_o = \sqrt{\nu L_2} \)

\( x = \) slip plane separation distance

\( \sigma = \) proportionality between \( L_1 \) and \( L_2 \)

\( D = \) the slip plane separation at which glide will just occur under the applied stress

\( \sigma = \) a constant of the system on the order of 0.1

\( D = \) vertical separation of sources

\( \nu \) = vertical separation of sources
3.4 MICROSTRAIN RESULTS

Extensive microstrain data was taken on the four magnesium samples listed in Table 3.1 in order to determine the behavior of the experimental variables of the Salama-Roberts relation as a function of total prestrain. The experimental variables of interest are namely: the flow stress, \( \tau_f \), the internal bias stress, \( \tau^* \), the slope of the \( \tau_f - \tau_a \) vs \( \dot{\gamma}^{1/4} \) plot, \( K \), and the total anelastic recovered microstrain, \( \Delta \gamma_{ro} \).

Figures 3.6 and 3.7 show the prestrain history of the two alloyed crystals M1A2A and M1A2B. In the case of crystal M1A2A all of the following presented data less than 5.15\% \( \gamma \) total prestrain was taken by Salama and Roberts and presented by permission. Figure 3.6 shows that for prestrain levels greater than 20\% \( \gamma \) the work hardening is practically constant at a value of \( \frac{G}{1 \times 10^5 \text{ dy cm}^{-2}} \). At prestrains less than 20\% \( \gamma \), the work hardening increases with decreasing strain to a value of \( \frac{G}{5.8 \times 10^3} \) at \( \gamma = 0.005 \). The time elapsed for room temperature recovery after a strain interval and unloading is shown on the figures. Recovery shows itself as a discontinuity in the flow stress of the crystal. It is clearly exemplified at .2\% in Fig. 3.6 where the crystal had remained 60 days at 300\^\circ K between strain intervals.
Fig. 3.6

MLA2A at 300°K

\( T_f \) vs \( Y_P \)

\( T_f \) vs (psi)

- 60 days
- 2 days
- 1 day
- 1 day
- 1 day
- 3 days @ 300 K
In comparison, the two relatively pure crystals M4A and M1B shown in Figs. 3.8 and 3.9 do not exhibit the above mentioned change in work hardening at low values of pre-strain. Crystal M4A, which will be discussed in detail in the following section, showed a consistently high work hardening coefficient of $\frac{G}{1 \times 10^3 \text{dy}(\text{cm})^{-2}}$ up to total shear strain of 0.32 $\gamma$.

Figures 3.10 through 3.13 are plots of the internal bias stress, $\tau^*$, as a function of prestrain. $\tau^*$, as deduced from the Salama-Roberts analysis, is the intercept on the stress axis of a plot of unloading stress, $\tau_f - \tau_a$, versus microstrain recovered to the one-quarter power. Its value is extremely sensitive to the slope of the above cited plot. $\tau^*$ was observed to exhibit a behavior similar to that described previously for $\tau_f$. This observation led this investigator to study in depth the experimental relation between $\tau^*$ and $\tau_f$. Fig. 3.14 is a plot of $\tau^*$ vs $\tau_f$ for representative data points obtained in the present study as well as those from the data of Salama and Roberts. Overlapping data points are eliminated. A least squares fit computer program has been applied to the data. The data points were found to fit a linear relation with slope of 0.548, intercept of -3.303, and an average deviation of 4.48, all of which are evident on the figure.
Fig. 3.9

$T_f$ vs $Y_p$

MIB

$T_f$ (psi)

0  150 days
5 days
14 days
300 K
77 K
300 K

0  150  200  250  300
Fig. 3.10

$\tau^* \text{ vs } \bar{Y}_p$

MLA2A at 300°F
Fig. 3.11

$\tau^* \text{ vs } \gamma_p$

MLA2B

at $300^\circ\text{K}$

$\tau^*(\text{psi})$

$\gamma_p$

$0 \quad 0.1 \quad 0.2 \quad 0.3 \quad 0.4 \quad 0.5 \quad 0.6 \quad 0.7 \quad 0.8$

$30 \quad 40 \quad 50 \quad 60 \quad 70$
Fig. 3.13

$\tau^* \text{ vs } \gamma_p$

M1B

$\tau^*(\text{psi})$

77$^\circ$K

300$^\circ$K

0

150

140

130

120

110

100

90

80

77$^\circ$K

300$^\circ$K

0

.1

.2

.3

.4

$\gamma_p$
Fig. 3.14

$\tau^*$ vs $\tau_f$

and least squares fit

$\tau^*$ (psi)

$\tau_f$ (psi)

M4A  M1A2A  M1B  M1A2B  M1B  M1B @ 77°K

Salama-Roberts
Figures 3.15 through 3.18 are plots of the slope, \( K \), of the \( \tau_f - \tau_a \) vs \( \gamma^{1/4} \) graph as it changes with percent prestrain. It was observed that the values of \( K \) for the alloyed crystals decreased sharply with prestrain for prestrains less than 5%. \( K \) then goes through a minimum around a prestrain of 15%. Lastly, \( K \) increases mildly with percent prestrain greater than 15% well into the stage I region. The effects of recovery are also observable in these curves. The pure crystals exhibit a markedly different behavior from the alloy crystal data, especially at low values of prestrain. Crystal M4A does not exhibit the drastic decrease of \( K \) with prestrain at low prestrains. This crystal exhibited \( K \) to consistently mildly linearly increase with prestrain. Crystal M1B shows a dramatic increase in the values of \( K \) at low percentage of prestrain.

In summary, then, no definite conclusions can be drawn regarding the behavior of \( K \) at values of total prestrain less than \( \approx 5\% \). This is probably due to the large scale rearrangement of the structural parameters operating at these low initial values of strain. For example, the dislocation blocking suggested by Seeger or the dislocation annihilation suggested by Hirsch and Lally may be settling down to a steady state in the early stages of prestrain.
Fig. 3.15

$K$ vs $\gamma_P$

M1A2A

at 300°K

$K(\text{psi})$

$\gamma_P$

1300
1200
1100
1000
900
800
700
600

0
0.1
0.2
0.3
0.4
0.5
0.6
Fig. 3.16

K vs Yp
MLA2B at 300°C
Fig. 3.17

$K$ vs $\gamma_p$

M4A

at $300^\circ$K

$K$ (psi)

$\gamma_p$

0 1 2 3
Figure 3.19a shows a plot of incremental recovered microstrain, $\Delta \gamma_{ro}$, vs total percent prestrain, $\gamma_p$. $\Delta \gamma_{ro}$ is the recovered microstrain observed after a prestrain increment $\Delta \gamma_p$. In Figures 3.19b and 3.19c are plotted respectively $\Delta \gamma_{ro}$ vs $\Delta \gamma_p$ and the total recovered microstrain, $\gamma_{ro}$, vs $\gamma_p$, the total amount of prestrain given each sample. $\Delta \gamma_{ro}$ was found to be one of the most accurately measured and well behaved experimental variables observed in this study. $\Delta \gamma_{ro}$ shows a linear increase with amount of prestrain for both pure and alloyed crystals at both 77°C and 300°C. It is interesting that the data from all crystals studied passes through the origin. Only the relative slopes change from crystal to crystal. The well behaved nature of $\Delta \gamma_{ro}$ with $\Delta \gamma_p$ suggests that we should utilize and emphasize this result in interpreting the microstrain models.

A study of the effect of temperature on the microstrain characteristics of these crystals was attempted. Macroscopically, the effects of temperature on the parameters of work hardening in hcp metals has been studied by Seeger [3.19]. He reports that the behavior of hcp metals is similar to the erratic behavior of fcc metals. For example, $\theta$ for Cu single crystals decreases by about a factor of two when going from 300°C to 77°C whereas Ni single crystals have relatively no temperature dependence over the same range. Seeger et al.'s stage I work hardening theory is an athermal theory and therefore should be
Fig. 3.19a

$\Delta \gamma_{f0} \text{ vs } \gamma_p$

- M1A2A
- M1A2B
- M4A
- M1B
- M1B 77°K
applicable to some specific temperature range where recovery effects are negligible. Because better agreement between experiment and theory than a factor of two was not hoped for, a temperature range was not clearly defined. Salama and Roberts have taken limited low temperature data on magnesium. Their results are reproduced in Fig. 3.1. Microstrain data at various macroscopic prestrain intervals were taken at 77°C on crystal MLB to further check out the athermal correctness of the various models discussed in this chapter.

The crystal exhibits a well behaved flow stress-macrostrain curve behavior, microscopic work hardening, $\Theta$, and incremental recovered microstrain, $\Delta \gamma_{ro}$, at this low temperature. The parameter $K$ changes from a 300°C value of 1400 psi to a 77°C value of 4200 psi over a 1.6% increment of prestrain. This more than two fold increase in the value of $K$ at 2% prestrain could be similar to the behavior of $K$ at small prestrains observed for this crystal at room temperature. Over this same strain interval, the flow stress increased from 150 psi at 300°C to 253 psi at 77°C which represents a 66% increase. It is possible the forest density of dislocations in the crystal is large with respect to the basal plane glide dislocation density. Consequently, the crystal may exhibit a larger ratio of thermal to athermal
component of flow stress generally observed in hcp metals. Also, smaller Frank-Read sources may be activated at low temperature causing an anomalous increase in the effective source density, $S$. The increase of the shear modulus, $G$, for the crystal between 298°C and 77°C should be 12.5%. These three effects might account for a two fold increase in $K$. It is difficult to evaluate if $n$ would increase or decrease with an increase in $S$. From Fig. 3.19 $\Delta \gamma_{r_0}$ appears not to change with temperature which may infer $A_{r_0}$ decreases with decreasing temperature. A two fold change in $n$ from 10-20 could account for the increase in $K$. It may be that at lower temperatures $S$ increases slightly but the higher absolute value of stress causes $n$ to be increased.

The change in the work hardening coefficient of Mg can be seen from the $\tau_f$ vs $\gamma_p$ graph. $\theta/G$ went from a value of $6.5 \times 10^{-5}$ at 300°C to a value of $45 \times 10^{-5}$ at 77°C at 2% $\gamma_p$ and from $8.1 \times 10^{-5}$ to $55 \times 10^{-5}$ at 27% $\gamma_p$. This six to seven fold increase is evidently one of the temperature effects which varies widely in hexagonal crystals and to which no general explanation appears available. Basinski [3.20] has observed a ten fold increase in the work hardening of magnesium at temperatures less than 200°C. His results are consistent with the present results.
In summary it seems that although the effects may vary among different metals or even different crystals, the above mentioned mechanism of decreased active Frank-Read source lengths and larger values of \( n \) seems to be a reasonable explanation of the macroscopically observed behavior and the observed microscopic parameter changes can be rationalized on this hypothesis.

3.5 MICROSCOPIC ANALYSIS

3.5.1 Introduction

The microscopic work hardening relation developed by Salama and Roberts contains three unknown dislocation structure arrangement parameters: \( S \), the density of dislocation sources; \( n \), the number of dislocations emitted per source during a strain increment; and \( A_{r_0} \), the total area swept out per dislocation bundle during strain recovery. There are, however, only two independent equations associated with the theory. It is therefore not possible to determine the arrangement parameters through microstrain behavior alone. Microstrain studies in conjunction with electron microscopy studies of surface slip line patterns after various
amounts of macroscopic prestrain can provide enough relations to determine and even check out the consistency of the unknown variables.

After a dislocation loop is created by one of the sources, it will move and expand under the externally applied stress during macroscopic deformation until it eventually, after numerous temporary blocks, pops out of the surface. In easy glide, the flux of dislocations emanating from the surface is just slightly less than the net flux released from sources. The Salama–Roberts relation assumes the sources are uniformly distributed throughout the sample and that the edge and screw components of the created rectangular dislocation loop are proportional in length. The measurement of both the slip line length and separation distance should yield a good estimate of the number of active dislocation sources per cubic centimeter, i.e., S. Knowledge of S by these means reduces our variables to two unknowns and two microstrain relations. This is assuming surface observations are compatible with microstrain dislocation activity.
3.5.2 Surface Replication

Prior to the application of the strain gauge, each sample was polished with a solution of HNO₃ and H₂O (3:1) to remove traces of previous slip lines and leave the surface polished. The samples were then given a macrostrain increment of approximately 10% γₚ. Microstrain data was subsequently taken during unloading and premacroyield stress loading. The strain gauge was then removed and the surface of the crystal was replicated using a two stage replication technique. The first stage of the replication process involves placing strips of 0.034 mm thick acetylcgellose film on the surface to be replicated after the film has been soaked in methyl acetate solvent for a moment. The film strips are cut slightly wider than an electron microscope grid and as long as the width of an optical microscope slide. After the acetylcgellose film has dried on the surface being replicated, it is removed and placed, replicated side up, in a vacuum evaporating system. The film is then shadowed at an angle and in a direction which is perpendicular to the slip lines. The shadowing was accomplished by the evaporation of a platinum-carbon alloy. A film of high purity carbon is subsequently evenly evaporated on the shadowed film to lend reinforcement. The films are
then taken from the vacuum evaporating system and cut into grid sizes with a razor blade. The acetylcellulose substrate is dissolved from the evaporated carbon film by soaking in methyl acetate solvent. The resolving power of this technique is about 100 Å which is satisfactory for slip line studies.

Figure 3.20 (E.M.L. #835-4)* is a micrograph of sample M1B taken at $1.1 \times 10^3$ magnification after a macroscopic prestrain of 10% $\gamma_p$ and is typical of those from which slip line data was obtained. Figure 3.21 (E.M.L. #828-8) is a replication of the surface of sample M4A taken at $2.1 \times 10^3$ magnification after a macroscopic shear strain increment of 10% $\gamma_p$, giving the sample a total amount of 20% macroscopic prestrain. The width and detail of these lines indicates clearly the resolution obtainable with the above described replication and shadowing technique. Figure 3.22 (E.M.L. #828-10) is a $75 \times 10^3$ magnification of one of the lines of Fig. 3.21. No fine structure within the slip band can be detected. Figure 3.23 (E.M.L. #5-3-72-23-8)** is a scanning electron

* E.M.L. - Electron Microscope Log for the electron microscope in the Materials Science Department of Rice University.

** Taken at the Metallurgy Section of the Manned Spacecraft Center, NASA, Houston, Texas.
micrograph taken at 760 magnification of a shadowed replica of sample M1A2B after a strain interval of 0.36 \( \gamma \) giving the sample a total prestrain of 81% \( \gamma_p \).

Figure 3.21 taken of sample M4A shows the traces of the climb behavior of the screw segments of the expanding dislocation loops. This phenomenon is unique to this crystal -- not being noticed in any of the other crystals even at much larger values of total prestrain. Screw dislocations do not have well defined slip planes and are therefore able to climb fairly easily between glide planes.

An estimate of the average slip line separation, \( \bar{d} \), was obtained by taking the arithmetic mean of a large number of measurements taken on all the micrographs obtained after a macroscopic strain interval. This observed separation, \( d_o \), was corrected for the orientation of the glide plane by the relation (3.13)

\[
\bar{d} = d_o \sin \theta
\]

where \( \theta \) is the angle between the face of observation and slip direction.

Table 3.3 shows the values obtained for all crystals studied.

An estimate of the value of the average slip line length, \( \bar{L} \), is more difficult to obtain because the
average length is generally larger than a single field of view at these magnifications. The slip line length was estimated from both optical and electron micrographs of moderate magnification. It can be reasoned that if \( n \) is the number of centimeters on the micrograph parallel to the slip lines, then there are \( 2n/L \) dislocation terminations in an area of \( L \) unit \( x n \). If \( m \) is the number of centimeters perpendicular to the slip lines, then there are \( m/d \) slip lines in \( m \) cm, and therefore \( m/2n \) \( \frac{m}{d} \) \( \frac{2n}{L} \) slip line terminations in area \( m \times n \). The average length of slip line can then be given by

\[
\bar{L} = \frac{2n}{M} \frac{d}{t} \tag{3.34}
\]

where \( M \) is the magnification of the micrograph, \( d \) is the number of dislocation lines in \( m \) centimeters, and \( t \) is the number of terminations in area \( n \times m \). This estimating technique applied to both optical and electron micrographs, including scanning electron micrographs of shadowed replicas, was compared to a more extensive method of making a series of electron micrographs while following a slip line bundle along the length (see Fig. 3.24). The order of magnitude agreement between the two techniques is considered to be within the range of scatter of the slip line lengths. Quantitative results are shown in Table 3.3 for all crystals.
In the light of the previous assumptions of uniformly dispersed sources and the existence of proportional lengths of screw and edge dislocation components, the number of active dislocation sources per unit volume is given by

$$ S = \left[ \frac{\bar{d}}{L_S} \frac{L_E}{L} \right]^{-1} $$

(3.35)

According to Van Bueren and Salama and Roberts, $L_S = L_E$; according to Seeger et al., $L_E = \alpha L_S$ where $\alpha > 1$; and according to Hirsch and Lally, $L_E = 3/2 L_S$. Calculated values of $\bar{S} = (\bar{L}^2 \bar{d})^{-1}$ are presented in Table 3.3 and will be discussed in the conclusion.

3.5.3 Transmission Electron Microscopy Studies

In order to get a better understanding of the dislocation density and arrangement in the strained magnesium samples, the investigation was extended by observing thinned sections of a strained sample by transmission electron microscopy techniques. The sample employed was M10B listed in Table 3.1. At the time of this investigation, the sample had a total of 20% shear strain. The sections were cut from the bulk sample parallel to the (0001) primary slip plane by employing a combined X-ray


| Table 3.3 |
| Experimentally Determined Values of Slip Line Separation Distance and Length with Dislocation Source Density |

<table>
<thead>
<tr>
<th></th>
<th>M1B</th>
<th>M1B</th>
<th>M1B</th>
<th>M4A</th>
<th>M4A</th>
<th>M4A</th>
<th>M1A2B</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2% $\gamma_P$</td>
<td>10% $\gamma_P$</td>
<td>27% $\gamma_P$</td>
<td>10% $\gamma_P$</td>
<td>20% $\gamma_P$</td>
<td>32% $\gamma_P$</td>
<td>81% $\gamma_P$</td>
</tr>
<tr>
<td>$d_0 \sin \theta \times 10^4 \text{cm}$</td>
<td>5.8</td>
<td>5.3</td>
<td>1.44</td>
<td>1.64</td>
<td>0.64</td>
<td>1.59</td>
<td>1.37</td>
</tr>
<tr>
<td>$\bar{L}^2 \times 10^4 \text{cm}$</td>
<td>24.0</td>
<td>9.0</td>
<td>10.3</td>
<td>41.0</td>
<td>36.0</td>
<td>55</td>
<td>250</td>
</tr>
<tr>
<td>$\bar{s} \times 10^{-6} (\text{cm})^{-3}$</td>
<td>0.68</td>
<td>2.1</td>
<td>6.6</td>
<td>1.5</td>
<td>4.3</td>
<td>1.15</td>
<td>0.27</td>
</tr>
<tr>
<td>$</td>
<td>\theta</td>
<td>/G$</td>
<td>$6.5 \times 10^{-5}$</td>
<td>$45 \times 10^{-5}$</td>
<td>$8.1 \times 10^{-5}$</td>
<td>$33 \times 10^{-5}$</td>
<td>$40 \times 10^{-5}$</td>
</tr>
<tr>
<td></td>
<td>300°K</td>
<td>77°K</td>
<td>55 $\times 10^{-5}$</td>
<td>77°K</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

171
and spark cutting technique.* The sections were then further chemically thinned by scanning the surface of the sections with a strong stream of diluted HNO₃ (10:1) while the sections were submerged in the etchant. Submersion prevents film from forming on the surface and retarding uniform dissolution.

Figures 3.25 through 3.27 show bright field micrographs of three different regions of a basal plane section. In general, the dislocations are relatively long indicating that the majority lie in the basal plane and the density of sources is relatively small. It appears from this transmission micrograph that the dislocation density is from 2-5 x 10⁶ per cm². The latter value is probably not sufficient to produce an appreciable extent of dislocation tangles. The regions are characterized by observable dislocation dipoles and some dislocation loops (see regions A and B, Fig. 3.25). We note at C (Fig. 3.26) the dislocations bowing out from a hole in the sample which is apparently acting as an operating dislocation source. Figure 3.26 partially supports the mechanism of the present theory whereby edge and screw dislocations emitted from neighboring sources impinge upon one another

* Spark cutter is a SERVOMET 197/430 made by Materials Research Ltd. of Cambridge, England.
and are uniformly blocked producing bundles which then mutually interact elastically. Figure 3.30 is a magnified picture of dislocations emanating from the hole in the film shown in Fig. 3.26. At B in Fig. 3.26 the bowing out of a dislocation from three dark points is noted. These points could be forest dislocations or impurity particles. A similar point is noticed at D (Fig. 3.26) overlapping the contrast of a dislocation slightly inclined to the basal plane. Figure 3.27 shows a region of dislocation tangles which might also be termed dislocation bundles. In the top half of the picture are observed what appear to be long vertical primary basal dislocations and dipoles. At A there appears to be a small dislocation pile-up of about five dislocations. This could indicate either a local source or a local barrier to their motion. At B is noticed what appears to be the initial formation of a dislocation helix. Figure 3.28 shows a more magnified section of Fig. 3.26. Here the details of a dislocation dipole is most evident. The pinched off effect at the tip of the dipole at point A is clearly seen. In the background are small protrusions from the surface which are evidently remnants of the spark cutting process. At points C and D three dislocations on overlapping glide planes are seen. The two nearly parallel dislocations are
seen to be of opposite sign by the way the contrast changes as they intersect the surface. The curves along the length of the dislocations seem to be a good example of how a screw and edge dislocation exert mutual torques on one another which tend to align them parallel to one another. The mechanism is shown schematically by the accompanying illustration which is consistent with the observed sign of the dislocations. Figure 3.29 is a 10\overline{1}0 dark field picture of a section of Fig. 3.27. Note the prismatic loops which are in contrast at A. Because they vanish in Fig. 3.27 they are perpendicular to the (0001) plane and have a \langle1\overline{1}20\rangle type burgers vector.
Figure 3.31 is a dark field 1120 reflection of Fig. 3.27. The primary basal dislocations at A, B, C, D and E vanish in this reflection indicating a burgers vector of a/3 (11\overline{2}0). From the orientation of the dislocations in Fig. 3.27 it can be seen that they have mainly edge components. There is a residual contrast in the dark field picture due to the \( \mathbf{b} \times \mathbf{\bar{e}} \) component of displacement around edge dislocations. The long dislocation at F is in contrast in this reflection but practically extinct in Fig. 3.29. This indicates its screw character with a burgers vector of a/3 (1\overline{2}10).

Figure 3.32 shows a section of Fig. 3.27 in three different 11\overline{2}0 type reflections taken to possibly detect the presence of partial dislocations. No appreciable extinction of dislocations is noticed indicating a very low occurrence of partial dislocations. This result was to be expected since partials are usually associated with various types of stacking faults and no such defects were found. In this series of 11\overline{2}0 type reflections the primary dislocations should be in contrast. Each picture is of a slightly different field of view of Fig. 3.27.

From these type observations no conclusive statement can be made in support of any one particular structural dislocation model over the others. Different degrees
of deformation and temperature have not been looked at. A few general conclusions can at least be cited. Quite a few dislocation bundles were observed in accord with the assumptions of the Salama-Roberts theory as well as the Hirsch and Lally and Hazzledine relations. Quite a few dislocation dipoles and loops were observed. These defects can be formed when moving dislocation loops elastically interact and the screw segments cross glide to annihilate [3.21]. This mechanism is in accord with the evidence of screw dislocation cross slip traces observed on sample M4A in the preceding section.
Fig. 3.27
Bright Field with diffraction pattern.
7,900 X
Fig. 3.29
Fig. 3.30 Magnified section of Fig. 3.26
Fig. 3.31
Dark Field of Fig. 3.27
7,900 X
Fig. 3.32 Dark Field. 1120 type reflection. 7,900 X.
3.6 CONCLUSION

It has now been demonstrated that the Van Bueren, Hirsch and Lally, Seeger et al., and Hazzledine macroscopic stage I work hardening theories adequately describe the macroscopic effects, but only the Salama-Roberts modification of the Van Bueren theory adequately and consistently predicts the microscopic work hardening in single crystal magnesium within the sensitivity of the $1/4$ power relation. The static and dynamic aspects of the microscopic and macroscopic parameters must now be investigated in the light of the results of the preceding microstrain and microscopic analysis.

There are a total of six parameters to be considered -- the three previously defined microscopic parameters which will be denoted by the tilde, $\tilde{S}$, $\tilde{n}$ and $\tilde{A}$, and the corresponding macroscopic parameters. From the anelastic region assumptions of Salama and Roberts, the incremental recovered microstrain, $\Delta \gamma_{r_0}$, and the slope of the $\tau_f - \tau_a$ vs $\gamma_r^{1/4}$ plot are both specified in terms of the microscopic parameters. The individual macroscopic theories give the macroscopic work hardening in terms of the macroscopic parameters. The microstrain analysis shows that $\Delta \gamma_{r_0}$ increases linearly with $\gamma_p$ and from the microscopic analysis an idea of $\overline{L}$, $\overline{d}$ and therefore $\overline{S}$ and $\overline{A}$ is obtained.
The set of equations relating the microscopic parameters under the Salama-Roberts microstrain relation, plus the additional relations of this analysis, are:

\[
K = \alpha G S^{1/4} (\tilde{n} b)^{3/4} \tag{3.36.1}
\]

\[
\gamma_{r_0} = \tilde{n} b \tilde{S} \tilde{A}_{r_0} \tag{3.36.2}
\]

\[
\frac{a}{G} = \frac{\alpha}{S^{1/2} A^{3/4}} = \alpha \left( \frac{d}{L_2} \right)^{1/2} \tag{3.36.3}
\]

\[
\frac{d \Delta \gamma_{r_0}}{d \gamma_p} = \text{constant} = \frac{\Delta \gamma_{r_0}}{\gamma_p} = \frac{\Delta (\tilde{n} \tilde{S} \tilde{A}_{r_0})}{n S A} \tag{3.36.4}
\]

\[
S = \frac{1}{d L_2^2} \tag{3.36.5}
\]

\[
A = L_1 L_2 \tag{3.36.6}
\]
Using the electron microscope technique the values of $\bar{d}$ as listed in Table 3.3 were found by an averaging technique and have an associated deviation of as much as two orders of magnitude (Fig. 3.20). The deviation in $\bar{d}$ was found to be at least one order of magnitude (Fig. 3.24). Taking an average value of $\theta/G$ to be $3 \times 10^{-4}$ and average values of $5 \times 10^{-2} \text{cm}$ and $1 \times 10^{-4} \text{cm}$ for $L$ and $d$ respectively, $(\frac{d}{L})^{1/2}$ has a value of $4 \times 10^{-2}$. In Eq. (3.36.3) the expression for $\alpha$ is

$$
\alpha = \frac{1}{8\pi(1-\nu)\alpha_L} \tag{3.37}
$$

where $\nu$ is Poisson's ratio and $\alpha_L$ is defined by $L_1 = \alpha_L L_2$. The Salama–Roberts relation assumes equal edge and screw slip trace lengths and therefore $\alpha_L$ is equal to unity. Assuming a value for $\alpha$ of 0.06, an average value of $\alpha(d/L)^{1/2}$ from the microscopically observed surface structure is found to be $30 \times 10^{-4}$. Compared to the above average value for the experimentally observed $\theta/G$ an order of magnitude agreement is obtained. From the scatter in this type of mechanical property data both in this analysis and that reported by Seeger (Fig. 3.2), agreement of this type is considered good. A slight correction could be injected by assigning a value to $\alpha_L$ which would correct for the edge dislocation slip trace and therefore the area swept
out. Hirsch and Lally assume a value of 3/2. This would enter into Eq. (3.36.3) only to the 1/4 power and is therefore negligible.

Macroscopically, therefore, the Salama-Roberts relation and the data of this investigation can be considered consistent. This result is also borne out by the agreement found by Salama and Roberts in their analysis of data reported by Seeger and mentioned at the beginning of this chapter.

Consistency in the microscopic region will be checked out by first making the assumption of equivalence of sources, i.e., \( S = \tilde{S} \), then by assuming equivalence of dislocations, i.e., \( nS = \tilde{n} \tilde{S} \). The first assumption simply states that whatever percentage of sources operate during macrostrain, the same percentage operate during unloading and microscopic strain recovery due to a flux of the newly created dislocation relaxing back to these sources.

From the results of the microstrain data, values of \( K, S, \frac{d\Delta \gamma_r}{d\gamma_p} \), and \( \gamma_r \) are taken at an appropriate prestrain, \( \gamma_p \), for each crystal. Equation 3.36.1 can then be solved to yield a value for \( \tilde{n} \). This value can then be put into Eq. (3.36.2) to yield a value for \( \tilde{\gamma}_{r_o} \).
the average microscopic area swept back during unloading. These two determined values can then be put into Eq. (3.36.4) to yield an estimate of $n$.

Under the second assumption, $nS = \tilde{n} \tilde{S}$, the total number of dislocations in each dislocation bundle is thought to participate in the microstrain recovery during unloading. Eq. (3.36.4) can be solved to give a value for $\tilde{\kappa}_{Ro}$ which can then be put into the simultaneous solution of 3.36.2 and 3.36.1 to give values for $\tilde{S}$ and $\tilde{n}$. Eq. (3.36.4) can then be used to give a value for $n$.

Table 3.4 summarizes the results of this procedure on the three crystals for which microscopic data was taken. The values used for each crystal are taken at one particular value of $\gamma_p$ from the microstrain section and from the microscopic data as shown in Table 3.3. Because absolute values of $\tilde{n}$, $\tilde{\kappa}_{Ro}$, $n$, and $\tilde{S}$ depend strongly on the microscopic data, which is accurate only to within orders of magnitude, the results of each assumption are given in terms of percentage. Ratios essentially null-out the dependence of the microstrain data on the amount of prestrain, $\gamma_p$, and will show more clearly the reasonableness of the equations themselves under each of the above assumptions. It is seen that very reasonable and consistent results are predicted by the above series of equations under both of the above assumptions, even over large variances of $\gamma_p$ and $d\Delta\gamma_{Ro}/d\gamma_p$. 
\[ d_0 \sin \theta = 1.37 \times 10^{-4} \text{cm} \]
\[ \frac{d}{L^2} = 250 \times 10^{-4} \text{cm}^2 \]
\[ \frac{d\Delta \gamma_r}{d\gamma_p} = 3.7 \times 10^{-3} \]
\[ K(0.8\gamma_p) = 6.9 \times 10^7 \text{ dy/cm}^2 \]
\[ S = 27 \times 10^8 \text{ cm}^{-3} \]
\[ \Delta \gamma_r (0.8\gamma_p) = 315 \times 10^{-5} \]

Assuming: \( S = S' \)
\[ \tilde{n} = 157 \]
\[ \tilde{\kappa}_r = 25 \times 10^{-4} \text{cm}^2 \]
\[ n = 4200 \]
\[ \frac{\tilde{n}}{n} = 3.7\% \]
\[ \frac{\tilde{\kappa}_r}{\kappa} = 10\% \]

Assuming: \( nS = \tilde{n} S' \)
\[ \tilde{n} = 30 \]
\[ \tilde{\kappa}_r = 0.9 \times 10^{-4} \text{cm}^2 \]
\[ \tilde{S} = 0.38 \times 10^8 \text{ cm}^{-3} \]
\[ n = 3800 \]
\[ \frac{\tilde{n}}{n} = 0.79\% \]
\[ \frac{\tilde{\kappa}_r}{\kappa} = 0.4\% \]
### TABLE 3.4

<table>
<thead>
<tr>
<th>M4A</th>
<th>M1B</th>
</tr>
</thead>
<tbody>
<tr>
<td>(d_o \sin \theta = 1.59 \times 10^{-4} \text{cm} )</td>
<td>(d_o \sin \theta = 1.44 \times 10^{-4} \text{cm} )</td>
</tr>
<tr>
<td>(\frac{L^2}{L^2} = 55 \times 10^{-4} \text{cm}^2 )</td>
<td>(\frac{L^2}{L^2} = 10.3 \times 10^{-4} \text{cm}^2 )</td>
</tr>
<tr>
<td>(\frac{d \Delta \gamma_r}{d \gamma_p} = 2.66 \times 10^{-3} )</td>
<td>(\frac{d \Delta \gamma_r}{d \gamma_p} = 0.5 \times 10^{-3} )</td>
</tr>
<tr>
<td>(K(3 \gamma_p) = 5.86 \times 10^7 \text{dy/cm}^2 )</td>
<td>(K(3 \gamma_p) = 17.2 \times 10^7 \text{dy/cm}^2 )</td>
</tr>
<tr>
<td>(S = 1.15 \times 10^6 \text{cm}^{-3} )</td>
<td>(S = 6.6 \times 10^6 \text{cm}^{-3} )</td>
</tr>
<tr>
<td>(\Delta \gamma_r (0.3 \gamma_p) = 80 \times 10^{-5} )</td>
<td>(\Delta \gamma_r (0.3 \gamma_p) = 15 \times 10^{-5} )</td>
</tr>
</tbody>
</table>

**Assuming:** \(S = \bar{S} \)

<table>
<thead>
<tr>
<th>M4A</th>
<th>M1B</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\tilde{n} = 77.8 )</td>
<td>(\tilde{n} = 179 )</td>
</tr>
<tr>
<td>(\tilde{A}_r = 3 \times 10^{-4} \text{cm}^2 )</td>
<td>(\tilde{A}_r = 0.04 \times 10^{-4} \text{cm}^2 )</td>
</tr>
<tr>
<td>(n = 1600 )</td>
<td>(n = 1471 )</td>
</tr>
<tr>
<td>(\tilde{n} )</td>
<td>(\tilde{n} )</td>
</tr>
<tr>
<td>(\tilde{n} = 4.8% )</td>
<td>(\tilde{n} = 12% )</td>
</tr>
<tr>
<td>(\tilde{A}_r / A = 5.5% )</td>
<td>(\tilde{A}_r / A = 0.39% )</td>
</tr>
</tbody>
</table>

**Assuming:** \(nS = \tilde{n} \bar{S} \)

<table>
<thead>
<tr>
<th>M4A</th>
<th>M1B</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\tilde{n} = 17.3 )</td>
<td>(\tilde{n} = 62 )</td>
</tr>
<tr>
<td>(\tilde{A}_r = 0.15 \times 10^{-4} \text{cm}^2 )</td>
<td>(\tilde{A}_r = 0.005 \times 10^{-4} \text{cm}^2 )</td>
</tr>
<tr>
<td>(\bar{S} = 1.03 \times 10^8 \text{cm}^{-3} )</td>
<td>(\bar{S} = 1.6 \times 10^8 \text{cm}^{-3} )</td>
</tr>
<tr>
<td>(n = 1549 )</td>
<td>(n = 1503 )</td>
</tr>
<tr>
<td>(\tilde{n} )</td>
<td>(\tilde{n} )</td>
</tr>
<tr>
<td>(\tilde{n} / n = 1.1% )</td>
<td>(\tilde{n} / n = 4.1% )</td>
</tr>
<tr>
<td>(\tilde{A}_r / A = 0.27% )</td>
<td>(\tilde{A}_r / A = 0.05% )</td>
</tr>
</tbody>
</table>
From the experimental observation that \( \frac{d\Delta \gamma_r}{d\gamma_p} \) is a constant for each crystal, in fact, \( \Delta \gamma_r \) is proportional to \( \gamma_p \) since the data goes through the origin, an experimentally determined value of the slope \( \frac{d\Delta \gamma_r}{d\gamma_p} \) should equal \( \frac{\gamma}{\tilde{\gamma} \tilde{r}_O} / \gamma \). The above relation can give the dynamic relation between the variables

\[
\frac{d \ln \tilde{r}_O}{d \ln \gamma} = \frac{d \ln \gamma}{d \ln \gamma_p} \tag{3.38}
\]

by employing the definitions of the individual terms.

Also, by differentiating \( K \) with respect to \( \gamma_p \) and looking at the limit of small prestrain there results the relation

\[
\lim_{\gamma_p \to 0} \frac{dK}{d\gamma_p} = \lim_{\gamma_p \to 0} \frac{\alpha}{4} b^{3/4} G \left[ \left( \frac{\tilde{\gamma}}{\tilde{\gamma}_0} \right)^{1/4} + \left( \frac{\tilde{\gamma}_0}{\tilde{\gamma}} \right)^{3/4} \right]
\]

\[
\tag{3.39}
\]
This shows that at low values of prestrain where either \( \tilde{S} \) or \( \tilde{n} \) is small, the slope of the \( K \) vs \( \gamma_p \) curve should go to infinity, which was confirmed experimentally on all crystals but the anomalous results found with crystal M1B.

From the slope of the \( K \) vs \( \gamma_p \) curves it is seen that \( K \) varies by about 15\% per strain interval for all the crystals. This effectively says that \( \tilde{S}^{1/4} \tilde{n}^{3/4} \) varies at this rate since \( \alpha, \gamma \) and \( b \) are constants. If \( \tilde{S} \) is assumed to vary by .23 as seen from the results of crystal M1B (see Table 3.3) then \( \tilde{n} \) would have to vary by .12 per strain interval which is not unreasonable. In a similar manner, \( \gamma_{r_o} \) was found to increase negligibly by 0.35\% per strain interval. By Eq. (3.36.2), \( \tilde{K}_{r_o} \) should then decrease at a rate approximately equal to that at which \( \tilde{S} \) plus \( \tilde{n} \) increases, approximately 0.35.

The integration constant, \( \tau^* \), of the Salama-Roberts relation is an average internal stress caused by surrounding dislocations acting on the mobile dislocations during microstrain loading and unloading. One of the important results of the present work is that the bias stress, \( \tau^* \), was found to obey the relation

\[
\tau^* = \frac{1}{2} \tau_f \quad (3.40)
\]
This implies that the mechanism operating to cause $\tau_F$ to vary during prestrain is the same mechanism controlling the internal bias stress. An interesting comparison can be made between the results just mentioned and results of Roberts and Brown [3.12]. They have shown that in unidirectional stress cycle damping loops, the frictional stress, $\tau_F$, acting on the mobile dislocations is related to the energy loss, $W_{\text{irr}}$, and the maximum anelastic strain of the loop, $\Delta \gamma$, as

$$\frac{dW_{\text{irr}}}{d(\Delta \gamma)} = 2 \tau_F$$

(3.41)

Employing this relation Salama and Roberts have shown that the frictional stress, $\tau_F$, was consistently one-half the value of the flow stress, $\tau_f$, again indicating similar operative mechanisms. They have given a relation between the frictional stress, $\tau_F$, flow stress, $\tau_f$, and bias stress, $\tau^*$, as

$$\tau_F = \frac{\tau_f(3\tau_f^2 + 8\tau^* \tau_f + 6\tau^{*2})}{7\tau_f^2 + 18\tau^* \tau_f + 12 \tau^{*2}}$$

(3.42)

If in Eq. (3.42) $\tau^*$ is assigned the value of 0.5 $\tau_f$ there results the relative identity that $\tau_F = (0.45)\tau_f$ in agreement with Salama and Roberts. There seems, then, to be a
correlation between the frictional stress and the bias stress. The model developed by Kressel and Brown [3.22] seems to be the only known theoretical analysis for energy dissipation and frictional stress analysis which can adequately and satisfactorily describe the $\tau_f'\tau_F$ relationship we find in this study.

In summary, it has been demonstrated experimentally that in the microstrain region the stress is proportional to $\gamma^{1/4}$. It was pointed out that only the Van Bueren macroscopic work hardening relation could predict the $1/4$ power dependence in the microscopic region under the Salama-Roberts assumptions of this region. This analysis has therefore contributed to the understanding of the macroscopic and microscopic parameters operating during stage I deformation by pointing out that the assumptions of Salama and Roberts in the microscopic region and the Van Bueren relation in the macroscopic region are intrinsically and extrinsically consistent, experimentally verifiable, and mutually complementary.
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ACKNOWLEDGEMENTS

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APPENDIX

Stress vs $\gamma_r^{1/4}$ for various crystals at various amounts of prestrain. Temperature is as noted in the individual figures.
Crystal M1A2A

Partial tensile strain of 
$0.2 \times 10^{-4}$

Total tensile strain of 
$0.568 \times 10^{-4}$

$T = 300^\circ K$

Slope = 1400 psi

$\tau^* = -34$ psi

Fig. A-1
\[ \tau_m - \tau_a \text{ psi} \]

\[ \gamma^{1/4} \]

Crystal MLA2A

Partial tensile strain of 0.0026

Total shear strain of 0.036

\[ T = 300^\circ K \]

Slope = 892 psi

\[ \tau^* = -38 \text{ psi} \]

Fig. A-2
\[ \tau_m - \tau_a \quad \text{psi} \]

Crystal M1A2A

Partial tensile strain of 0.0113

Total shear strain of 0.203

Slope = 830 psi

\[ T = 300^\circ \text{K} \]

\[ \tau^* = -49 \quad \text{psi} \]

\[ \gamma^{1/4} \]

Fig. A-3
Crystal MLA2B
Partial Shear Strain of
Slope = \( K = 1003 \text{ psi} \)
\( \gamma_p = 0.00034 \)
\( T = 300^\circ \text{K} \)
\( \tau^* = -24 \text{ psi} \)

\[ \tau_m - \tau_a \text{ psi} \]

Fig. A-4
$\tau_m - \tau_a$

psi

Crystal M1A2B

Partial shear strain of 0.01

Total shear strain of 0.09

Slope = 850 psi

$T = 300^\circ K$

$\tau^* = -37.5$ psi

Fig. A-5
Crystal M1A2B

Partial shear strain of 0.05
Total shear strain of 0.64
Slope = 1060 psi
$T = 300^\circ K$
$\tau^* = -69$ psi

Fig. A-6
$\tau_m - \tau_a$

psi

Crystal M4A

Partial tensile strain of 0.0036

Total shear strain of 0.089

Slope = 840 psi

$T = 300^\circ K$

$\tau^* = -20$ psi

Fig. A-7
Crystal M4A

Partial tensile strain of 0.0067
Total shear strain of 0.20
Slope = 760 psi
$T = 300^\circ$K
$\tau^* = -30$ psi

Fig. A-8
\( \tau_m - \tau_a \) psi

Crystal M4A

Partial tensile strain of 0.0064

Total shear strain of 0.33

Slope = 950 psi

\( T = 300^\circ K \)

\( \tau^* = -42 \text{ psi} \)

Fig. A-9
Crystal MLB

Partial tensile strain of 0.0025

Total shear strain of 0.016

Slope = 1400 psi

\( T = 300^\circ \text{K} \)

\( \tau^* = -75 \text{ psi} \)

Fig. A-10
Crystal M1B.

Partial tensile strain of 0.0025

Total shear strain of 0.11

Slope = 6400 psi

$T = 77{}^\circ K$

$\tau^* = -160$ psi

Fig. A-11
Crystal M1B

Partial tensile strain of 0.013
Total shear strain of 0.37
Slope = 3590 psi
T = 77°C
\( \tau^* = -158 \text{ psi} \)

Fig. A-12