Title
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Publication Date
1966-08-01

UCRL-17066

University of California

Ernest O. Lawrence Radiation Laboratory

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Berkeley, California

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AEC Contract No. W-7405-eng-48

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Arthur Caetano Nunes, Jr.

(Ph.D. Thesis)

August, 1966

CONTENTS

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September, 1966

ABSTRACT

The energy to constrict a dissociated dislocation is calculated using linear isotropic elasticity theory coupled with a core energy model containing parameters based on the Morse potential calculation of Doyama and Cotterill for copper. No assumption is made restricting the curvature of the partial dislocations to small values, but the shape of the partials are assumed to be exponential curves specified by a single parameter with respect to which the energy is minimized.

The results are very sensitive to the core model. A least squares fit of a linear log-log relation to the calculated points gives for the edge constriction

$$\frac{\Delta E}{Gb^3} = 0.0124 \left(\frac{d_\tau}{b}\right)^{1.36}$$

and for the screw constriction

$$\frac{\Delta E}{Gb^3} = 0.0077 \left(\frac{d_\tau}{b}\right)^{1.45}$$

where ΔE is the constriction energy; G, the elastic shear modulus; b, the Burgers vector; and d_τ, the separation distance between partials. These results are more accurate than those previously obtained using the line energy model of a dislocation.

INTRODUCTION

Before cross-slip or intersection can take place a dissociated dislocation must constrict.* A constricted dislocation has a higher energy than an unconstricted dislocation, thus an energy barrier exists between the states prior to and after the above processes.

The determination of the energy of a simple constriction at a point of a dissociated dislocation has been undertaken by a number of investigators. Stroh,[3] Seeger,[4] and Dorn and Mitchell[5] have made calculations based on the line tension model of a dislocation. Schöck and Seeger[6] have made a similar calculation based on an extension of Peierls' calculation[7] of the width of a dislocation. Kröner, Seeger, and Wolf[8] have made use of a technique similar to the one used in this paper for calculating the energy of a constriction where one partial dislocation remains straight.

In this paper the energy of a symmetrical constriction of assumed exponential shape in an isotropic linear elastic medium is calculated for both edge and screw extended dislocations. In addition to the purely elastic terms the effects of the core and stacking fault are included. It is believed that this calculation is the most accurate one that has been made to date. Better models involving anisotropy or departure from a continuum approach must be pair for in limited applicability or greatly increased complication.

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*There is also the possibility of cross-slip by formation of a stair-rod dislocation[1] with no constriction but the strong attraction between the strair-rod and cross-slipped dislocation segments make such a process unlikely.[2] A pure edge dislocation jog formed during constriction may split with a slight lowering of energy, but for dislocations not purely edge the required length of step makes for splitting makes the phenomenon energetically unfavorable.[2] Only the constriction model will be considered in the following investigation.

THE ELASTIC ENERGY

When the significance of the dislocation for the plastic deformation process in crystalline material was realized[9,10,11] in 1934, the dislocation of the elasticians had been on the scene for roughly thirty years; the classic treatise was that of V. Volterra,[12] "Sur l'équilibre des corps élastiques multiplement connexes"; the English name of "dislocation" had been given by A. E. H. Love.[13]

While the energy of a dislocation loop of arbitrary shape may be calculated on an entirely classical basis,[14] this calculation will be described here in terms of Kröner's "Kontinuumstheorie der Versetzungen und Eigenspannungen"[15] as expounded in English by R. deWit.[16]

The method involves the evaluation of a double line integral, the origination of which is as follows:

The energy, E, of an elastically strained body of volume V may be written as the volume integral

$$E = \frac{1}{2} \int_V \sum_i \sum_j \sigma_{ij} \, \varepsilon_{ij} \, dV \qquad (1')$$

where σ_{ij} and ε_{ij} are the stress and strain respectively acting upon volume element dV. The convention of summing on repeated indices will be followed in all subsequent equations, hence equation (1') will be written

$$E = \frac{1}{2} \int_V \sigma_{ij} \, \varepsilon_{ij} \, dV \qquad (1)$$

which means exactly the same thing as equation (1').

The volume integral (1) can be converted into a surface integral through the relations

$$\varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{2}$$

where u_i is a displacement of a point in the elastic body away from the initial unstrained position,

$$\sigma_{ij} = \sigma_{ji} \tag{3}$$

and the divergence theorem

$$\int_V \frac{\partial T}{\partial x_i} \, dV = \int_A T \, dA_i \tag{4}$$

where T is a tensor of any rank and dA_i is a vector normal to and equal in magnitude to an element of surface area of A enclosing volume V. The sign of dA_i is positive when directed away from volume V.

The result is

$$E = \frac{1}{2} \int_A \sigma_{ij} \, u_j \, dA_i \tag{5}$$

When a dislocation loop is created in an initially unstressed elastic body, all surfaces but the loop surface being held rigid, the process may be visualized as follows.

First a "wormhole" must be cut out along the boundary of the loop to allow slipping of loop surfaces over one another without generating infinite stresses. This "wormhole" region is referred to as the "core" region of the dislocation.

Secondly a cut is made over the surface of the loop, the surfaces are slipped relative to one another by vector b_j, the Burgers vector of the dislocation, and the surfaces are rewelded.

Thirdly the core material is reinserted in place.

Assuming that the cutting and welding processes require no net expenditure of energy the energy of the dislocation loop may be decomposed into three terms:

(i) The energy required to slip one surface with respect to the other for the loop

$$E_1 = \frac{b_j}{2} \int \sigma_{ij} \, dA_i \quad (6)$$

(ii) The disturbance in the elastic energy of the elastic continuum outside the dislocation core upon reinsertion of the core material referred to as the "core traction energy" and labeled E_2.

(iii) The energy of the core material itself, labeled E_3.

Only E_1 will be considered for the moment. For convenience a stress function χ_{ln} may be defined such that

$$\sigma_{ij} = -2G \, \varepsilon_{ikl} \, \varepsilon_{jmn} \frac{\partial^2}{\partial x_k \partial x_m} \left(\chi_{ln} + \frac{\nu}{1-\nu} \chi_{pp} \, \delta_{ln}\right) \quad (7)$$

while ε_{ikl} and ε_{jmn} are permutation symbols defined so that they are zero unless all the indices are different and if they are different

$$\varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1$$

$$\varepsilon_{132} = \varepsilon_{321} = \varepsilon_{213} = -1$$

δ_{ln} is a Kronecker delta defined such that it is unity when $l = n$ and zero when $l \neq n$, and G and ν are the shear modulus and Poisson's ratio respectively for the material. The stress function χ_{ln} may be thought of as a generalization of a scalar potential.

Kröner expresses the stress function in terms of a dislocation density:

$$\chi_{ln} = \frac{1}{8\pi} \left[\int_{V'} \varepsilon_{nrs} \, \alpha_{ls} \, (r') \frac{\partial R}{\partial x_r} \, dV' \right]^S \qquad (8)$$

where R is the distance $\sqrt{x'^2 + y'^2 + z'^2}$ from the coordinate origin at which χ_{ln} is being evaluated, and $\alpha_{ls}(r')$ is the dislocation density defined so that upon completing a Burger's circuit about a local area element dA_l the closure failure is $db_s = \alpha_{ls} dA_l$. The $[\quad]^S$ means that only the symmetrical part of the tensor is to be taken. To calculate the energy of a dislocation loop one writes

$$\alpha_{ls}(r') \, dV' = [\alpha_{ls}(r') \, dA_l'] \, dl_l' \qquad (9)$$

$$= b_s' \, dl_l'$$

that is, one expresses the core volume, which is assumed to contain the entire dislocation, as the product of an area times a length, combines the area with the dislocation density tensor and obtains the Burgers' vector of the dislocation line b_s'. dl_l' represents a differential line element along the dislocation line.

Combining equations (6), (7), (8) and (9) and making use of the relations:

$$\varepsilon_{jmn}\,\varepsilon_{nrs} = \delta_{jt}\,\delta_{ms} - \delta_{mr}\,\delta_{js} \tag{10}$$

and Stokes' theorem

$$\int_{A_i} \varepsilon_{ikl} \frac{\partial T}{\partial x_k}\, dA_i = \oint_l T dl_l \tag{11}$$

and

$$\int_l \frac{\partial R}{\partial x_k}\, dl_k = \int_A \varepsilon_{ijk} \frac{\partial}{\partial x_j} \frac{\partial R}{\partial x_k}\, dA_i = 0 \tag{12}$$

the expression for E_1 is obtained

$$E_1 = -\frac{Gb_i b_j'}{16\pi} \oint \oint \frac{\partial^2 R}{\partial x_k \partial x_k} \left(dl_j' dl_i + \frac{2\nu}{1-\nu}\, dl_i'\, dl_j\right)$$

$$+ \frac{2}{1-\nu} \left(\frac{\partial^2 R}{\partial x_j \partial x_i} - \delta_{ij} \frac{\partial^2 R}{\partial x_l \partial x_l}\right) dl_k'\, dl_k \tag{13}$$

Equation (13) is a much more complicated expression than it appears at first sight when the compact notation of the summation convention is translated into the solution of an actual problem. Some illustrative calculations using equation (13) are presented in Appendix I.

If a second loop is created in the continuum the energy becomes:

$$E = \frac{1}{2} \int_V \left(\sigma_{ij}^1 + \sigma_{ij}^2\right)\left(\varepsilon_{ij}^1 + \varepsilon_{ij}^2\right) dV \tag{14}$$

where the superscripts denote the loop. Expression (14) can be written because superposition of stress and strain are allowed in linear elasticity theory. Hence

$$E = \frac{1}{2} \int \sigma^1_{ij} \; \varepsilon^1_{ij} \; dV + \frac{1}{2} \int \sigma^2_{ij} \; \varepsilon^2_{ij} \; dV$$

$$+ \frac{1}{2} \int \left(\sigma^2_{ij} \; \varepsilon^1_{ij} + \sigma^1_{ij} \; \varepsilon^2_{ij}\right) dV \qquad (15)$$

$$= E^{11} + E^{22} + E^{12}$$

E^{11} and E^{22} are the self-energies of loops 1 and 2 respectively and E^{12} is the interaction energy of the pair of loops. By constructing loops 1 and 2 at the same time or by first constructing one and then the other it is seen that

$$E^{12} = \frac{1}{2} \int_V \left(\sigma^2_{ij} \; \varepsilon^1_{ij} + \sigma^1_{ij} \; \varepsilon^2_{ij}\right) dV = \int_V \sigma^2_{ij} \; \varepsilon^1_{ij} \; dV = \int_V \sigma^1_{ij} \; \varepsilon^2_{ij} \; dV \qquad (16)$$

Thus the interaction energy of a pair of loops may be calculated from (13) but it is required that (13) be evaluated for each loop and added together or that double the value for a single loop be taken.

From Appendix I the values

$$\frac{\partial^2 R}{\partial x_k \partial x_k} = \frac{2}{R} \qquad (17)$$

and

$$\frac{\partial^2 R}{\partial x_j \partial x_i} = \frac{\delta_{ij}}{R} - \frac{X_i X_j}{R^3} \qquad (18)$$

may be taken and inserted into (13) to give

$$E_1 = -\frac{Gb_i b_j'}{8\pi} \oint \oint \frac{1}{R} \left(dl_j' dl_i + \right.$$

$$\left. \frac{2\nu}{1-\nu} dl_i' dl_j \right) - \frac{1}{1-\nu} \left(\frac{\delta_{ij}}{R} + \frac{X_i X_j}{R^3} \right) dl_k' dl_k \tag{19}$$

where X_i is defined as $(x_i - x_i')$ and R is the distance between segments dl_i and dl_j'.

It can be seen that in equation (19) the inverse of the separation between dislocation segments will become infinite as the segments approach one another closer and closer. The situation is saved by remembering that interactions within the core are not the same as linear elasticity predicts. It is assumed that all interactions over a distance shorter than one Burgers vector[6] must be treated separately in the core energy analysis and all such interactions are eliminated in performing the integration, which then converges. Thus a point on the dislocation line does not interact with any other point inside a sphere of radius b. These spheres of no interaction mark off a tubular core region about each partial dislocation which is shown in Fig. 5a. (Pg. 21)

The dislocations depicted in Fig. 2 may be characterized by their shape equations

$$y_1 = y_1 (x) \tag{20}$$

$$y_2 = y_2 (x) \tag{21}$$

and their Burgers vectors b_1 and b_2.

Initially

$$y_{10} = \frac{1}{2} d_\tau \tag{22}$$

$$y_{20} = -\frac{1}{2} d_\tau \tag{23}$$

To determine the elastic energy of a constricted dislocation by means of equation (19) requires the integration of (19) over the two closed loops shown in Fig. 1.

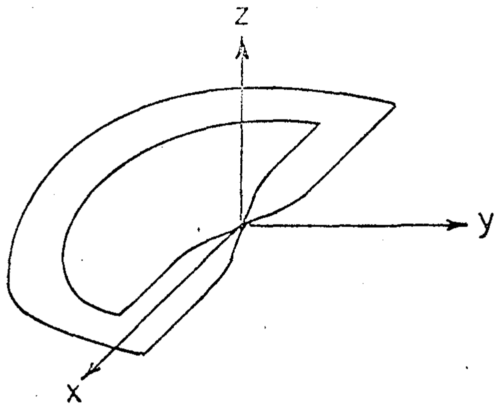


Fig. 1. Constricted Dislocation Shown with Closing Loop

But we are really only interested in the change in energy ΔE_1 produced upon constriction of the dislocation. Consideration of the physics of the situation leads to the expectation that the constriction process should be localized and not very dependent upon the configuration of dislocations outside of its immediate neighborhood.

In Appendix II the effect of the closing loop on the energy change ΔE_1 is shown to be nonzero in general, but a closing loop contour is found for which integration over the unclosed dislocation lines depicted in Fig. 2 yields the same results as for integration over a loop. It seems reasonable to pick such a loop as most representative of the conditions present in an actual medium.

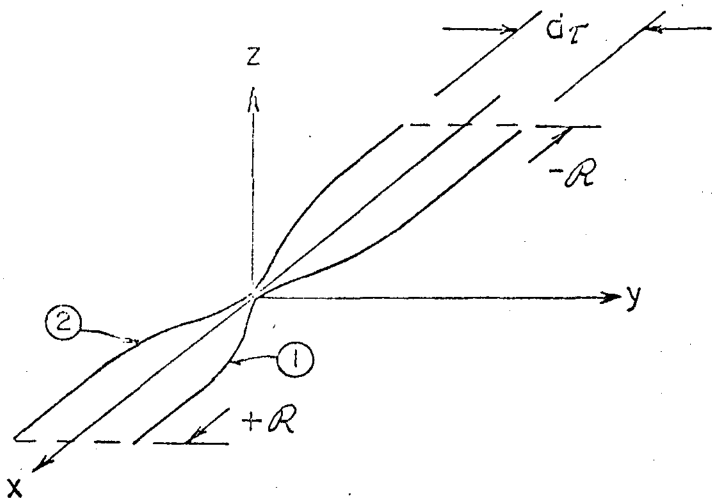


Fig. 2. Constricted Dislocation Ranges of Integration.

In Appendix III equation (19) is evaluated for the general configuration shown below in Fig. 3.

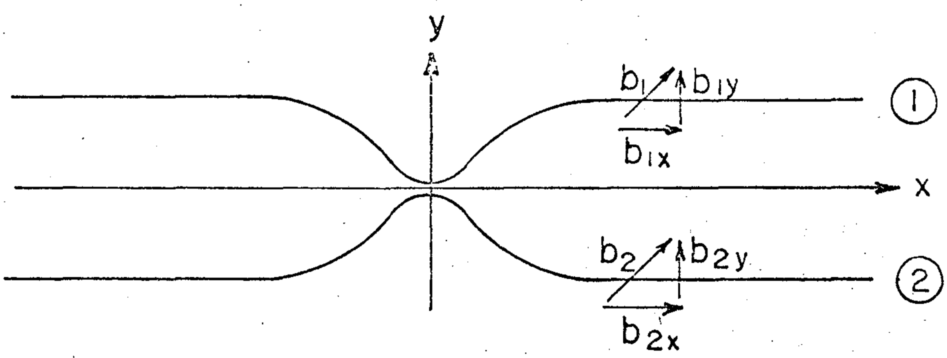


Fig. 3. General Constricted Dislocation.

For a screw dislocation $\vec{b}_1$ and $\vec{b}_2$ add to give a vector $\vec{b}$ in the x-direction. The angle that $\vec{b}_1$ makes with $\vec{b}_{1x}$ and $\vec{b}_2$ with $\vec{b}_{2x}$ must be 30°; this is required by the geometry of the f.c.c. lattice.

For an edge dislocation $\vec{b}_1$ and $\vec{b}_2$ must add to give a Burgers vector $\vec{b}$ in the y-direction. $\vec{b}_1$ and $\vec{b}_2$ make 30° angles with $\vec{b}_{1y}$ and $\vec{b}_{2y}$ respectively in this case.

The configuration of Burgers vectors is shown in Fig. 4 and the partial Burgers vectors are given in terms of the total Burgers vector in Table I.

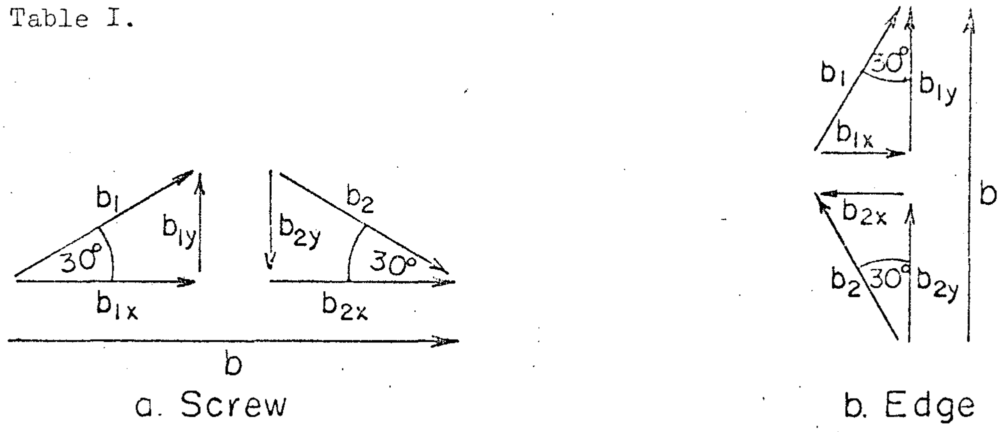


Fig. 4. Burgers Vector Configurations

Table I

Partial Burgers Vectors

	Screw	Edge
b_{1x}	$+\frac{b}{2}$	$+\frac{b}{2\sqrt{3}}$
b_{1y}	$+\frac{b}{2\sqrt{3}}$	$+\frac{b}{2}$
b_{2x}	$+\frac{b}{2}$	$-\frac{b}{2\sqrt{3}}$
b_{2y}	$-\frac{b}{2\sqrt{3}}$	$+\frac{b}{2}$

Symmetry considerations can simplify the expression derived in Appendix III for the screw dislocation case. A plane of mirror symmetry along the x-axis requires that

$$y_2\ (x) = -y_1\ (x) \qquad (24a)$$

$$y_2'\ (x') = -y_1'\ (x') \qquad (24b)$$

provided that the external stresses and barrier don't destroy the symmetry. Such a simplification does not exist for the edge dislocation.

The complexity of the integrals of Appendix III makes the exact solution even to the relatively simplified model taken by us, where we have neglected anisotropy and nonlinearity, impracticable. An exact solution relative to the model chosen would require finding the minimum energy configuration of the system:

$$\delta\ (\Delta E_c) = 0 \qquad (25)$$

where ΔE_c represents the total energy required to constrict the dislocation, including stacking fault and core energies as well as strictly elastic terms. The variation of ΔE_c takes place under conditions:

$$y_1\ (0) = y_2\ (0) = 0 \qquad (26a,b)$$

and

$$y_1\ (+\mathcal{R}) = y_1\ (-\mathcal{R}) = +\frac{d_\tau}{2} \qquad (27a,b)$$

$$y_2\ (+\mathcal{R}) = y_2\ (-\mathcal{R}) = -\frac{d_\tau}{2} \qquad (27c,d)$$

and similarly for primed functions. (Note that $\mathcal{R}$ and R are not the same; $\mathcal{R}$ is a limit, and R is a function equal to $\sqrt{X_i X_i}$.)

Therefore it is necessary to limit our objectives to the extraction of a good approximate solution for the constriction energy. This can be done by means of an assumption about the shape of the partial dislocations comprising the constriction.

THE ASSUMED CONFIGURATION

Algebraic complexity prevented the solution of equation (25) in a general way. An approximate solution can be obtained, however, in the following way. A shape function depending on a single parameter is specified, and the energy is minimized with respect to this parameter. This shape function prescribes a curve which is not in equilibrium as prescribed by equation 25. The energy calculated using the shape function is thus that of equilibrium shape plus that due to the application of constraint forces necessary to distort the equilibrium shape to the assumed shape. Since the energy error due to using the assumed shape depends upon the square of these constraint forces, the approximate energy obtained will be only slightly higher than the exact energy provided that the shape assumed is close enough to the true equilibrium shape to make the constraint forces small. It is assumed that a good enough shape for the purposes of an energy calculation is represented by the curve:

$$y = y_o \left(1 - e^{-\frac{\beta x}{y_o}}\right) \tag{28}$$

in the positive y-x quadrant with reflection symmetry about the x and y axes.

β is the parameter with respect to which energies are minimized. Differentiation of equation (28) shows β to be the slope at the origin of of partial dislocation in the positive quadrant. When β is high the constriction is sharp, and when β is low the constriction is gradual.

A semilog plot from Stroh's[3] Fig. 1 shows that his curve shape may be represented to a good approximation by equation (28) with β approximately 0.5. Our resultant β's turn out to be nearer unity, and as the core decreases in importance the values of β go toward (but do not reach) 0.5.

THE CORE TRACTION ENERGY

As pointed out by Bullough and Foreman[17] in their calculation of the elastic energy of a rhombus shaped loop and as indicated in the previous section on the elastic energy of the constriction, a core traction energy, E_2, must be accounted for.

Making the assumption that the core traction energy is localized very close to the core of the dislocation, E_2 may be approximated by integrating along the dislocations the difference in energy of a unit length of straight dislocation that has and that has not had the core tractions eliminated by an appropriate stress function.

In Appendix IV it is calculated that

$$\Delta E_2 = \frac{G}{16\pi(1-\nu)^2} \Delta \int b^2_{edge} \, dl \qquad (29)$$

where the subscript "edge" refers to the edge component of dislocation of line increment dl. Only edge dislocations contribute core traction energy. $\Delta \int b^2_{edge} \, dl$ is evaluated for the assumed curve shape in Appendix V.

THE CORE ENERGY

In the linear elastic treatment of the bulk elastic energy of a dislocation there exists a singularity at the core of the dislocation which would give an infinite energy if it were not eliminated. In real substances nonlinearities smooth out and eliminate such singularities. Therefore the core region of a dislocation is cut out of the bulk energy and its energy is treated in a completely different way.

Before proceeding with a discussion of what the energy of the material inside the region of nonlinear behavior should be, let us consider how much of the continuum about the dislocation has been eliminated in the elastic calculations. The transformation of the energy integral from a space integral to a double line integral complicates matters. In the space of the double line integral the interactions between segments less than a Burgers vector apart are eliminated; in fact this test is made directly in the course of the numerical integration. Thus in the space in which the double line integral is performed, the core region may be said to lie inside a region generated by sweeping a sphere of Burgers vector radius along all dislocation lines present. As the space is the same for the volume integral associated with the energy (although the form of the integral is different) as for the double line integral, the region of core cut out is identified with that for the line integrals. Thus the core region is that swept out by a sphere of Burgers vector radius translated along the dislocation lines. It may be noted in passing that the cut out process may result in negative bulk elastic energies when the overall energy of constriction is small. The core energy contribution (and other energy contributions such as core traction) must be such as to compensate for any such negative bulk elastic energy to give a total positive constriction energy.

The energy of a unit length of core region should depend upon the energy density and the volume of the core. We have chosen to consider a core radius of one Burgers vector. Any extension of the actual core beyond this radius is considered to be approximately accounted for by the elastic energy of the model localised in the region just outside the Burgers vector radius.

Research by Doyama and Cotterill[18,19] (Morse potential core energy calculations for copper) indicates that core radii of 1.5b and 2.0b may be expected for edge and screw dislocations respectively in copper. For a partial dislocation with a maximum partial Burgers vector of $b/\sqrt{3}$ a core radius of one Burgers vector seems reasonable if the core radius is roughly proportional to the Burgers vector. If the core transition takes place at approximately the same stress, which is proportional to the Burgers vector and inversely proportional to the distance from the dislocation center in the elastic model, one would expect the core radius to be proportional to the Burgers vector.

A calculation based upon the analysis of Doyama and Cotterill yields a strong dependence of the core energy density on the orientation of the Burgers vector. The energy density associated with an edge dislocation is about five times that of a screw dislocation. The energy density of the core of a mixed dislocation has not be investigated, but it might be estimated by some kind of interpolation function dependent on the relative edge and screw components. As the energy density depends on the magnitudes of edge and screw components and not on their signs the interpolation function should involve the squares of the edge and screw Burgers vector components. The simplest function that can be constructed is a linear function of these squares of the edge and screw Burgers vector components. Thus the energy per unit length of dislocation will be taken as

$$\frac{dE_3}{dl} = \frac{\alpha_c G}{4\pi} \left\{ \frac{b^2_{edge}}{1-\nu} + f\, b^2_{screw} \right\} \tag{30}$$

in order to account for the change in orientation of Burgers vector with respect to the partial dislocation. Equation 30 is usually written[2] without the f, which is included here for the sake of generality.

As customarily used Equation 30 interpolates between cores of different size. Thus when the Doyama and Cotterill values of 1.0 eV per {112} plane and 0.2 eV per {110} plane for edge and screw dislocations respectively are used with an assumed value of Gb^2 for copper equal to 4.3 eV, the results (α_c = 1.12 and f = 0.52) have to be modified to eliminate the effect of change in core size which has already been accounted for in the elastic energy, albeit crudely. If a uniform energy density distribution is assumed within the core, multiplying f by $\left(\frac{1.5b}{2.0b}\right)^2$ cuts down the effective size of the screw core to that of the edge giving f = 0.3. Multiplying α_c by $\left(b/\frac{1.5}{3}b\right)^2$ accounts for some additional material contained in the core assuming a strict proportionality of core radius to Burgers vectors giving α_c = 1.5, but this calculation is not very meaningful as it lies well within the wide bounds of indeterminacy to which this calculation is subject.

To reveal the magnitude of the energy dependency on the core parameters chosen calculations are also made using $\alpha_c = 1.0$ and $f = 1.0$.

An additional contribution to the core energy due to the stacking fault lying between the core edge and the core centerline is present in any analysis that calculates the stacking fault area from the centerline of the core instead of from its edge. Due to the high deformation in the core region the concept of a stacking fault, which implies a region of partially slipped but not highly deformed or jumbled up material, loses its meaning. For this reason as well as to isolate the effect of the material in the core region the stacking fault is eliminated from the core regions. This will be discussed later in conjunction with the stacking fault energy.

THE REGION OF CORE OVERLAP

A constriction in a dissociated dislocation refers to recombination of the partials at a point. As long as dislocations are thought of as strictly linear imperfections such a point should have no effect on the core energy because it occupies no volume. In this model a discontinuous change occurs in the core energy when $\beta = 0$, i.e. when the gradually constricted partials reach the limit at which they recombine. At this limit the Burgers vectors and not the energies are additive; otherwise the core energies of the nonoverlapping partials are simply additive.

Because of the tendency in nature for avoidance of such discontinuous jumps and because of the overlapping of real cores of finite radius near the constriction point it seems reasonable that a portion of the overlap core region might better be replaced by the core of a recombined dislocation, the length of the recombined portion increasing as β decreases, so as to change the core character smoothly to that of a recombined dislocation at $\beta = 0$.

In Fig. 5 the region of overlap is shown. A characteristic length, $2x'$, varying from zero to infinity may be found for the overlap region of the assumed configuration such that

$$x' = -\frac{y_o}{\beta} \ln \frac{V}{\beta} \qquad (31)$$

where V is the root immediately below β of the equation

$$V^4 - 2\beta V^3 + (1+\beta^2)V^2 - 2\beta V + \beta^2\left(1 - \frac{b^2}{y_o^2}\right) = 0 \qquad (32)$$

(See Appendix V)

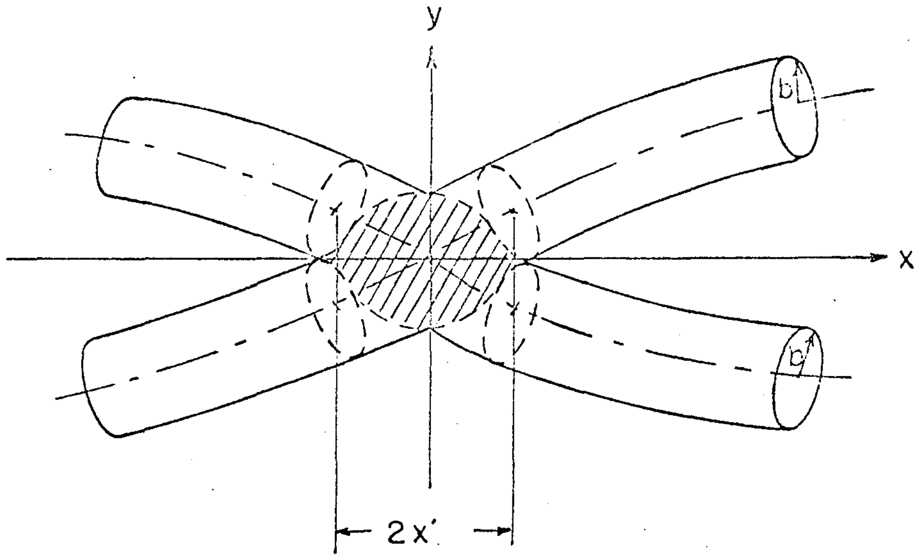


Figure 5. Region of Overlap of a Constricted Dislocation

Because only part of the region between $\pm x'$ actually overlaps the recombined region is taken only between $\pm\frac{x'}{2}$. In this region the energy contribution of the two partial dislocations including core traction energy as well as core energy proper is subtracted out of the constriction energy and the core and core traction energies of a recombined dislocation added in their place. The energy change resulting from the above substitution is called the recombination energy and is given the symbol ΔE_4. In the range of β's for which calculations are made it is usually negative for the screw constriction and positive for the edge constriction. The magnitude of the recombination energy is shown in Figs. 8 and 9 for a case where the separation of partials is small with respect to the core diameter.

THE STACKING FAULT ENERGY

The energy resident in a region of material between a pair of partial dislocations, conceived as due to an unstable phase produced by a shear transformation on passage of the first partial and not yet wiped out by passage of the second partial, is usually characterized by a stacking fault energy, γ, per unit area of stacking fault.

This represents a fifth contribution to the constriction energy

$$\Delta E_5 = \gamma \Delta A \qquad (33)$$

where ΔA is the area change of the stacking fault due to the constriction.

The area change ΔA is considered to be that between the inner core boundaries and not that between centerlines, which is simply $-\frac{2y_o^2}{\beta}$, as shown in Appendix V.

$$\Delta A = -\frac{2y_o^2}{\beta} - \frac{4y_o b}{\beta}\{\frac{y_o}{b}[1 - \frac{V}{\beta} + \left(1 - \frac{b}{y_o}\right) \ln \frac{V}{\beta}]$$

$$+ 1 + \ln\left(\frac{1+\sqrt{1+V^2}}{2}\right) - \frac{1+\beta V}{1+V^2}$$

$$+ \frac{\beta}{2}\frac{b}{y_o}[\tan^{-1} V + \frac{V}{1+V^2}] \qquad (34)$$

where V is the solution to Eq. (32) mentioned previously.

In order to express the constriction energy in the nondimentional form $\Delta E/Gb^2 d_\tau$, where d_τ is the equilibrium separation distance between partials ($d_\tau = 2y_o$), an expression for γ in terms of G, B, and d_τ

must be obtained. The configuration of the unconstricted partials is shown in Fig. 6.

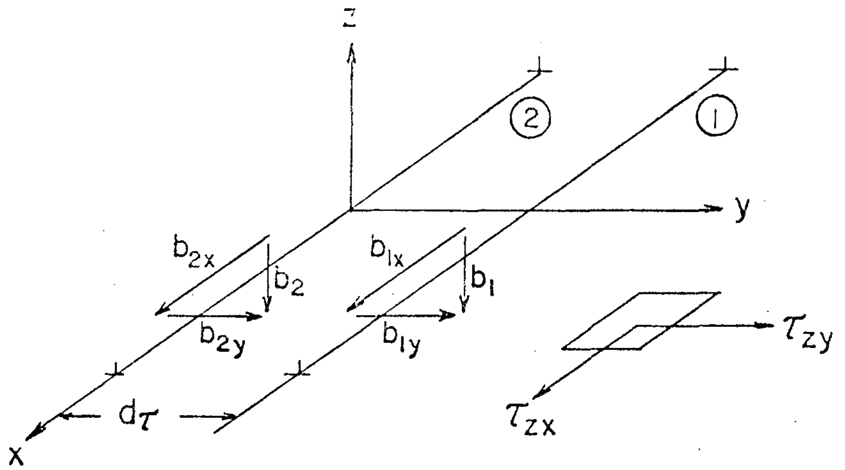


Fig. 6. Configuration of Unconstricted Partials

The force, dFi, acting on a dislocation segment, dl_k, may be written in terms of stresses acting at the dislocation segment:[21]

$$dF_i = \epsilon_{ijk} \sigma_{jm} b_m dl_k \tag{35}$$

Requiring equilibrium for a segment of dislocation 1 in Fig. 5 along the y-direction:

$$-\gamma + \sigma_{zx} b1_x + \sigma_{zy} b1_y = 0 \tag{36a}$$

and for dislocation 2:

$$+\gamma + \sigma_{zx} b2_x + \sigma_{zy} b2_y = 0 \tag{36b}$$

The externally acting stresses are τ_{zx} and τ_{zy}. The stress contribution due to a dislocation may be obtained from Appendix IV for the edge component and from Cottrell's book[20] for the screw. Hence:

$$\gamma = \left(\frac{Gb_{2_x}}{2\pi d_\tau} + \tau_{zx}\right) b_{1_x} + \left(\frac{Gb_{2_y}}{2\pi(1-\nu)d_\tau} + \tau_{zy}\right) b_{1_y} \quad (37a)$$

$$= -\left(-\frac{Gb_{1_x}}{2\pi d_\tau} + \tau_{zx}\right) b_{2_x} - \left(-\frac{Gb_{1_y}}{2\pi(1-\nu)d_\tau} + \tau_{zy}\right) b_{2_y} \quad (37b)$$

or, averaging (33a) and (33b):

$$\gamma = \frac{G}{2\pi d_\tau} \left[b_{1_x} b_{2_x} + \frac{b_{1_y} b_{2_y}}{1-\nu}\right]$$

$$+ \tau_{zx} \left[\frac{b_{1_x} - b_{2_x}}{2}\right]$$

$$+ \tau_{zy} \left[\frac{b_{1_y} - b_{2_y}}{2}\right] \quad (37c)$$

Making the terms of the equation nondimensional:

$$\frac{\gamma}{Gb} = \frac{b}{d_\tau} \left(\frac{1}{2\pi}\right) \left[\frac{b_{1_x}}{b} \frac{b_{2_x}}{b} + \left(\frac{1}{1-\nu}\right) \frac{b_{1_y}}{b} \frac{b_{2_y}}{b}\right]$$

$$+ \frac{\tau_{zx}}{G} \left(\frac{1}{2}\right) \left[\frac{b_{1_x}}{b} - \frac{b_{2_x}}{b}\right]$$

$$+ \frac{\tau_{zy}}{G} \left(\frac{1}{2}\right) \left[\frac{b_{1_y}}{b} - \frac{b_{2_y}}{b}\right] \quad (37d)$$

BOUNDARY STRESSES

A constricted dislocation is generally under a state of long range stress, σ_{ij}, which may be considered as due to the stresses acting on the boundary of the region containing the dislocation. Designating the internal stresses due to the dislocation configuration by σ_{ij}^{I} the total elastic energy of the body may be written

$$E = \frac{1}{2} \int_{v} \left(\sigma_{ij}^{B} + \sigma_{ij}^{I}\right) \left(\varepsilon_{ij}^{B} + \varepsilon_{ij}^{I}\right) dv \qquad (38)$$

where ε_{ij}^{B} and ε_{ij}^{I} are the strains due to the boundary and internal stresses respectively and the integral is taken over the total volume of material neglecting the dislocation cores. The effect of the internal stresses alone has already been accounted for through E_1 and E_2. Using the divergence theorem and the condition of local equilibrium the energy can be transformed to a surface integral.

$$E = \frac{1}{2} \int_{A} \left(\sigma_{ij}^{B} + \sigma_{ij}^{I}\right) \left(u_{j}^{B} + u_{j}^{I}\right) dA_{i}$$

$$= E_1 + E_2 + \frac{1}{2} \int \sigma_{ij}^{B} \left(u_{j}^{B} + 2u_{j}^{I}\right) dA_{i} \qquad (39)$$

where u_{j}^{B} represents the jth component of a displacement due to the boundary stresses, dA_i represents the ith component of a differential surface area, etc.

The principle of superposition of stresses and strains implies that if σ_{ij}^{B} is held constant, which will be the case for all of the following analysis, u_j^B must be constant too. The change in energy may then be written:

$$\Delta E = \Delta E_1 + \Delta E_2 + \Delta \int \sigma_{ij}^B u_k^I \, dA_i \tag{40}$$

The sketch in Fig. 7 showing schematically the stresses and displacements on the surface of a cut which is to have its surfaces relatively displaced to form a new slipped area, ΔA_i, and the stresses and displacements acting on the exterior surface of a unit cube of material containing the cut clarifies the method of evaluation of the last term in equation (40).

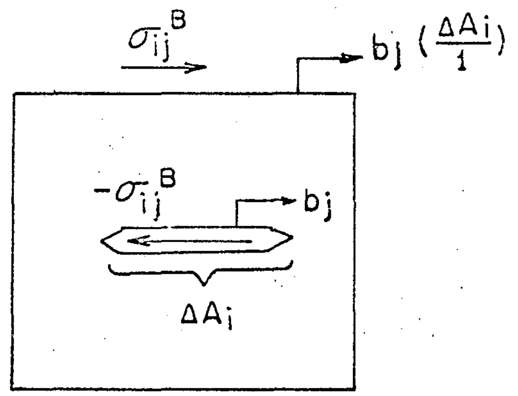


Fig. 7. Stresses and Displacements

Hence

$$\Delta \int \sigma_{ij}^B u_j^I \, dA_i = (\text{work done by } \sigma_{ij}^B \text{ on exterior surface})$$

$$+ (\text{work done by } \sigma_{ij}^B \text{ on internal slip surface})$$

$$= \sigma_{ij}^B b_j \Delta A_i + (-\sigma_{ij}^B) b_j \Delta A_i = 0 \tag{41}$$

Thus there is no change in elastic energy stored in the material <u>directly</u> due to the boundary stresses when the latter are held constant. It is, or course, possible that elastic energy may be stored in the specimen as it deforms under a constant stress since the term evaluated in equation (41) does not represent an energy balance. If the effect of the dislocation configuration within the material is to alter the stress acting at the slipped surface by $\Delta\sigma_{ij}^{I}$, then an energy balance may be written (for a quasi equilibrium situation):

$$\Delta E = \sigma_{ij}^{B} b_j \Delta A_i + \left(-\sigma_{ij}^{B} + \Delta\sigma_{ij}^{I}\right) b_j \Delta A_i$$

$$= \Delta\sigma_{ij}^{I} b_j \Delta A_i$$

$$= \Delta E_1 + \Delta E_2 \qquad (42)$$

From equation (42) it can be seen that although the elastic energy increase is supplied by the external stresses, it appears in the internal stresses.

Thus the fraction of energy stored elastically (the remainder being dissipated as heat) is

$$\frac{\text{Energy Stored}}{\text{Energy Input}} = \frac{\Delta\sigma_{ij}^{I}}{\sigma_{ij}^{B}} \qquad (43)$$

To find the equilibrium configuration of a constriction subject to a long range stress one can proceed in two ways. The minimization of energy principle applies to internal forces and displacements of an isolated system. Therefore one can consider the source of the external stress as a part of the system, the energy of which is to be minimized, along with the elastic continuum containing the dislocation. The result of this procedure is an additional contribution to the energy to be minimized:

$$\Delta E_6 = -\sigma_{ij}^{B}\, b_j\, \Delta A_i \tag{44}$$

ΔE_6 represents the energy change of the external system exerting the stress σ_{ij}^{B}.

The alternative viewpoint is to consider the elastic system as infinitely extended with fixed boundaries. If this system is initially stressed at the level σ_{ij}^{B}, slip of dislocations will change the energy of the continuum itself without appreciably changing the long range state of stress, provided that the dislocation rearrangement is finite in extent. In this case equation (44) is again obtained as an additional energy change that must be considered in energy minimization for the continuum.

The case in which the long range shear stresses τ_{zx} and τ_{zy} act at the constriction yields the result:

$$\Delta E_6 = -Gb \left\{ \left[\frac{\tau_{zx}}{G} \left(\frac{b_{1x}}{b}\right) + \frac{\tau_{zy}}{G} \left(\frac{b_{1y}}{b}\right) \right] \Delta A^1 + \left[\frac{\tau_{zx}}{G} \left(\frac{b_{2x}}{b}\right) + \frac{\tau_{zy}}{G} \left(\frac{b_{2y}}{b}\right) \right] \Delta A^2 \right\} \tag{45a}$$

where ΔA^1 and ΔA^2 refer to areas slipped by dislocations 1 and 2 respectively.

The form of (45a) can be altered to make it similar to that of the stacking fault energy in (37d):

$$\frac{\Delta E_5}{Gb(\Delta A^1-\Delta A^2)} = -\left\{\frac{\tau_{zx}}{G}\left(\frac{b_{1x}}{b} + \frac{b_{2x}}{b}\right) + \frac{\tau_{zy}}{G}\left(\frac{b_{1y}}{b} + \frac{b_{2y}}{b}\right)\right\} \qquad (45b)$$

where $(\Delta A^1 - \Delta A^2)$ is ΔA between the partial dislocation centerlines.

BARRIER STRESSES

In order for the constricting dislocation to be in equilibrium under the action of the externally imposed stresses τ_{zx} and τ_{zy} a barrier must be present to exert the necessary equilibrating counterforce.

Two kinds of barriers may be distinguished: those exerting long range back stresses for which the effective external stresses at the dislocation are zero and those exerting very short range stresses which require the dislocation to contract under the action of external stresses on the trailing partial dislocation. Cases in between may be roughly handled by use of a barrier parameter α_B. The leading dislocation is considered to be always in equilibrium, although the external stresses remaining when the "long range" barrier stresses have been subtracted from τ_{zx} and τ_{zy} are considered to contribute to ΔE_5 on the barrier side as well as the trailing dislocation.

Rewriting equation (36b):

$$\gamma + \left(- \frac{Gb_{1_x}}{2\pi d_\tau} + \alpha_B \tau_{zx}\right) b_{zx} + - \frac{Gb_{1_y}}{2\pi(1-\nu)d} + \alpha_B \tau_{zy}) b_{zy} = 0 \qquad (46)$$

results in a revised value of ΔE_5:

$$\frac{\Delta E_5}{Gb(\Delta A^1 - \Delta A^2)} = - \frac{1}{2\rho} \left(\frac{b_{1_x}}{b} \frac{b_{2_x}}{b} \frac{b}{d_\tau}\right)$$

$$- \frac{1}{2\pi(1-\nu)} \left(\frac{b_{1_y}}{b} \frac{b_{2_y}}{b} \frac{b}{d_\tau}\right)$$

$$+ \alpha_B \left(\frac{\tau_{zx}}{G} \frac{b_{2x}}{b} + \frac{\tau_{zy}}{G} \frac{b_{2y}}{b}\right) \quad (43)$$

Similarly a revised value of ΔE_6 is obtained

$$\frac{\Delta E_6}{Gb\Delta A^1} = - \alpha_B \left\{ \left(\frac{\tau_{zx}}{G} \frac{b_{1x}}{b} + \frac{\tau_{zy}}{G} \frac{b_{1y}}{b}\right) + \left(\frac{\tau_{zx}}{G} \frac{b_{2x}}{b} + \frac{\tau_{zy}}{G} \frac{b_{2y}}{b}\right) \frac{\Delta A^2}{\Delta A^1} \right\} \quad (47)$$

For a "long range" barrier

$$\alpha_B = 0 \quad (48a)$$

and for a "short range" barrier

$$\alpha_B = 1 \quad (48b)$$

For this work it will be assumed that the stresses τ_{zx} and τ_{zy} are zero or very small, and we will not concern ourselves with the nature of the barrier except for having already indicated how the barrier can be accounted for in crude approximation. In a pileup of n screw dislocations the assumption that τ_{zx} is n times the external τ_{zx} gives contractions in rough (order of magnitude) agreement with those of Wolf's[8] Figure 4 when using equation (46) above with $\alpha_B = 1$.

RESULTS AND DISCUSSION

Upon carrying out the computation program delineated in the previous sections one finds that the bulk elastic energy and the stacking fault energy contributions to the constriction energy tend to cancel each other when the core is of appreciable size in comparison with the separation between partial dislocations. This is apparent in Figs. 8 and 9 where the components of the constriction energy are plotted for the case where the separation is only four times the core radius. In the case of the edge dislocation the stacking fault term actually overpowers the bulk elastic term and without the recombination energy a negative constriction energy results at low values of β, i.e. gradual constrictions.

Because of the cancellation of the largest energy contributions the smaller contributions due to the core become extremely important for small separations. Two conclusions can be drawn from this: first, for small separations the accuracy of our calculation is only as good as the accuracy of the core energy, which is known only to the extent of its order of magnitude; and second extrapolations to smaller separations than those for which the calculations were made are even more doubtful. Figs. 10 and 11 show the difference made by a slightly different assumption about the core.

An approximate equation can be given for the constriction energy giving a straight line least squares fit to the curves shown in Fig. 11.

For the edge dislocation the constriction energy, ΔE, is given by

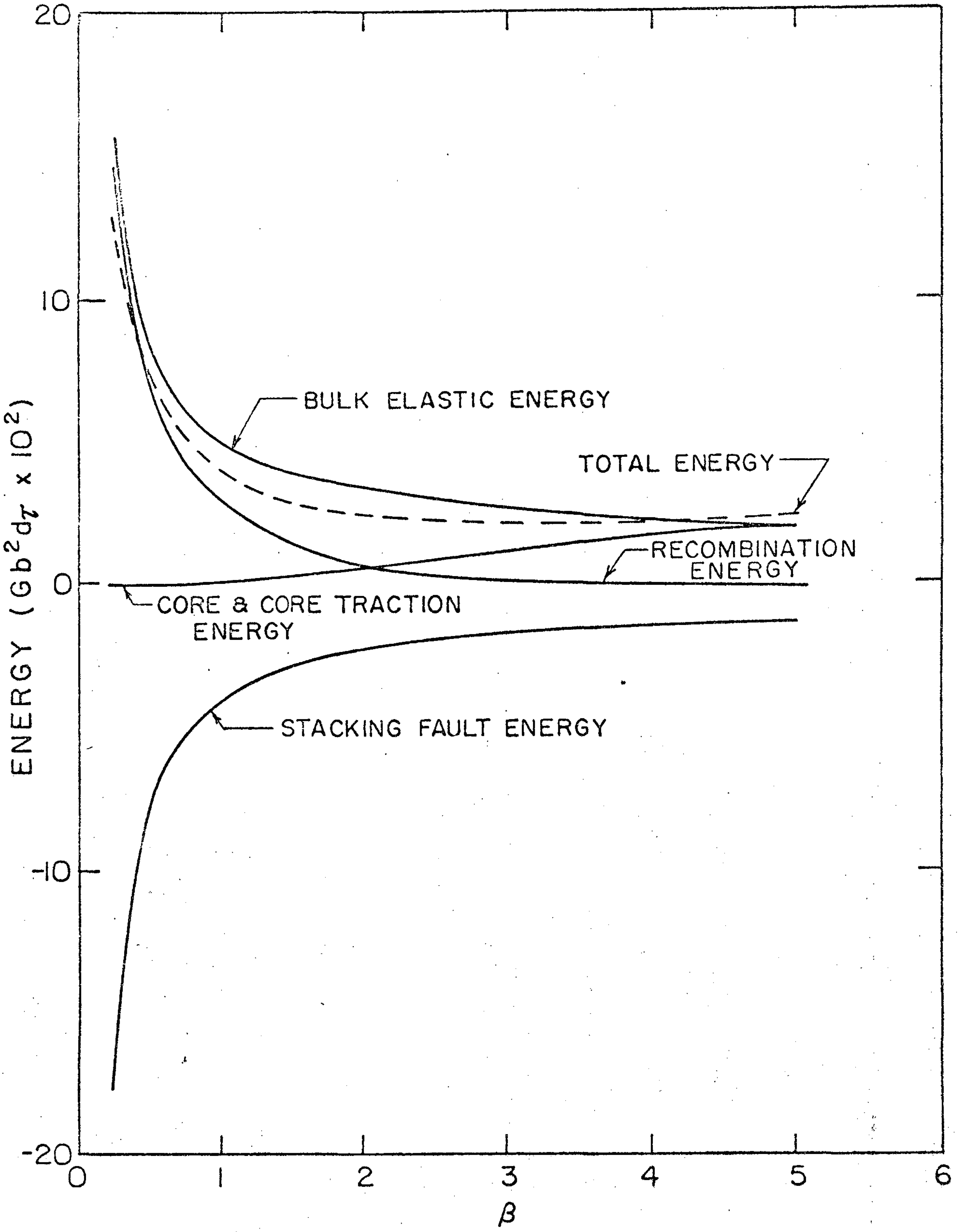


FIG. 8 ENERGY vs. β PARAMETER.
EDGE CONSTRICTION $\frac{d\tau}{b} = 4$, $\alpha_c = 1.5$, $f = 0.3$.

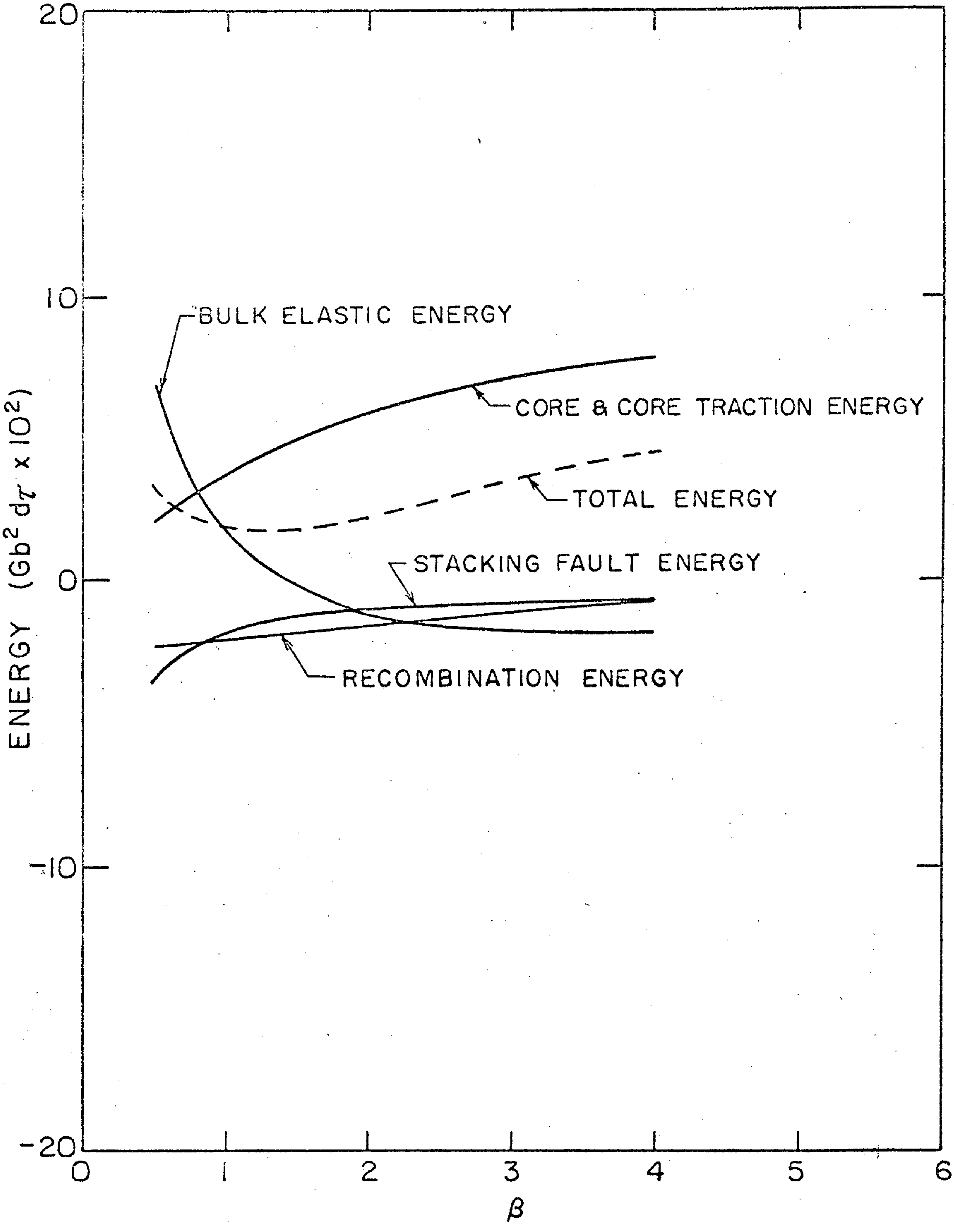


FIG. 9 ENERGY vs. β PARAMETER.
SCREW CONSTRICTION $\frac{d\tau}{b} = 4$, $\alpha_c = 1.5$, $f = 0.3$.

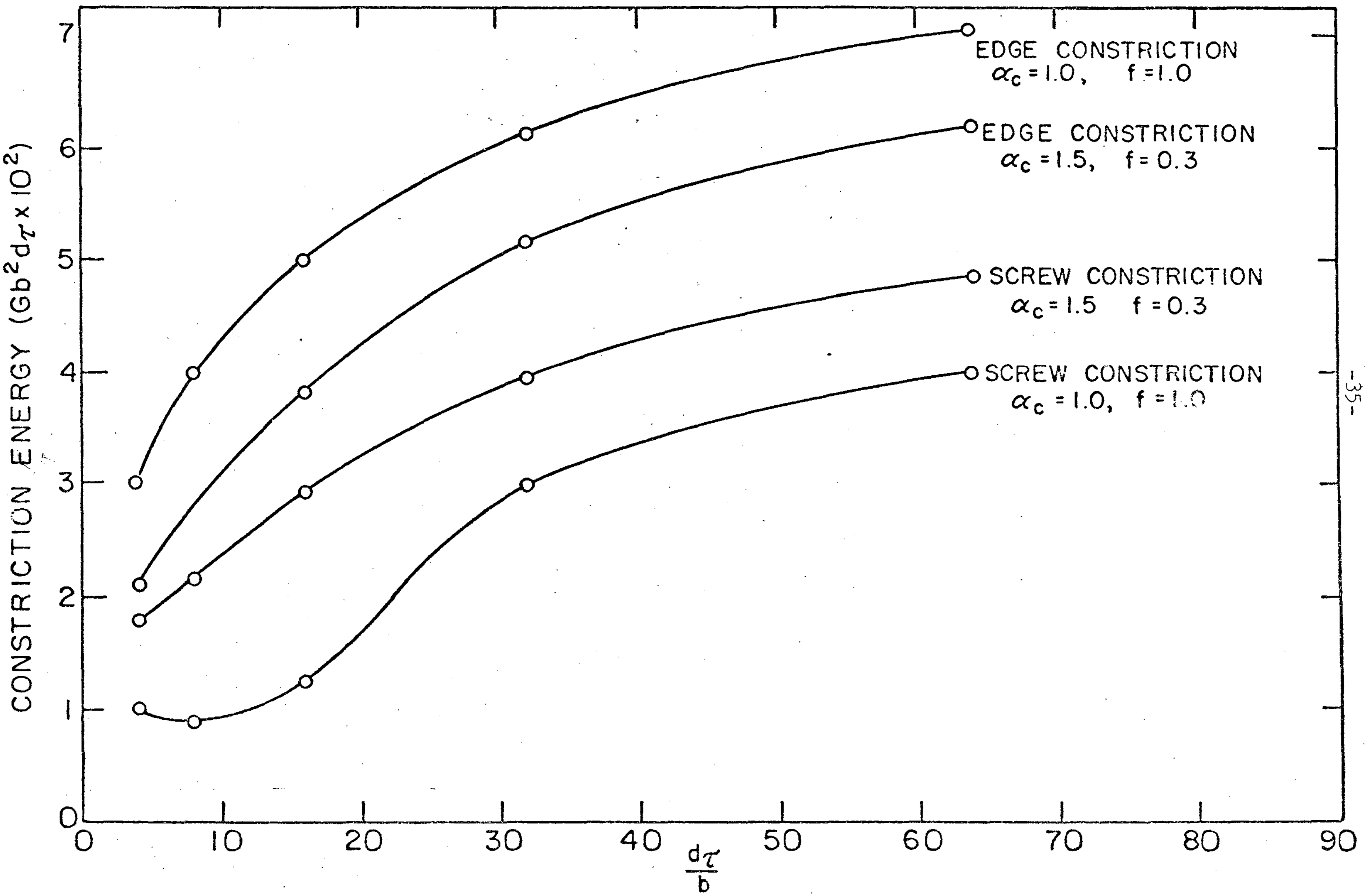


FIG. 10 CONSTRICTION ENERGY vs. STACKING FAULT WIDTH.

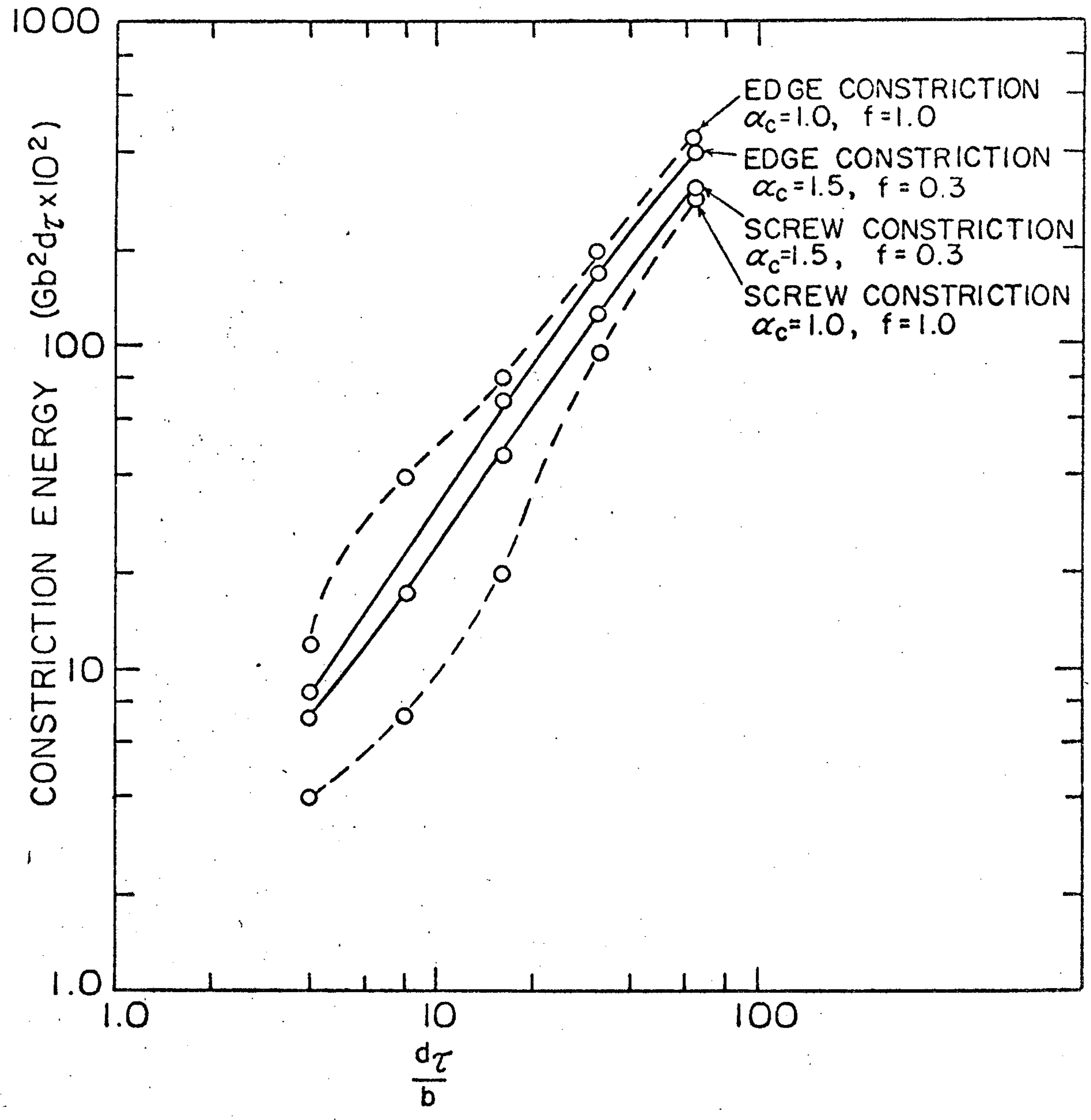


FIG.11 CONSTRICTION ENERGY vs. STACKING FAULT WIDTH.

$$\frac{\Delta E}{Gb^3} = 0.0124 \left(\frac{d_\tau}{b}\right)^{1.36} \tag{49}$$

and for the screw constriction, by

$$\frac{\Delta E}{Gb^3} = 0.0077 \left(\frac{d_\tau}{b}\right)^{1.45} \tag{50}$$

Experimental confirmation of these results is difficult to obtain because for those cases where the stacking fault width can be measured the activation energy for a process involving constriction is so high that the process would not be expected to occur; and where activation energies are measurable the stacking fault width is too small to measure. It is possible, however, to estimate the stacking fault energy indirectly[22] by relating it to the energy of a twin boundary and relating the twin boundary energy to that of a grain boundary. By this means the energy of a stacking fault in aluminum is estimated at roughly 200 ergs/cm^2 and in copper, 40 ergs/cm^2. The constriction energies (Table II) based on these values are tabulated and compared with: (1) some theoretical values obtained by Schöck and Seeger[3] based on an extension of the Peierls extended dislocation model, (2) experimental values of the activation energy for stage III hardening given by Berner,[23] and (3) an experimental value of the activation energy for thermally activated low temperature deformation of aluminum obtained by Mukherjee, Mote and Dorn.[24]

The activation energies cited are the total energies required to surmount the associated short range barriers to dislocation motion.

Table II

Comparison of Results with Experiment and Other Theory

Material	Dislocation Type	Constriction Energy		Stage III Deformation Activation Energy after Berner[21]	Low Temperature Deformation Activation Energy after Mukherjee Mote and Dorn[22]
		Obtained by Us	Obtained by Schöck & Seeger[3]		
Al	Edge	0.10 eV	0.21 eV	0.13 eV	0.18 to 0.19 eV
	Screw	0.02 eV	0.11 eV		
Cu	Edge	1.6 eV	3.9 eV	0.414 eV	-----
	Screw	0.38 eV	0.84 eV		

This has not been obtained for the low temperature deformation of copper because[25] no athermal regime of behavior is encountered when flow stress is plotted vs. temperature. Because cross slip may be expected to require the formation of a pair of constrictions, the constriction energy should be[2] of the order of half the stage III activation energies or larger depending upon aid given to the cross slip process by the shear stress on the cross slip plane. The mechanism governing the low temperature deformation of aluminum, when considered to be the intersection process, may be expected to require the formation of a pair of constrictions and jogs for each unit intersection process. As Stroh points out,[3] however, because the dislocation segments forming the constriction about a jog are on different planes the attractive forces between them are not the same as for a planar constriction especially for small separations as for aluminum. Only for large d_τ/b does he estimate the energy of a single jog by means of his equation for the constriction:

$$\frac{\Delta E}{Gb^3} \simeq .03 \frac{d_\tau}{b} \sqrt{\ln \frac{d_\tau}{b}} \qquad (51)$$

for which he takes the logarithm term equal to unity. For small separations as in aluminum he bases his jog energy estimate on the core energy and obtains a value of about 0.1 Gb^2 with which a calculation of Seeger[22] agrees although Friedel[26] estimates both calculations to be several times too high.

It should also be noted that stress gradients, e.g. a forward force on the rear partial blocked by a backward acting barrier force on the front partial, can reduce d_τ/b. Another correction is also involved in this case to account for the work done by the stresses during constriction as has been discussed in the sections on boundary and barrier stresses. This effect has not been accounted for in the results obtained and can lower the constriction energy significantly.

CONCLUSIONS

From the foregoing analysis it may be concluded that:

(1) The model chosen for the dislocation core strongly affects the calculated constriction energy over the entire range of constriction energies considered.

(2) For the core model chosen (based on Morse potential calculations[18,19] for copper) the constriction energies may be represented approximately by the equations:

$$\frac{\Delta E}{Gb^3} = 0.0124 \left(\frac{d_\tau}{b}\right)^{1.36}$$

for an edge constriction and

$$\frac{\Delta E}{Gb^3} = 0.0077 \left(\frac{d_\tau}{b}\right)^{1.45}$$

for a screw constriction, or by the curves in Figs. 10 and 11.

From comparison with reported experimental data it may also be concluded that:

(3) The activation energies for stage III hardening of Al and Cu and that for low temperature deformation of Al are of the order of magnitude of the estimated constriction energies.

ACKNOWLEDGEMENTS

The author would like to acknowledge the contributions of Professor John E. Dorn, who suggested the problem and provided indispensible advice and criticism throughout the working out of the analysis, and of Mr. Jon Wallace, whose mathematical assistance particularly with the bulk elastic energy integrals and computer programming and whose suggestions and criticisms were extensive and essential in performing the calculations.

This work was prepared as part of the activities of the Inorganic Materials Research Division of the Lawrence Radiation Laboratory of the University of California, Berkeley, and was done under the auspices of the U. S. Atomic Energy Commission.

APPENDICES

Appendix I

Illustrative Calculations Using Equation (13)

A. The Line Energy of a Screw Dislocation.

The use of equation (13) in the body of this report may be illustrated in a calculation of the line energy of a screw dislocation. The configuration used is shown below in Fig. I-1.

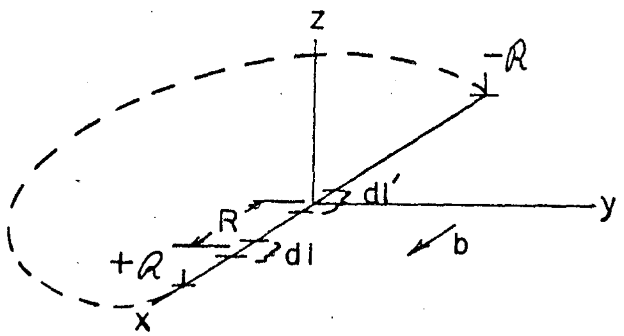


Figure I-1. Screw Dislocation.

$dl' = (dx', 0, 0)$

$dl = (dx, 0, 0)$

$b_i = (b, 0, 0)$

$b'_j = (b, 0, 0)$

The energy of the line segment dl' can be represented by the integral

$$\frac{dE'}{dl'} = - \frac{Gb^2}{16\pi} \oint \frac{\partial^2 R}{\partial x_k \partial x_k} \left(dx + \frac{2\nu}{1-\nu} dx \right)$$

$$+ \frac{2}{1-\nu} \left(\frac{\partial^2 R}{\partial x^2} - \frac{\partial^2 R}{\partial x_1 \partial x_1} \right) dx \tag{I-1}$$

Care must be taken in evaluation of the derivatives of R. Defining $X_i = (x_i - x'_i)$:

$$R = \sqrt{X_i X_i} = \sqrt{(x-x')^2 + (y-y')^2 + (z-z')^2} \tag{I-2}$$

$$\frac{\partial R}{\partial x} = \frac{x-x'}{\sqrt{(x-x')^2 + (y-y')^2 + (z-z')^2}} = \frac{x-x'}{R} \tag{I-3}$$

and in general

$$\frac{\partial R}{\partial x_i} = \frac{X_i}{R} \tag{I-4}$$

Similarly

$$\frac{\partial^2 R}{\partial x^2} = \frac{1}{\sqrt{(x-x')^2 + (y-y')^2 + (z-z')^2}} -$$

$$\frac{(x-x')^2}{[(x-x')^2 + (y-y')^2 + (z-z')^2]^{3/2}}$$

$$= \frac{1}{R} - \frac{(x-x')^2}{R^3} \tag{I-5}$$

and

$$\frac{\partial^2 R}{\partial y \partial x} = - \frac{(x-x')(y-y')}{[(x-x')^2 + (y-y')^2 + (z-z')^2]^{3/2}}$$

$$= - \frac{(x-x')(y-y')}{R^3} \tag{I-6}$$

Thus in general

$$\frac{\partial^2 R}{\partial x_j \partial x_i} = \frac{\partial_{ij}}{R} - \frac{X_i X_j}{R^3} \tag{I-7}$$

Formally we may calculate

$$* \quad \frac{\partial^2 R}{\partial x_i \partial x_i} = \frac{\delta_{ii}}{R} - \frac{X_i X_i}{R^3}$$

$$= \frac{3}{R} - \frac{R^2}{R^3} = \frac{2}{R} \qquad \text{(I-8)}$$

by use of the summation convention. The same result would have been arrived at by differentiation of the less compact expressions. Therefore

$$\frac{dE'}{dl'} = -\frac{Gb^2}{16\pi} \oint \frac{2}{R} \left(dx + \frac{2\nu}{1-\nu} dx\right)$$

$$+ \frac{2}{1-\nu}\left[\frac{1}{R} - \frac{(x-x')^2}{R^3} - \frac{2}{R}\right]dx \qquad \text{(I-9)}$$

$$= \frac{Gb^2}{8\pi} \oint \frac{dx}{|x|}$$

Since $R = |x-x'| = |x|$.

Integrating over the ranges

$$-\mathcal{R} \leq (x-x') \leq -b$$

$$b \leq (z-z') \leq +\mathcal{R}$$

the relation

$$\frac{dE'}{dl'} = \frac{Gb^2}{4\pi} \ln \frac{\mathcal{R}}{b} \qquad \text{(I-10)}$$

---

*Note to readers unfamiliar with tensor algebra:

$\delta_{ii} = \delta_{11} + \delta_{22} + \delta_{33} = 1 + 1 + 1 = 3$

is obtained. The expression represents in a sense the effect of a length $2\mathcal{R}$ of dislocation on an element at the origin, interactions from dislocation line closer than a distance b to the origin being forbidden. Neglect of the rest of the loop is unjustified and in this case the infinite loop having $\mathcal{R} = \infty$ would have $\frac{dE'}{dl'} = \infty$ too. The result is similar to that obtained by the classical use of a specified displacement field of a screw dislocation in a cylinder (see Appendix IV).

The elastic energy of the material in a cylinder of outer radius r_o with a small cylindrical region of radius r_i removed from the center, the site of a screw dislocation of Burgers vector b is given by the expression

$$E = \frac{Gb^2}{4\pi} [\ell n \frac{r_o}{r_i} - 1] \qquad \text{(I-11)}$$

The constant term is due to a balancing couple required for equilibrium. Otherwise the energy expressions in (I-10) and (I-11) are the same in form, and exactly the same if the cutoff terms b and r_o are identified and also the outer radius r_o and the integration range $\mathcal{R}$.

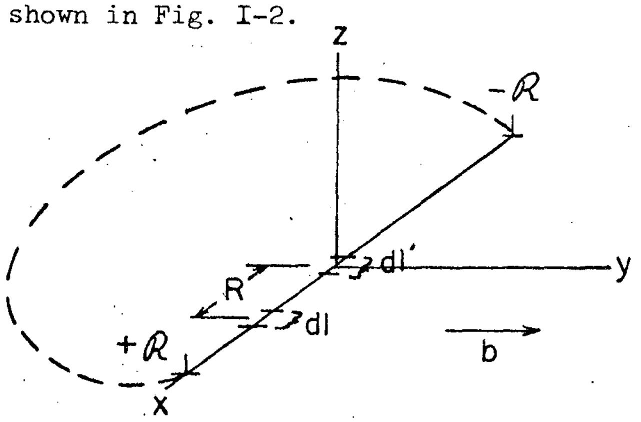
If a term due to the remainder of the loop connecting $x = +\mathcal{R}$ to $x = -\mathcal{R}$ taken as a semicircle is added to the energy, the energy is changed by a constant term (see Appendix II):

$$\frac{dE'}{dl'} = \frac{Gb^2}{4\pi} [\ell n \frac{\mathcal{R}}{b} - \frac{8-3\nu}{3(1-\nu)}] \qquad \text{(I-12)}$$

In our constriction calculations $\mathcal{R}$ is extended to infinity as we are calculating differences in energy which remain finite as $\mathcal{R}$ becomes large in contrast with absolute energies which become infinite in this situation. The cutoff radius b, however, must be specified. In the above special case it can be identified with the core radius of the dislocation. Following the lead of Jøssang, Lothe, and Skylstad[27] the cutoff in the integration, b, will <u>in general</u> be considered as the core radius of the dislocation and will be taken to be one Burgers vector in magnitude.

B. The Line Energy of an Edge Dislocation.

The energy of a small segment of edge dislocation may be calculated in a manner similar to that of the screw segment. The configuration is shown in Fig. I-2.



$$dl' = (dx', 0, 0)$$
$$dl = (dx, 0, 0)$$
$$b_i = (0, b, 0)$$
$$b_j' = (0, b, 0)$$

Figure I-2. Edge Dislocation.

The line energy integral may be written

$$\frac{dE'}{dl'} = -\frac{Gb^2}{16\pi} \oint \frac{2}{1-\nu} \left(\frac{\partial^2 R}{\partial y^2}\right) dx$$

$$= -\frac{Gb^2}{16\pi} \oint \frac{2}{1-\nu} \left(\frac{1}{R} - \frac{2}{R}\right) dx$$

$$= \frac{Gb^2}{8\pi(1-\nu)}\left[\int_{-\mathcal{R}}^{-b} -\frac{dx}{x} + \int_{b}^{\mathcal{R}} \frac{dx}{x}\right]$$

$$= \frac{Gb^2}{4\pi(1-\nu)} \ln \frac{\mathcal{R}}{b} \qquad \text{(I-13)}$$

This expression agrees with the calculation for a dislocation in a cylinder of radius r_o and internal cutout cylinder of radius r_i:

$$E = \frac{Gb^2}{4\pi(1-\nu)}\left[\ln \frac{r_o}{r_i} - \frac{3-4\nu}{4(1-\nu)}\right] \qquad \text{(I-14)}$$

Adding on the hemicircular closing loop changes (I-13) to

$$\frac{dE'}{dl'} = \frac{Gb^2}{4\pi(1-\nu)}\left[\ln \frac{\mathcal{R}}{b} - \frac{5}{3}\right] \qquad \text{(I-15)}$$

The constant terms in (I-14) are due partly to core traction terms and partly to the free surface of the cylinder. The constant terms thus may be thought of as due to different "boundary" conditions and should not be expected to be the same for dislocations having different environments. The meaning of this consideration for the constriction is more fully discussed in Appendix II.

Appendix II

Closing Loop Energy Contribution

Let us consider the energy change (elastic) when a dissociated dislocation loop is deformed within a region P as shown in Fig. II-1.

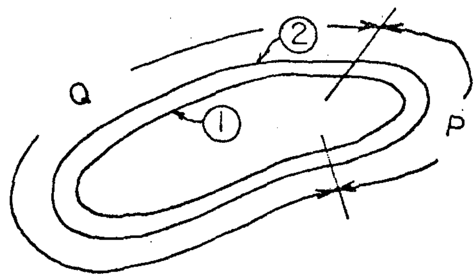


Figure II-1. Dislocation Loop

One partial dislocation is labelled "1" and the other "2"; Q is the closure loop region and remains undeformed. The energy change ΔE_1 may be decomposed:

$$\Delta E_1 = \Delta E^P + \Delta E^Q + \Delta E^{PQ} \tag{II-1}$$

Since Q is undeformed

$$\Delta E^Q = 0 \tag{II-2}$$

The interaction term ΔE^{PQ} is written in terms of an integral:

$$\Delta E^{PQ} = \Delta \left\{ - \frac{Gb_i^P b_j^Q}{16\pi} \int_P \int_Q \frac{2}{R_{PQij}} \left(dl_j^Q dl_i^P \right. \right.$$

$$\left. + \frac{2}{1-\nu} dl_i^Q dl_j^P \right) - \frac{2}{1-\nu} \left(\frac{\delta_{ij}}{R_{PQij}} \right.$$

$$+ \frac{X_i^{PQ} X_j^{PQ}}{R^3_{PQij}} \Big) dl_k^P dl_k^Q \Bigg\} \qquad \text{(II-3)}$$

As the distance from P to Q is increased R_{PQij} increases but so does the length of dislocation line over which integration is carried out. Equations (I-12) and (I-15) in Appendix I show contributions to the line energy of an element at the origin due to the closure loops considered, which clearly imply that an alteration of shape in region P changes the elastic energy of the system differently depending upon the closure loop shape.

In this appendix the calculations will be made. The closing loop for a screw dislocation segment is shown in Fig. II-2.

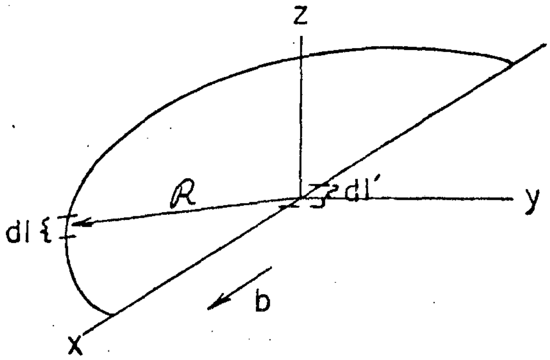


Figure II-2. Closing Loop

The line energy is written (from equation (19))

$$\frac{dE'}{dl'} = - \frac{Gb^2}{16\pi} \int_{\phi=0}^{\phi=\pi} \frac{2}{\ } (dx + \frac{2\nu}{1-\nu} dx)$$

$$- \frac{2}{1-\nu} \left(\frac{1}{R} + \frac{(R\sin\phi)^2}{R^3}\right) dx$$

$$= -\frac{Gb^2}{8\pi\mathcal{R}} \int_{\phi=0}^{\phi=\pi} \left[\left(1 + \frac{2\nu}{1-\nu} - \frac{2}{1-\nu}\right)\left(1 + \sin^2\phi\right)\right] \cdot$$

$$\cdot \left[(\mathcal{R} d\phi)(-\sin\phi)\right]$$

$$= -\frac{Gb^2}{8\pi} \int_{\phi=0}^{\phi=\pi} \left(1 + \frac{2\sin^2\phi}{1-\nu}\right) \sin\phi \, d\phi$$

$$= \frac{Gb^2}{8\pi} \int_{1}^{-1} \left(\frac{3-\nu}{1-\nu} - \frac{2}{1-\nu}\zeta^2\right) d\zeta$$

where $\zeta = \cos\phi$

$$= -\frac{Gb^2}{4\pi}\left[\frac{8-3\nu}{3(1-\nu)}\right] \qquad \text{(II-4)}$$

The picture for the edge case is similar to that of Fig. II-2 with the Burgers vector direction along the y-axis. The energy expression is:

$$\frac{dE'}{dl'} = -\frac{Gb^2}{16\pi} \int_{\phi=0}^{\phi=\pi} -\frac{2}{1-\nu}\left(\frac{1}{\mathcal{R}} + \frac{(\sin\phi)^2}{\mathcal{R}^3}\right).$$

$$\left[(\mathcal{R} d\phi)(-\sin\phi)\right]$$

$$= +\frac{Gb^2}{8\pi(1-\nu)} \int_{\phi=0}^{\phi=\pi} (1 + \sin^2\phi)(-\sin\phi \, d\phi)$$

$$= \frac{Gb^2}{8\pi(1-\nu)} \int_{1}^{-1} (2 - \zeta^2)\, d\zeta$$

$$= -\frac{Gb^2}{4\pi(1-\nu)} \left(\frac{5}{3}\right) \qquad \text{(II-5)}$$

The need to consider the above type of interactions can, however, be removed without violating the closing loop requirement. Since P is confined to the x-y plane it is possible to choose Q, or rather critical regions of Q, such that $dl_k^P\, dl_k^Q$ is zero by taking dl_k^Q normal to the x-y plane. Since the Burgers vectors are also restricted to the x-y plane $dl_j^P = dl_i^Q = 0$ in (II-3). These regions of Q can be extended from the boundaries of P normal to the plane of P for an indefinite distance. Thus the connection between the branches of Q which are normal to the plane can be brought farther and farther away from P without increasing its size and although this part of Q must have components of extension parallel to the x-y plane, its effect may be made as small as desired. For this closing loop (shown in Fig. II-3):

$$\Delta E^{PQ} = 0 \qquad \text{(II-6)}$$

and

$$\Delta E_1 = \Delta E^P$$

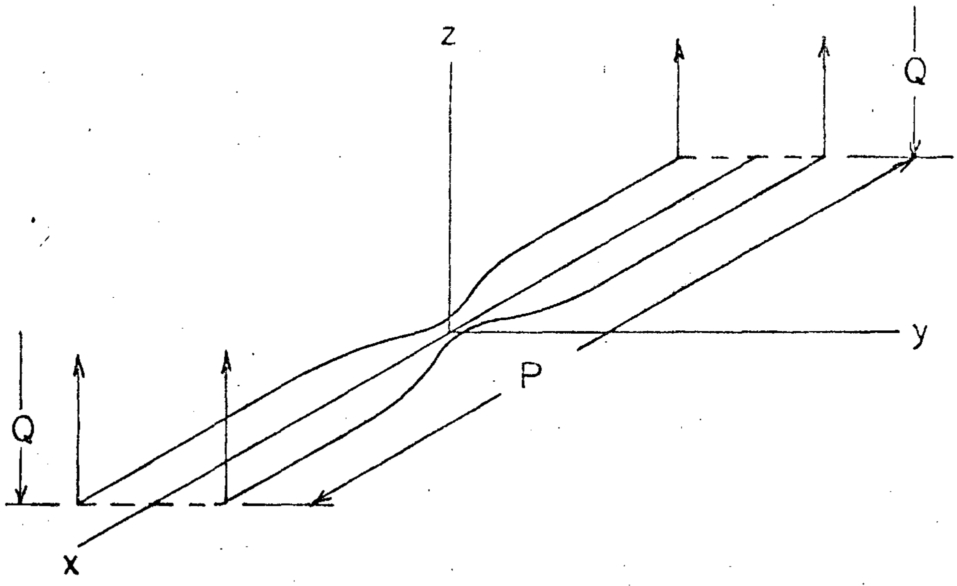


Figure II-3. Closing Loop Q Having No Effect on ΔE_1.

Appendix III

Calculation of ΔE_1

The calculation of ΔE_1 is helped by a few decompositions:

$$\Delta E_1 = \Delta E_1^{11} + \Delta E_1^{22} + \Delta E_1^{12} \qquad \text{(III-1)}$$

$$\Delta E_1^{11} = \Delta E_1^{11xx} + \Delta E_1^{11yy} + \Delta E_1^{11xy} \qquad \text{(III-2)}$$

$$\Delta E_1^{22} = \Delta E_1^{22xx} + \Delta E_1^{22yy} + \Delta E_1^{22xy}$$

$$\Delta E_1^{12} + \Delta E_1^{12xx} + \Delta E_1^{12yy} + \Delta E_1^{12xy} \qquad \text{(III-4)}$$

where 1 and 2 refer to the dislocation lines and x and y refer to Burgers vector components.

$$\Delta E_1^{11xx} = -\frac{G(b_{1x})^2}{8\pi} \int_{-\mathcal{R}}^{+\mathcal{R}} \int_{-\mathcal{R}}^{+\mathcal{R}} \frac{1}{R^{11xx}} (dx'dx$$

$$+ \frac{2\nu}{1-\nu} dx'dx) - \frac{1}{1-\nu} \frac{1}{R^{11xx}} - \frac{(x-x')^2}{(R^{11xx})^3}.$$

$$(dx'dx + dy'dy) - \frac{1}{R_o^{11xx}} (dx'dx +$$

$$\frac{2\nu}{1-\nu} dx'dx) + \frac{1}{1-\nu} \left(\frac{1}{R_o^{11xx}} - \frac{(x-x')^2}{R_o^{11xx}}\right) dx'dx) \qquad \text{(III-5)}$$

where

$$R^{11xx} = \sqrt{(y_1 - y_1')^2 + (x-x')^2} \qquad \text{(III-6)}$$

$$y_1 = y_1(x) \qquad y_1' = y_1(x') \qquad \text{(III-7)}$$

and

$$R_o^{11xx} = \sqrt{(x-x')^2} \qquad \text{(III-8)}$$

$$\Delta E_1^{11xx} = -\frac{G(b_{1x})^2}{8\pi} \int_{-\mathcal{R}}^{+\mathcal{R}} \int_{-\mathcal{R}}^{+\mathcal{R}}$$

$$\frac{\nu}{1-\nu} \left[\frac{1}{\sqrt{(y_1-y_1')^2 + (x-x')^2}} - \frac{1}{\sqrt{(x-x')^2}}\right] dx'dx$$

$$- \frac{1}{1-\nu} \left[\frac{(x-x')^2}{[(y_1-y_1')^2 + (x-x')^2]^{3/2}} - \frac{1}{\sqrt{(x-x')^2}}\right] dx'dx$$

$$- \frac{1}{1-\nu} \left[\frac{(x-x')^2}{[(y_1-y_1')^2 + (x-x')^2]^{3/2}}\right] \left(\frac{dy_1'}{dx'} \frac{dy_1}{dx}\right) dx'dx \qquad \text{(III-9)}$$

$$\Delta E_1^{11yy} = -\frac{G(b_{1y})^2}{8\pi} \int_{-\mathcal{R}}^{+\mathcal{R}} \int_{-\mathcal{R}}^{+\mathcal{R}} \frac{1}{R^{11yy}} (dy'dy +$$

$$\frac{2\nu}{1-\nu} dy'dy) - \frac{1}{1-\nu} \left(\frac{1}{R^{11yy}} + \frac{(y-y')^2}{(R^{11yy})^3}\right).$$

$$(dx'dx + dy'dy) + \frac{1}{1-\nu}\left(\frac{1}{R_o^{11yy}}\right) dx'dx \qquad \text{(III-10)}$$

where

$$R^{11yy} = \sqrt{(y_1-y_1')^2 + (x-x')^2} \qquad \text{(III-11)}$$

$$R_o^{11yy} = \sqrt{(x-x')^2} \qquad \text{(III-12)}$$

$$\Delta E_1^{11yy} = -\frac{G(b_{1y})}{8}\int_{-\mathcal{R}}^{+\mathcal{R}}\int_{-\mathcal{R}}^{+\mathcal{R}}$$

$$\frac{\nu}{1-\nu}\left[\frac{1}{\sqrt{(y_1-y_1')^2 + (x-x')^2}}\right]\left(\frac{dy_1'}{dx'}\frac{dy_1}{dx}\right) dx'dx$$

$$-\frac{1}{1-\nu}\left[\frac{(y_1-y_1')^2}{[(y_1-y_1')^2 + (x-x')^2]^{3/2}}\right]\left[1 + \frac{dy_1'}{dx'}\frac{dy_1}{dx}\right] dx'dx$$

$$-\frac{1}{1-\nu}\left[\frac{1}{\sqrt{(y_1-y_1')^2 + (x-x')^2}} - \frac{1}{\sqrt{(x-x')^2}}\right] dx'dx \qquad \text{(III-13)}$$

$$\Delta E_1^{11xy} = -2\,\frac{G(b_{1x}b_{1y})}{8\pi}\int_{-\mathcal{R}}^{+\mathcal{R}}\int_{-\mathcal{R}}^{+\mathcal{R}}\frac{1}{R^{11xy}}\,(dy_1'\,dx$$

$$+ \frac{2\nu}{1-\nu} (dx' dy_1) - \frac{1}{1-\nu} \left(\frac{(y_1 - y_1')\ (x-x')}{(R^{11^{xy}})^3} \right) \cdot$$

$$(dx' dx + dy_1' dy_1) - 0 \qquad \text{(III-14)}$$

where

$$R^{11^{xy}} = \sqrt{(y_1 - y_1')^2 + (x-x')^2} \qquad \text{(III-15)}$$

$$\Delta E_1^{11^{xy}} = \frac{G b_{1x} b_{1y}}{4\pi} \int_{-R}^{+R} \int_{-R}^{+R}$$

$$\left[\frac{1}{\sqrt{(y_1 - y_1')^2 + (x-x')^2}} \quad \frac{dy_1'}{dx'} \right] dx' dx$$

$$+ \frac{2}{1-\nu} \left[\frac{1}{\sqrt{(y_1 - y_1')^2 + (x-x')^2}} \cdot \frac{dy_1}{dx} \right] dx' dx$$

$$- \frac{1}{1-\nu} \left[\frac{(y_1 - y_1')(x-x')}{[(y_1 - y_1')^2 + (x-x')^2]^{3/2}} \left(\frac{dy_1'}{dx'} \quad \frac{dy_1}{dx} + 1 \right) \right] dx'\ dx \qquad \text{(III-16)}$$

$$\Delta E_1^{22^{xx}} = - \frac{G(b_{2x})^2}{8\pi} \int_{-R}^{+R} \int_{-R}^{+R}$$

$$\frac{\nu}{1-\nu}\left[\frac{1}{\sqrt{(y_2-y_2')^2+(x-x')^2}} - \frac{1}{\sqrt{(x-x')^2}}\right] dx'dx$$

$$-\frac{1}{1-\nu}\left[\frac{(x-x')^2}{\sqrt{(y_2-y_2')^2+(x-x')^2}} - \frac{1}{\sqrt{(x-x')^2}}\right] dx'dx$$

$$-\frac{1}{1-\nu}\left[\frac{(x-x')^2}{[(y_2-y_2')^2+(x-x')^2]^{3/2}}\right]\left(\frac{dy_2'}{dx'}\quad\frac{dy_2}{dx}\right) dx'dx \qquad \text{(III-17)}$$

by similarity with $\Delta E_1^{11^{xx}}$

$$\Delta E_1^{22^{yy}} = -\frac{G(b_{2y})^2}{8\pi}\int_{-R}^{+R}\int_{-R}^{+R} .$$

$$\frac{\nu}{1-\nu}\left[\frac{1}{\sqrt{(y_2-y_2)^2+(x-x')^2}}\right]\left(\frac{dy_2'}{dx'}\quad\frac{dy_2}{dx}\right) dx'dx$$

$$\frac{1}{1-\nu}\left[\frac{(y_2-y_2')^2}{[(y_2-y_2')^2+(x-x')^2]^{3/2}}\right]\left[1+\frac{dy_2'}{dx'}\quad\frac{dy_2}{dx}\right] dx'\ dx$$

$$-\frac{1}{1-\nu}\left[\frac{1}{\sqrt{(y_2-y_2')^2+(x-x')^2}} - \frac{1}{\sqrt{(x-x')^2}}\right] dx'dx \qquad \text{(III-18)}$$

by similarity with $E_1^{11^{yy}}$

$$\Delta E_1^{22^{xy}} = - \frac{G b_{1x} b_{1y}}{4\pi} \int_{-R}^{+R} \int_{-R}^{+R}$$

$$\left[\frac{1}{\sqrt{(y_2 - y_2')^2 + (x-x')^2}} \quad \frac{dy_2'}{dx'} \right] dx' dx$$

$$+ \frac{2\nu}{1-\nu} \left[\frac{1}{\sqrt{(y_2-y_2')^2 + (x-x')^2}} \quad \frac{dy_2}{dx} \right] dx' dx$$

$$- \frac{1}{1-\nu} \left[\frac{(y_2-y_2')\ (x-x')}{[(y_2-y_2')^2 + (x-x')^2]^{3/2}} \left(\frac{dy_2'}{dx'} \quad \frac{dy_2}{dx} + 1 \right) \right] dx' dx$$

(III-19)

by similarity with $\Delta E_1^{11^{xy}}$

$$\Delta E_1^{12^{xx}} = - 2 \frac{G b_{1x} b_{2x}}{8\pi} \int_{-R}^{+R} \int_{-R}^{+R} \frac{1}{R^{12^{xx}}} (dx' dx$$

$$+ \frac{2\nu}{1-\nu} dx' dx) - \frac{1}{1-\nu} \frac{1}{R^{12^{xx}}} + \left(\frac{(x-x')^2}{(R^{12^{xx}})^3} \right).$$

$$(dx' dx + dy_1' dy_2) - \frac{1}{R_o^{12^{xx}}} (dx' dx +$$

$$\frac{2\nu}{1-\nu} dx' dx) + \frac{1}{1-} \left(\frac{1}{R_o^{12^{xx}}} + \frac{(x-x')^2}{(R_o^{12^{xx}})^3} \right).$$

$$(dx'dx + dy_1'dy_2) - \frac{1}{R_o^{12^{xx}}} (dx'dx +$$

$$\frac{2\nu}{1-\nu} dx'dx) + \frac{1}{1-\nu} \left(\frac{1}{R_o^{12^{xx}}} + \frac{(x-x')^2}{(R_o^{12^{xx}})^3} \right) (dx'dx) \qquad \text{(III-20)}$$

where

$$R^{12^{xx}} = \sqrt{(y_2-y_1')^2 + (x-x')^2} \qquad \text{(III-21)}$$

$$R^{12^{xx}} = \sqrt{d_t^{\ 2} + (x-x')^2} \qquad \text{(III-22)}$$

(d_t = separation of partials before constriction)

$$\Delta E_1^{12^{xx}} = - \frac{Gb_{1x}b_{2x}}{4\pi} \int_{-R}^{+R} \int_{-R}^{+R}$$

$$\frac{\nu}{1-\nu} \left[\frac{1}{\sqrt{(y_2-y_1')^2 + (x-x')^2}} - \frac{1}{\sqrt{d_t^{\ 2} + (x-x')^2}} \right] dx'dx$$

$$- \frac{1}{1-\nu} \left[\frac{(x-x')^2}{[(y_2-y_1')^2 + (x-x')^2]^{3/2}} - \frac{(x-x')^2}{[d_t^2 + (x-x')^2]^{3/2}} \right] dx'dx$$

$$- \frac{1}{1-\nu} \left[\frac{(x-x')^2}{[(y_2-y_1') + (x-x')^2]^{3/2}} \left(\frac{dy_y'}{dx'} \quad \frac{dy_2}{dx} \right) \right] dx'dx \qquad \text{(III-23)}$$

$$\Delta E_1^{12^{yy}} = - 2 \frac{Gb_{1y}b_{2y}}{8\pi} \int_{-R}^{+R} \int_{-R}^{+R} \frac{1}{R^{12^{yy}}} (dy_2 dy_1'$$

$$+ \frac{2\nu}{1-\nu} dy_2 dy_1') - \frac{1}{1-\nu} \left(\frac{1}{R^{12^{yy}}} + \frac{(y_2-y_1')^2}{(R^{12^{yy}})^3} \right) \cdot$$

$$(dx'dx + dy_2 dy_1') + \frac{1}{1-\nu} \left(\frac{1}{R_o^{12^{yy}}} \right.$$

$$\left. + \frac{d_t^{\,2}}{(R_o^{12^{yy}})^3} \right) dx'dx \qquad \text{(III-24)}$$

where

$$R^{12^{yy}} = \sqrt{(y_2-y_1')^2 + (x-x')^2} \qquad \text{(III-25)}$$

$$R_o^{12^{yy}} = \sqrt{d_\tau^{\,2} + (x-x')^2} \qquad \text{(III-26)}$$

$$\Delta E_1^{12^{yy}} = - \frac{Gb_{1y}b_{2y}}{4\pi} \int_{-R}^{+R} \int_{-R}^{+R}$$

$$\frac{\nu}{1-\nu} \left[\frac{1}{\sqrt{(y_2-y_1')^2 + (x-x')^2}} \right] \left(\frac{dy_2}{dx} \quad \frac{dy_1'}{dx'} \right) dx'dx$$

$$- \frac{1}{1-\nu} \left[\frac{1}{\sqrt{(y_2-y_1')^2 + (x-x')^2}} - \frac{1}{\sqrt{d_\tau^2 + (x-x')^2}} \right] dx'dx$$

$$- \frac{1}{1-\nu} \left[\frac{(y_2-y_1')^2}{[(y_2-y_1')^2+(x-x')^2]^{3/2}} - \frac{d_t^{\,2}}{[d_\tau^{\,2} + (x-x')^2]^{3/2}} \right] dx'dx$$

$$- \frac{1}{1-\nu} \left[\frac{(y_2-y_1')^2}{[(y_2-y_1')^2+ (x-x')^2]^{3/2}} \right] \left(\frac{dy_2}{dx} \frac{dy_1'}{dx'} \right) dx'dx \qquad \text{(III-27)}$$

$$\Delta E_1^{12^{xy}} = - 2(2) \frac{Gb_{1x}b_{2y}}{8\pi} \int_{-R}^{+R} \int_{-R}^{+R} \frac{1}{R^{12^{xy}}} \ (dy_2 dx_1'$$

$$+ \frac{2\nu}{1-\nu} \ dy_1'dx) - \frac{1}{1-\nu} \left(\frac{(y_2-y_1')(x-x')}{(R^{12^{xy}})^3} \right) \cdot$$

$$(dxdx' + dy_1'dy_2) - \frac{1}{1-\nu} \left(\frac{d_\tau(x-x')}{(R_o^{12^{xy}})^3} \right) \quad (dxdx') \qquad \text{(III-28)}$$

where

$$R^{12^{xy}} = \sqrt{(y_2-y_1')^2+(x-x')^2} \qquad \text{(III-29)}$$

$$R_o^{12^{xy}} = \sqrt{d_\tau^{\,2} + (x-x')^2} \qquad \text{(III-30)}$$

$$\Delta E_1^{12^{xy}} = -\frac{Gb_{1x}b_{2y}}{2\pi}\int_{-R}^{+R}\int_{-R}^{+R}$$

$$\left[\frac{1}{\sqrt{(y_2-y_1')^2+(x-x')^2}}\left(\frac{dy_2}{dx}+\frac{2\nu}{1-\nu}\frac{dy_1'}{dx'}\right)\right]dx'dx$$

$$-\frac{1}{1-\nu}\left[\frac{(y_2-y_1')(x-x')}{[(y_2-y_1')^2+(x-x')^2]^{3/2}}-\frac{d_t(x-x')}{[d_\tau^2+(x-x')^2]^{3/2}}\right]dx'dx$$

$$-\frac{1}{1-\nu}\left[\frac{(y_2-y_1')(x-x')}{[(y_2-y_1')^2+(x-x')^2]^{3/2}}\left(\frac{dy_1'}{dx'}\frac{dy_2}{dx}\right)\right]dx'dx \qquad \text{(III-31)}$$

The expression for $\Delta E_1/Gb^2d_t$ that results from summing the component parts above is of the form

$$\frac{\Delta E_1}{Gb^2d_\tau} = E\!\!\int_{-\infty}^{+\infty}\!\!C \quad E\!\!\int_{-\infty}^{+\infty}\!\!C \quad f(u,u')\,du\,du' \qquad \text{(III-32)}$$

where u and u' represent the nondimensionalized lengths $\frac{x}{yo}$ and $\frac{x'}{yo}$ respectively, and the notation E C refers to the elimination of core terms in the course of performing the integration (see below).

Decomposing the integrals

$$\frac{\Delta E_1}{Gb^2d_\tau} = \left(E\!\!\int_{-\infty}^{0}\!\!C + E\!\!\int_{0}^{\infty}\!\!C\right)\left(E\!\!\int_{-\infty}^{0}\!\!C + E\!\!\int_{0}^{\infty}\!\!C\right) f(u,u')\,du\,du' \qquad \text{(III-33a)}$$

$$= E\int_{-\infty}^{0} C \; E\int_{-\infty}^{0} C + E\int_{0}^{\infty} C \; E\int_{0}^{\infty} C + E\int_{-\infty}^{0} C \; E\int_{0}^{\infty} C + E\int_{-\infty}^{\infty} C \; E\int_{-\infty}^{0} C$$

$$f(u,u') \, dudu' \qquad \text{(III-33b)}$$

$$= E\int_{0}^{\infty} C \; E\int_{0}^{\infty} C \; f(-u,-u') \, dudu'$$

$$+ E\int_{0}^{\infty} C \; E\int_{0}^{\infty} C \; f(u,u') \, dudu'$$

$$+ E\int_{0}^{\infty} C \; E\int_{0}^{\infty} C \; f(-u,u') \, dudu'$$

$$+ E\int_{0}^{\infty} C \; E\int_{0}^{\infty} C \; f(u,-u') \, dudu' \qquad \text{(III-33c)}$$

$$= E\int_{0}^{\infty} C \; E\int_{0}^{\infty} C \; [f(-u,-u') + f(u,u')$$

$$+ f(-u,u') + f(u,-u')] \; dudu' \qquad \text{(III-33d)}$$

Using the transformation of (III-33d) plus the above energy expressions for the case where $\nu = \frac{1}{3}$ and the Burgers vectors are given as in Table I equations (III-34) and (III-35) are obtained. These may be machine integrated to finite upper limits using Simpson's rule and extrapolated to infinite limits. For the screw dislocation

$$\frac{\Delta E_1}{Gb^2 d_\tau} = -\frac{1}{96\pi} \quad E\int_0^\infty C \quad E\int_0^\infty C \left\{ \frac{-8\beta^2 e^{-\beta(u+u')}}{\sqrt{(u-u')^2 + (e^{-\beta u} - e^{-\beta u'})^2}} \right.$$

$$+ \frac{8\beta^2 e^{-\beta(u+u')}}{\sqrt{(u+u')^2 + (e^{-\beta u} - e^{-\beta u'})^2}}$$

$$- \frac{[9(u-u')^2 + 3(e^{-\beta u} - e^{-\beta u'})^2][1 + \beta^2 e^{-\beta(u+u')}]}{[(u-u')^2 + (e^{-\beta u} - e^{-\beta u'})^2]^{3/2}}$$

$$- \frac{[9(u+u')^2 + 3(e^{-\beta u} - e^{-\beta u'})^2][1 - \beta^2 e^{-\beta(u+u')}]}{[u+u')^2 + (e^{-\beta u} - e^{-\beta u'})^2]^{3/2}}$$

$$+ \frac{9}{\sqrt{(u-u')^2}} + \frac{9}{\sqrt{(u+u')^2}}$$

$$+ \frac{6 + 10\beta^2 e^{-\beta(u+u')}}{\sqrt{(u-u')^2 + (2 - e^{-\beta u} - e^{-\beta u'})^2}}$$

$$+ \frac{6 - 10\beta^2 e^{-\beta(u+u')}}{\sqrt{(u\ u')^2 + (2 - e^{-\beta u} - e^{-\beta u'})^2}}$$

$$\frac{[9(u-u')^2 - 3(2 - e^{-\beta u} - e^{-\beta u'})^2][1 - \beta^2 e^{-\beta(u+u')}]}{[(u-u')^2 + (2 - e^{-\beta u} - e^{-\beta u'})^2]^{3/2}}$$

$$- \frac{[9(u+u')^2 - 3(2-e^{-\beta u}-e^{-\beta u'})^2][1 + \beta^2 e^{-\beta(u+u')}]}{[(u\ u')^2 + (2-e^{-\beta u}-e^{-\beta u'})^2]^{3/2}}$$

$$- \frac{6}{\sqrt{(u-u')^2 +4}} - \frac{6}{\sqrt{(u+u')^2 + 4}}$$

$$+ \frac{9(u-u')^2 - 12}{[(u-u')^2 + 4]^{3/2}} + \frac{9(u+u')^2 - 12}{[(u+u')^2 + 4]^{3/2}} \Bigg\} \quad du du' \qquad \text{(III-34)}$$

where the $E\!\int\!C$ integration sign means that the core is eliminated from the range of integration by equating terms involving distances of interaction less than a Burgers vector to zero. Each sum of squares in the denominator, for example $(u-u')^2 + (e^{-\beta u}-e^{-\beta u'})^2$ in the first term in (III-34), represents the square of a distance between two elements du and du'. If the square of the distance is equal to or greater than $(b/yo)^2$, since the u's are distances nondimensionalized with respect to yo, then the term is included in the integral. If not, the term is equated to zero.

For the edge dislocation

$$\frac{\Delta E_1}{Gb^2 d_\tau} = - \frac{1}{96\,\pi} \; E\!\!\int_0^\infty\! C \;\; E\!\!\int_0^\infty\! C \left\{ \frac{-8}{\sqrt{(u-u')^2 + (e^{-\beta u}-e^{-\beta u'})^2}} \right.$$

$$\frac{-8}{\sqrt{(u+u')^2 + (e^{-\beta u}-e^{-\beta u'})^2}}$$

$$- \frac{[3(u-u')^2 + 9(e^{-\beta u}-e^{-\beta u'})^2][1 + \beta^2 e^{-\beta(u+u')}]}{[(u-u')^2 + (e^{-\beta u}-e^{-\beta u'})^2]^{3/2}}$$

$$- \frac{[3(u+u')^2 + 9(e^{-\beta u} - e^{-\beta u'})^2][1 - \beta^2 e^{-\beta(u+u')}]}{[(u+u')^2 + (e^{-\beta u} - e^{-\beta u'})^2]^{3/2}}$$

$$+ \frac{11}{\sqrt{(u-u')^2}} + \frac{11}{\sqrt{(u+u')^2}}$$

$$- \frac{10 + 6\beta^2 e^{-\beta(u+u')}}{\sqrt{(u-u')^2 + (z-e^{-\beta u} - e^{-\beta u'})^2}}$$

$$- \frac{10 - 6\beta^2 e^{-\beta(u+u')}}{\sqrt{(u+u')^2 \quad (z-e^{-\beta u} - e^{-\beta u'})^2}} + \frac{10}{\sqrt{(u-u')^2 + 4}}$$

$$+ \frac{10}{\sqrt{(u+u')^2 + 4}} + \frac{36}{\sqrt{[(u-u')^2 + 4]^{3/2}}}$$

$$+ \frac{36}{[(u+u')^2 + 4]^{3/2}}$$

$$- \frac{[3(u-u')^2 - 9(2-e^{-\beta u} - e^{-\beta u'})^2][1 - \beta^2 e^{-\beta(u+u')}]}{[(u-u')^2 + (z-e^{-\beta u} - e^{-\beta u'})^2]^{3/2}}$$

$$+ \frac{[3(u+u')^2 - 9(2-e^{-\beta u} - e^{-\beta u'})^2][1 + \beta^2 e^{-\beta(u+u')}]}{[(u+u')^2 \quad (2-e^{-\beta u} - e^{-\beta u'})^2]^{3/2}}$$

$$- \frac{3(u-u')^2}{[(u-u')^2 + 4]^{3/2}} - \frac{3(u+u')^2}{[(u+u')^2 + 4]^{3/2}} \Bigg\} du\,du' \qquad \text{(III-35)}$$

A tabulation of the results of evaluation of the integrals is given in Tables III-1 and III-2.

Table III-1. Bulk Elastic Energy Screw Constriction

dt/b ↓ β →	.10	.25	.5	.625	.75	1.15	1.5	2.5	3.0	3.5	4.0	4.5
4			6.96		3.63	1.034	-.178		-1.878		-1.940	
8		13.96	6.03		3.00		-.727		-2.98			
16	34.5		5.89		3.16		-.195		-1.94			
32		13.07	6.22		3.78		.895	-.670		-1.58		-2.155
64		13.25		5.44	4.64		2.32			.540		

Table III-2. Bulk Elastic Energy Edge Constriction

$d\tau/b$ \ β	.25	.50	.90	1.00	1.50	2.00	2.50	3.00	3.50	4.00	4.50	5.00
4	15.84	8.28		4.98	3.91			2.61				1.92
8	23.87	12.40		7.26	5.59							
16	27.66	14.52	9.31	8.67	6.69			4.52				
32	29.6	15.77		9.71	7.95			5.83				
64	30.6	16.57		10.71	9.03	8.25	7.76	7.41	7.13	6.76		

APPENDIX IV

Core Traction Energy Calculations

A. The Core Traction Energy of an Edge Dislocation

A straight edge dislocation embedded in the center of a straight cylinder as shown in Fig. (IV-1) may be described in terms

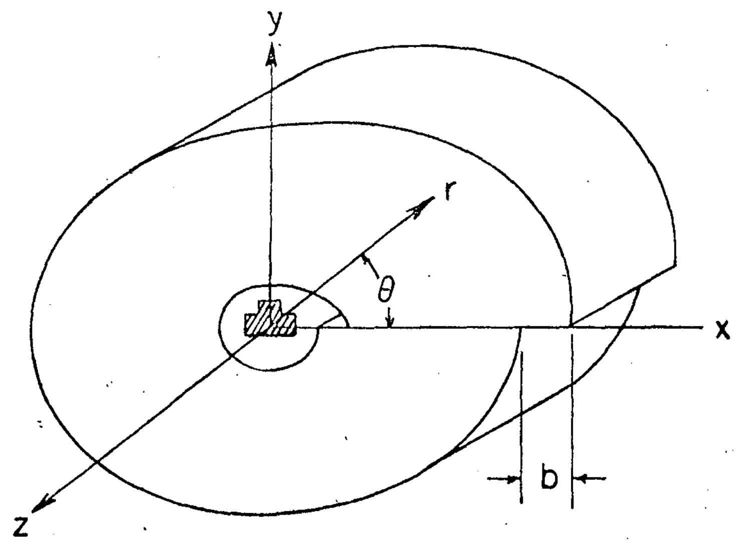


Figure IV-1. Straight Edge Dislocation in Cylinder

of a stress function[20], χ, in terms of which the local stresses, σ_{ij}, may be calculated by differentiation:

$$\begin{bmatrix} \sigma_{rr} & \sigma_{r\theta} & \sigma_{rz} \\ \sigma_{\theta r} & \sigma_{\theta\theta} & \sigma_{\theta z} \\ \sigma_{zr} & \sigma_{z\theta} & \sigma_{zz} \end{bmatrix} = \begin{bmatrix} \frac{1}{r}\frac{\partial\chi}{\partial r} + \frac{1}{r}\frac{\partial^2\chi}{\partial\theta^2} & -\frac{\partial}{\partial r}\frac{1}{r}\frac{\partial\chi}{\partial\theta} & 0 \\ -\frac{\partial}{\partial r}\frac{1}{r}\frac{\partial\chi}{\partial\theta} & \frac{\partial^2\chi}{\partial r^2} & 0 \\ 0 & 0 & -\nu\,(\sigma_{rr} + \sigma_{\theta\theta}) \end{bmatrix} \qquad \text{(IV-1)}$$

The above formulation assumes no displacements (or strains) along the axis of the dislocation. Any χ that is specified must automatically satisfy the equilibrium condition on the stresses.

The stress function characterizing the edge dislocation of Fig. (IV-1) is

$$\chi_o = Dr \ln r \sin\theta \qquad \text{(IV-2)}$$

where

$$D = \frac{Gb}{2\pi(1-\nu)} \qquad \text{(IV-3)}$$

The stresses due to the dislocation may then be calculated to be:

$$[\sigma_{ij}] = \begin{bmatrix} \frac{D \sin\theta}{r} & -\frac{D\cos\theta}{r} & 0 \\ -\frac{D\cos\theta}{r} & \frac{D\sin\theta}{r} & 0 \\ 0 & 0 & -\frac{2\nu D \sin\theta}{r} \end{bmatrix} \qquad \text{(IV-4)}$$

These stresses fall off from a singularity at the origin to zero at infinity and may be considered to represent a dislocation in a cylinder of infinite radius with a "full" core. The elastic energy, E, stored in the stress field of a region between radii r_o and R_a is given by the volume integral

$$E = \frac{1}{2} \int_{r=r_o}^{r=R_c} \sigma_{ij}\sigma_{ij} \, dv \qquad \text{(IV-5)}$$

where ε_{ij}, the local strain, is related to the stress tensor by Hooke's law:

$$\begin{bmatrix} \varepsilon_{rr} & \varepsilon_{r\theta} & \varepsilon_{rz} \\ \varepsilon_{\theta r} & \varepsilon_{\theta\theta} & \varepsilon_{\theta z} \\ \varepsilon_{zr} & \varepsilon_{z\theta} & \varepsilon_{zz} \end{bmatrix} =$$

$$\frac{1}{2G} \begin{bmatrix} \sigma_{rr} - \frac{\nu}{1+\nu}(\sigma_{rr}+\sigma_{\theta\theta}+\sigma_{zz}) & \sigma_{r\theta} & \sigma_{rz} \\ \sigma_{\theta r} & \sigma_{\theta\theta} - \frac{\nu}{1+\nu}(\sigma_{rr}+\sigma_{\theta\theta}+\sigma_{zz}) & \sigma_{\theta z} \\ \sigma_{zr} & \sigma_{z\theta} & \sigma_{zz} - \frac{\nu}{1+\nu}(\sigma_{rr}+\sigma_{\theta\theta}+\sigma_{zz}) \end{bmatrix} \quad \text{(IV-6)}$$

Since the stress tensor may be written

$$[\sigma_{ij}] = \begin{bmatrix} \sigma_{rr} & \sigma_{r\theta} & 0 \\ \sigma_{r\theta} & \sigma_{\theta\theta} & 0 \\ 0 & 0 & \nu(\sigma_{rr}+\sigma_{\theta\theta}) \end{bmatrix} \quad \text{(IV-7)}$$

the strain tensor simplifies to

$$[\varepsilon_{ij}] = \frac{1}{2G} \begin{bmatrix} \sigma_{rr}-\nu(\sigma_{rr}+\sigma_{\theta\theta}) & \sigma_{r\theta} & 0 \\ \sigma_{r\theta} & \sigma_{\theta\theta}-\nu(\sigma_{rr}+\sigma_{\theta\theta}) & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \text{(IV-8)}$$

The energy integral then becomes

$$E = \frac{1}{2} \frac{1}{2G} \int \{\sigma_{rr}[\sigma_{rr} - \nu(\sigma_{rr} + \sigma_{\theta\theta})]$$

$$+ 2\sigma_{r\theta}^{2} + \sigma_{\theta\theta}[\sigma_{\theta\theta} - \nu(\sigma_{rr} + \sigma_{\theta\theta})]\} \, dv$$

$$= \frac{1}{4G} \int \{(1-\nu)(\sigma_{rr}^{\ 2} + \sigma_{\theta\theta}^{\ 2}) - 2\nu\sigma_{rr}\sigma_{\theta\theta}$$

$$+ 2\sigma_{r\theta}^{\ 2}\} \, dv \qquad \text{(IV-9)}$$

Inserting the stresses due to the dislocation stress function:

$$E = \frac{1}{4G} \int \{(1-\nu) \frac{D^2}{r^2} (2 \sin^2\theta)$$

$$- 2\nu \frac{D^2}{r^2} (\sin^2\theta) + 2 \frac{D^2}{r^2} (\cos^2\theta)\} \, dv \qquad \text{(IV-10)}$$

or for a unit length of dislocation

$$E = \frac{D^2}{2G} \int_{r=r_o}^{r=R_c} \int_{\theta=0}^{\theta=2\pi} \frac{1-2\nu\sin^2\theta}{r^2} \, r d\theta dr$$

$$= \frac{\pi D^2}{G} \ln \frac{R_c}{r_o} (1-\nu)$$

$$= \frac{Db}{2} \ln \frac{R_c}{r_o}$$

$$= \frac{Gb^2}{4\pi(1-\nu)} \ln \frac{R_c}{r_o} \qquad \text{(IV-11)}$$

Another stress function, χ_c, may be added to that of the dislocation, χ_o, to remove the effect of the core material by eliminating forces exerted by the core material on the surrounding region, i.e. by eliminating "core tractions". This stress function is

$$\chi_c = \frac{B\sin\theta}{r} \tag{IV-12}$$

where B is a constant.

The stresses associated with χ_c are:

$$[\sigma_{ij}]_c = \begin{bmatrix} \frac{-2B\sin\theta}{r^3} & \frac{2B\cos\theta}{r^3} & 0 \\ \frac{2B\cos\theta}{r^3} & \frac{2B\sin\theta}{r^3} & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{IV-13}$$

which have the proper symmetry to eliminate σ_{rr} and $\sigma_{r\theta}$ on a surface of constant r. As σ_{rz} is already zero and is not affected by χ_c this stress function can be seen to eliminate core tractions when it is seen that the stresses drop off in magnitude and do not influence the stresses at the surface of an infinite cylinder. In passing it should be noted that there exists another stress function of similar stress symmetry that increases in magnitude with r and may be used to eliminate tractions on the surface of a cylinder about the dislocation: this device is used when one wishes to consider a finite cylinder containing a dislocation. For the sake of simplicity we will work with an infinite cylinder, which will not affect the core traction energy term because the surface terms will be negligible in regions of small r, provided R_c, the cylinder diameter is very large.

Thus at r_o, the core surface

$$-\frac{2B\sin\theta}{r_o^{\,3}} + \frac{D\sin\theta}{r_o} = 0 \qquad \text{(IV-14a)}$$

and (equivalently)

$$\frac{2B\cos\theta}{r_o^{\,3}} - \frac{D\cos\theta}{r_o} = 0 \qquad \text{(IV-14b)}$$

which requires that

$$B = \frac{Dr_o^{\,2}}{2} \qquad \text{(IV-15)}$$

The new stress tensor becomes

$$[\sigma_{ij}] = \begin{bmatrix} D\left(\frac{1}{r} - \frac{r_o^{\,2}}{r^3}\right)\sin\theta & D\left(-\frac{1}{r} + \frac{r_o^{\,2}}{r^3}\right)\cos\theta & 0 \\ D\left(-\frac{1}{r} + \frac{r_o^{\,2}}{r^3}\right)\cos\theta & D\left(\frac{1}{r} + \frac{r_o^{\,2}}{r^3}\right)\sin\theta & 0 \\ 0 & 0 & -\frac{2\nu D\sin\theta}{r} \end{bmatrix} \qquad \text{(IV-16)}$$

The stresses are different now that the core has been removed but the expression for the elastic energy of the hollow cylinder in terms of stresses is the same. Hence for the hollow cylinder

$$E_h = \frac{1}{4G}\int \{(1-\nu)\frac{D^2}{r^2}[(1 - \frac{r_o^{\,2}}{r^2}) + (1 + \frac{r_o^{\,2}}{r^2})^2]\sin^2\theta$$

$$- 2\nu \frac{D^2}{r^2} \left[\left(1 - \frac{r_o^{\ 2}}{r^2}\right)\left(1 + \frac{r_o^{\ 2}}{r^2}\right)\right] \sin^2\theta$$

$$+ 2 \frac{D^2}{r^2} [(-1 + \frac{r_o^{\ 2}}{r^2})^2] \cos^2\theta\} \, dv$$

$$= \frac{1}{4G}\int \{(1 - \nu) \frac{D^2}{r^2} [2 + 2 \frac{r_o^{\ 4}}{r^4}] \sin^2\theta$$

$$- 2\nu \frac{D^2}{r^2} [1 - \frac{r_o^{\ 4}}{r^4}] \sin^2\theta$$

$$+ 2 \frac{D^2}{r^2} [1 - \frac{r_o^{\ 2}}{r^2} + \frac{r_o^{\ 4}}{r^4}] \cos^2\theta\} \, dv$$

$$= E + \frac{D^2}{2G}\int \{\frac{r_o^{\ 4}}{r^6} - \frac{2r_o^{\ 2}}{r^4} \cos^2\theta\} \, dv \qquad \text{(IV-17)}$$

The core traction energy, E_2, for a unit length of edge dislocation becomes

$$E_2 = E - E_h = - \frac{D^2}{2G} \int_{\theta=0}^{\theta=2\pi} \int_{r=r_o}^{r=R} \left(\frac{r_o^{\ 4}}{r6} - \frac{2r_o^{\ 2}}{r^4} \cos^2\theta\right) r d\theta dr$$

$$= - \frac{D^2}{2G} \int_{r_o}^{R} 2\pi \left(\frac{r_o^{\ 4}}{r^5} - \frac{r_o^{\ 2}}{r^3}\right) dr$$

$$= - \frac{\pi D^2}{G} \cdot - \left[\frac{r_o^{\ 4}}{4r^4} + \frac{r_o^{\ 2}}{2r^2}\right]_{r_o}^{R}$$

$$= - \frac{\pi D^2}{G} \left[- \frac{1}{4} + \frac{1}{2} \left(\frac{r_o}{R} \right)^2 - \frac{1}{4} \left(\frac{r_o}{R} \right)^4 \right]$$

$$= \frac{\pi D^2}{4G} \left[1 - \left(\frac{r_o}{R} \right)^2 \right]^2 \qquad \text{(IV-18)}$$

$$= \frac{Gb^2}{16\pi(1-\nu)^2} \left[1 - \left(\frac{r_o}{R} \right)^2 \right]^2 \qquad \text{(IV-18)}$$

If $r_o = b$ and $R = 2b$

$$E_2 = [1 - \left(\frac{1}{2} \right)^2]^2 \; (E_2)_{Total} = \frac{9}{16} \; (E_2)_{Total} \qquad \text{(IV-19)}$$

so that a little over half the energy due to the core tractions lies within a Burgers vector of the core surface. This is our justification for treating the energy as localized along the length of a dislocation.

The magnitude of the effect of the core region on the interactions of dislocations is obtained by calculating the percent change in shear stress, $\sigma_{r\theta}$, for $\theta = 0$ when the core is added to a hollow dislocation:

$$\frac{\Delta\sigma_{r\theta}}{\sigma_{r\theta}} = \frac{\sigma - \sigma_n}{\sigma} = \frac{-\frac{D}{r} - \left(-\frac{D}{r} + \frac{Dr_o^{\,2}}{r^3} \right)}{-\frac{D}{r}} = \frac{r_o^{\,2}}{r^3} \qquad \text{(IV-20)}$$

Thus there is an effect of 25% of the magnitude of the hollow core stress at twice the core radius, 11% at three times the core radius, 6% at four times, etc.

If the length of dislocation where the cores of the partial dislocations are closer together than, say, 5 or 6 Burgers vectors is very influential in the constriction energy calculation, then the effect of the core becomes important in the elastic as well as the core energy proper. We assume this effect to be negligible.

Two ways to handle the situation where the core traction stresses cannot be separated from the elastic stress field of the hollow dislocation are:

(1) Describe the dislocation in terms of a distributed dislocation density; this would be equivalent to a three-dimensional generalization of Peierls' calculation[7] of the width of a dislocation. Computer calculations of the configuration of f.c.c. dislocations have been made[18,19] assuming Morse potential interactions. Either a simplifying assumption or extensive analysis of this would be required here.

(2) Integrate the more general form of the Kröner elastic energy expression where the double line integral becomes a quadruple integral involving coordinates of integration normal to the lines.[16] This approach would still involve the assumptions of isotropy and a given dislocation shape; it would probably not be worth the trouble unless one were lucky enough to hit upon some unexpected simplification, say by a clever choice of a dislocation density distribution profile across the dislocation core.

Thus the core traction energy of a curved edge dislocation is taken to be

$$E_2 = \int_{\substack{\text{length of}\\ \text{dislocation}}} \frac{Gb^2_{edge}}{16\pi(1-\nu)^2} |d\ell| \qquad \text{(IV-21)}$$

assuming $R >> r_o$, where $d\ell$ is an increment along the dislocation line. The integral is always positive, not depending on the sign of $d\ell$ as is the case for the Kröner line integrals of which one is the result of an application of Stokes' theorem and the other depends on the relative direction of the Burgers vector.

B. The Core Traction Energy of a Screw Dislocation

When a similar calculation to the above is performed for a screw dislocation, it is found that the core traction energy is zero. Rather than repeat the details of the calculation a physical argument justifying the absence of core traction energy will be given.

In forming a screw dislocation the displacements made are all parallel to the dislocation axis; also the displacements are the same whether the core is empty or full. The only work that screw tractions can do during formation is to provide a frictional force, but not a force that can distort material in the elastic matrix around the core after the dislocation has been formed except for local pinching or stretching on the atomic level, which we neglect, and which would require detailed knowledge of core structure to calculate. Thus we conclude that there is no elastic core traction energy associated with a screw dislocation.

Appendix V

Some Line and Area Integrals

A. Introduction

In order to determine the core and core traction energies associated with a particular constriction configuration it is necessary to evaluate the integrals $\Delta \int b_{edge}^2 \, dl$ and $\Delta \int b_{screw}^2 \, dl$ which represent the change in squares of the edge and screw Burgers vectors associated with a unit length of dislocation line. Later in the analysis a portion of the core is removed to be replaced by a recombined segment. This requires the calculation of the integrals $\int_{-x/2}^{+x/2} b_{edge}^2 \, dl$ and $\int_{-x/2}^{+x/2} b_{screw}^2 \, dl$. It is also necessary to evaluate the change in area of stacking fault, ΔA, that occurs when the constriction is made. These quantities are calculated in this appendix.

B. The Integrals $\Delta \int b_{edge}^2 \, dl$ and $\Delta \int b_{screw}^2 \, dl$

Let the Burgers vector of a partial dislocation be written

$$\vec{b}_p = b_x \vec{i} + b_y \vec{j} \qquad \text{(V-1)}$$

where $\vec{i}$ and $\vec{j}$ are unit vectors along the x and y axes respectively. The tangent vector to the dislocation line is given by:

$$\frac{d\vec{l}}{dl} = \frac{dx \, \vec{i} + dy \, \vec{j}}{dl}$$

and the local screw component is given by:

$$\vec{b}_{screw} = (\vec{b}_p \cdot \frac{d\vec{l}}{dl})\frac{d\vec{l}}{dl}$$

$$= (b_x \frac{dx}{dl} + b_y \frac{dy}{dl})\frac{d\vec{l}}{dl} \qquad \text{(V-3)}$$

The local edge component is

$$\vec{b}_{edge} = \vec{b}_p - \vec{b}_{screw} \qquad \text{(V-4)}$$

and its square is

$$b^2_{edge} = b^2_p + b^2_{screw} - 2\vec{b}_p \cdot \vec{b}_{screw}$$

$$= b^2_p - b^2_{screw}$$

$$= \left(b^2_x + b^2_y\right) - \left[b^2_x \left(\frac{dx}{dl}\right)^2 + b^2_y \left(\frac{dy}{dl}\right)^2 + 2b_x b_y \frac{dx}{dl}\frac{dy}{dl}\right]$$

$$= \left[1 + \left(\frac{dx}{dl}\right)^2\right] b^2_x + \left[1 + \left(\frac{dy}{dl}\right)^2\right] b^2_y + \left[2 \frac{dx}{dl}\frac{dy}{dl}\right] b_x b_y \qquad \text{(V-5)}$$

Consequently:

$$\Delta \int b^2_{edge}\, dl = \int \left\{ \left[1 - \left(\frac{dx}{dl}\right)^2\right] b_x^2 + \left[1 - \left(\frac{dy}{dl}\right)^2\right] b_y^2 \right.$$

$$\left. - \left[2\,\frac{dx}{dl}\,\frac{dy}{dl}\right] b_x b_y \right\} dl - \left\{ \left[1 + 1^2\right] b_x^2 + \left[1 + 0^2\right] b_y^2 \right.$$

$$\left. + [2(1 \cdot 0]\, b_x b_y \right\} dx$$

$$= \int \left\{ \left[1 - 2\,\frac{dx}{dl} - \left(\frac{dx}{dl}\right)^2\right] b_x^2 + \left[1 - \left(\frac{dy}{dl}\right)^2\right] b_y^2 \right.$$

$$\left. - \left[2\,\frac{dx}{dl}\,\frac{dy}{dl}\right] b_x b_y \right\} dl \qquad \text{(V-6)}$$

Similarly

$$\Delta \int b^2_{screw}\, dl = \int \left\{ \left[b_x^2 \left(\frac{dx}{dl}\right)^2 + b_y^2 \left(\frac{dy}{dl}\right)^2 \right. \right.$$

$$\left. + 2b_x b_y\,\frac{dx}{dl}\,\frac{dy}{dl} \right] dl - \left[b_x^2 \cdot 1^2 + b_y^2 \cdot 0^2 \right.$$

$$\left. \left. + 2b_x b_y \cdot 1 \cdot 0 \right] dx \right\}$$

$$= \int \left\{ \left[\left(\frac{dx}{dl}\right)^2 - \frac{dx}{dl} \right] b_x^2 + \left(\frac{dy}{dl}\right)^2 b_y^2 \right.$$

$$\left. + \left[2\,\frac{dx}{dl}\,\frac{dy}{dl}\right] b_x b_y \right\} dl \qquad \text{(V-7)}$$

In performing the integration one must remember to integrate over <u>all</u> of the partial dislocation lines between $-\infty$ and $+\infty$. Letting

$$P = \ln \frac{4}{\beta^2} \left(\frac{\sqrt{1 + \beta^2} - 1}{\sqrt{1 + \beta^2} + 1} \right) \qquad \text{(V-8)}$$

$$Q = \frac{\sqrt{1 + \beta^2} - 1}{\beta} \qquad \text{(V-9)}$$

the evaluated integrals are:

For the edge constriction

$$\Delta \int b^2_{edge}\, dl = \frac{b^2 d_\tau}{12} [3P + 2Q] \qquad \text{(V-10)}$$

$$\Delta \int b^2_{screw}\, dl = \frac{b^2 d_\tau}{12} [P + 6Q] \qquad \text{(V-11)}$$

For the screw constriction

$$\Delta \int b^2_{edge}\, dl = \frac{b^2 d_\tau}{12} [P + 6Q] \qquad \text{(V-12)}$$

$$\Delta \int b^2_{screw}\, dl = \frac{b^2 d_\tau}{12} [3P + 2Q] \qquad \text{(V-13)}$$

C. The Integrals $\int_{-x/2}^{+x/2} b^2_{edge}\, dl$ and $\int_{-x/2}^{+x/2} b^2_{screw}\, dl$

Recalling Equations (V-3) and (V-5)

$$\int_{-x/2}^{+x/2} b^2_{edge}\, dl = \int_{-x/2}^{+x/2} \left\{ \left[1 - \left(\frac{dx}{dl}\right)^2 \right] b_x^2 + \left[1 - \left(\frac{dy}{dl}\right)^2 \right] b_y^2 \right.$$

$$- 2\left[\frac{dx}{dl}\frac{dy}{dl}\right] b_x b_y \Big\} dl \qquad (V-14)$$

and

$$\int_{-x/2}^{+x/2} b^2_{screw}\, dl = \int_{-x/2}^{+x/2} \left\{ \left[\left(\frac{dx}{dl}\right)^2\right] b_x^2 + \left[\left(\frac{dy}{dl}\right)^2\right] b_y^2 \right.$$

$$\left. + \left[2\,\frac{dx}{dl}\frac{dy}{dl}\right] b_x b_y \right\} dl \qquad (V-15)$$

One must be careful to integrate over all the partial dislocation lines between $-x/2$ and $+x/2$.

Defining

$$T = \frac{1}{\beta}\ \ln\left(\frac{\sqrt{1+\beta V} + 1}{\sqrt{1+\beta^2} + 1}\right)\left(\frac{\sqrt{1+\beta^2} - 1}{\sqrt{1+\beta V} - 1}\right) \qquad (V-16)$$

$$U = \frac{\sqrt{1+\beta^2} - \sqrt{1+\beta V}}{\beta} \qquad (V-17)$$

where

$$V = \beta\, e^{-\frac{\beta x}{y_o}} \qquad (V-18)$$

the evaluated integrals are:

For the edge constriction:

$$\int_{-x/2}^{+x/2} b^2_{edge}\, dl = \frac{b^2 d_T}{12}\,[3T + 2U] \qquad (V-19)$$

$$\int_{-x/2}^{+x/2} b^2_{screw}\, dl = \frac{b^2 d_\tau}{12} [T + 6U] \qquad (V\text{-}20)$$

For the screw constriction:

$$\int_{-x/2}^{+x/2} b^2_{edge}\, dl = \frac{b^2 d_\tau}{12} [T + 6U] \qquad (V\text{-}21)$$

$$\int_{-x/2}^{+x/2} b^2_{screw}\, dl = \frac{b^2 d_\tau}{12} [3T + 2U] \qquad (V\text{-}22)$$

In contrast to the energy differences calculated in Eqs. (V-10) to (V-13), which remain finite, these energy terms go to infinity at the limit where x goes to ∞ and V goes to zero.

D. The Stacking Fault Area

The stacking fault area change upon constriction may be decomposed into two parts for convenience: (1) the area change when the stacking fault is considered to extend to the centerline of the partials, ΔA_1, and (2) the area change necessary to exclude the stacking fault from the core region, ΔA_2. The stacking fault area change, ΔA, may then be written:

$$\Delta A = \Delta A_1 + \Delta A_2 \qquad (V\text{-}23)$$

ΔA_1 is shown in Fig. V-1. It is easily calculated.

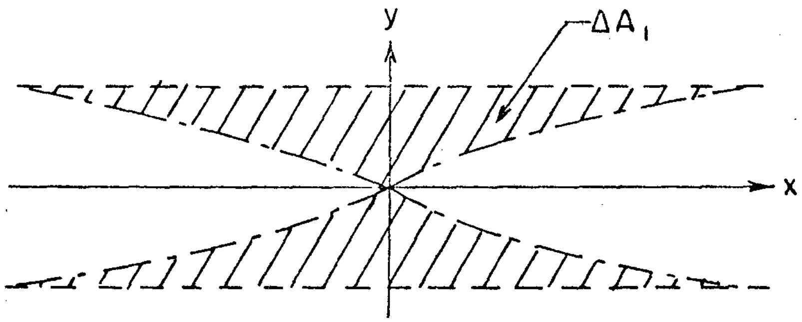


Figure V-1. Stacking Fault Area Change Including Stacking Fault Between Partial Centerlines and Core Boundary.

$$\Delta A_1 = -4\int_0^{y_o} x\,dy$$

$$= -4\int_0^{y_o} -\frac{y_o}{\beta}\ln\left(1-\frac{y}{y_o}\right)\,dy$$

$$= -\frac{4y_o^{\,2}}{\beta} = -\frac{d_\tau^{\,2}}{\beta} \qquad \text{(V-24)}$$

The sign is negative because the area of the stacking fault decreases when the constriction is produced.

The stacking fault contained in the core is shown in Fig. V-2.

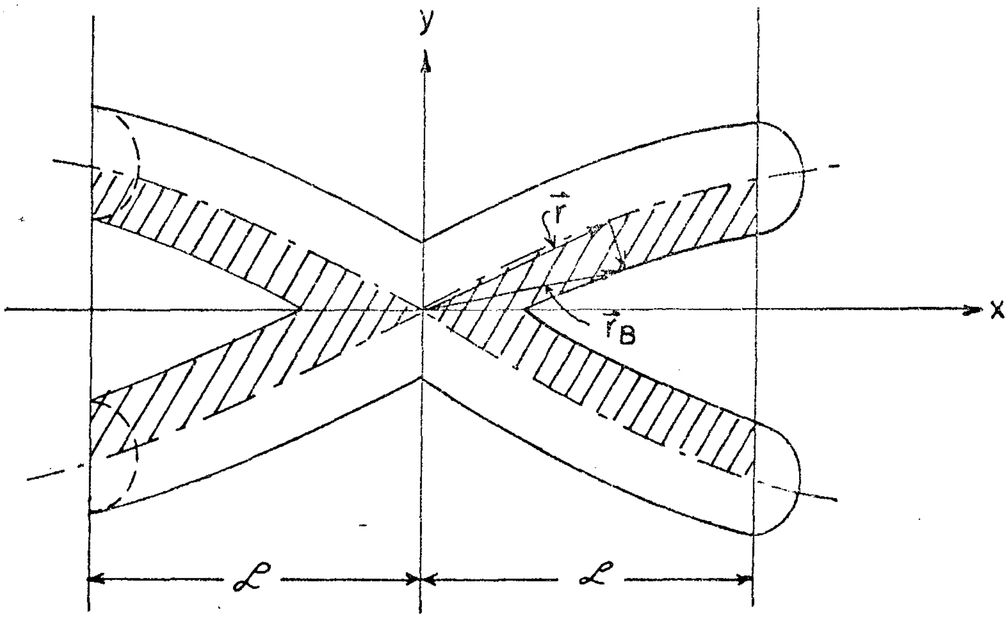


Figure V-2. Stacking Fault Contained in Cores of Partial Dislocations

Let the initial area of stacking fault within the core in a region $x = -\mathcal{L}$ to $x = +\mathcal{L}$ about the constriction be A_I and let the area of stacking fault in the core of the constricted dislocation within the same region be A_{II}. Then

$$\Delta A_2 = \lim_{\mathcal{L}\to\infty} (A_{II} - A_I) \qquad \text{(V-25)}$$

A_I is easy to calculate

$$A_I = 4b\mathcal{L} \qquad \text{(V-26)}$$

but A_{II} requires further computation.

The vector to a point on the centerline of the partial in the positive quadrant is given by:

$$\vec{r} = x\vec{i} + y\vec{j}$$

$$= x\vec{i} + y_o(1 - e^{-\frac{\beta x}{y_o}})\,\vec{j} \qquad \text{(V-27)}$$

The vector to a point on the inner boundary of the core is given by

$$\vec{r}_B = \vec{r} + b\left\{\frac{\frac{d^2\vec{r}}{ds^2}}{\left|\frac{d^2 r}{ds^2}\right|}\right\}$$

$$= \left[x + \frac{b\beta e^{-\frac{\beta x}{y_o}}}{\sqrt{1 + \beta^2 e^{-\frac{2\beta x}{y_o}}}}\right]\vec{i}$$

$$+ \left[y_o(1 - e^{-\frac{\beta x}{y_o}}) - \frac{b}{\sqrt{1 + \beta^2 e^{-\frac{2\beta x}{y_o}}}}\right]\vec{j} \qquad \text{(V-28)}$$

where use was made of a Frenet-Serret formula to obtain a unit normal to the centerline curve.

Then

$$A_{II} = 4\int_{x=0}^{x=\ell} y_o(1 - e^{-\frac{\beta x}{y_o}})\; dx$$

$$x + \frac{b\beta e^{-\frac{\beta x}{y_o}}}{\sqrt{1 + \beta^2 e^{-\frac{\beta x}{y_o}}}} = \mathcal{L}$$

$$- 4 \int \left[y_o(1 - e^{-\frac{\beta x}{y_o}}) - \frac{b}{\sqrt{1 + \beta^2 e^{-\frac{2\beta x}{y_o}}}} \right] d \left[x + \frac{b\beta e^{-\frac{\beta x}{y_o}}}{\sqrt{1 + \beta^2 e^{-\frac{2\beta x}{y_o}}}} \right]$$

$$y_o(1 - e^{-\frac{\beta x}{y_o}}) - \frac{b}{\sqrt{1 + \beta^2 e^{-\frac{2\beta x}{y_o}}}} = 0 \qquad \text{(V-29)}$$

Integrating and taking the limit one gets:

$$\Delta A_2 = - \frac{4y_o b}{\beta} \left\{ \frac{y_o}{b} \left[1 - \frac{V}{\beta} + (1 - \frac{b}{y_o}) \ \ln \ \frac{V}{\beta} \right] \right.$$

$$+ 1 + \ln \ (\frac{1 + \sqrt{1 + V^2}}{2}) - \frac{1 + \beta V}{\sqrt{1 + V^2}}$$

$$\left. + \frac{\beta}{2} \ \frac{b}{y_o} \left[\tan^{-1} V + \frac{V}{1 + V^2} \right] \right\} \qquad \text{(V-30)}$$

where $V(= \beta e^{-\frac{\beta x}{y_o}})$ is the root of the equation

$$V^4 - 2\beta V^3 + (1 + \beta^2)V^2 - 2\beta B$$

$$+ \beta^2(1 - \frac{b^2}{y_o^2}) = 0 \qquad \text{(V-31)}$$

nearest to and less than β.

Appendix VI

Size of Overlap Region

In Appendix V a vector following the inner edge of the core of the partial dislocation in the positive quandrant was derived:

$$\vec{r}_B = \left[x + \frac{b\beta e^{-\frac{\beta x}{y_o}}}{\sqrt{1 + \beta^2 e^{-\frac{2\beta x}{y_o}}}} \right] \vec{i}$$

$$+ \left[y_o(1 - e^{-\frac{\beta x}{y_o}}) - \frac{b}{\sqrt{1 + \beta^2 e^{-\frac{2\beta x}{y_o}}}} \right] \vec{j} \qquad \text{(V-28)}$$

The overlap region ends when the end of $\vec{r}_B$ just touches the x-axis. Defining x' as the x at which this occurs then

$$y_o(1 - e^{-\frac{\beta x'}{y_o}}) - \frac{b}{\sqrt{1 + \beta^2 e^{-\frac{2\beta x}{y_o}}}} = 0 \qquad \text{(VI-1)}$$

or defining

$$x' = -\frac{y_o}{\beta} \ln \frac{V}{\beta} \qquad (31)$$

$$V^4 - 2\beta V^3 + (1 + \beta^2)V^2 - 2\beta V + \beta^2(1 - \frac{b^2}{y_o^2}) = 0 \qquad (32)$$

Since x' must be positive only roots such that $V < \beta$ are acceptable, and since $V \simeq \beta$ (and $x' \simeq 0$) for large β, the solution of Eq. (32) giving physically acceptable behavior is that just below β. This solution may be found by computer by starting evaluations of the polynomial at β and then decreasing β until the sign of the polynomial changes; any desired accuracy may be obtained by backing off to the point just before the sign change and proceeding again with a finer β interval.

APPENDIX VII

Minimization Curves

Figures VII-1 through VII-4 show plots of constriction energy vs. the β-parameter. The minima of the energy curves are taken as the equilibrium values of the constriction energy.

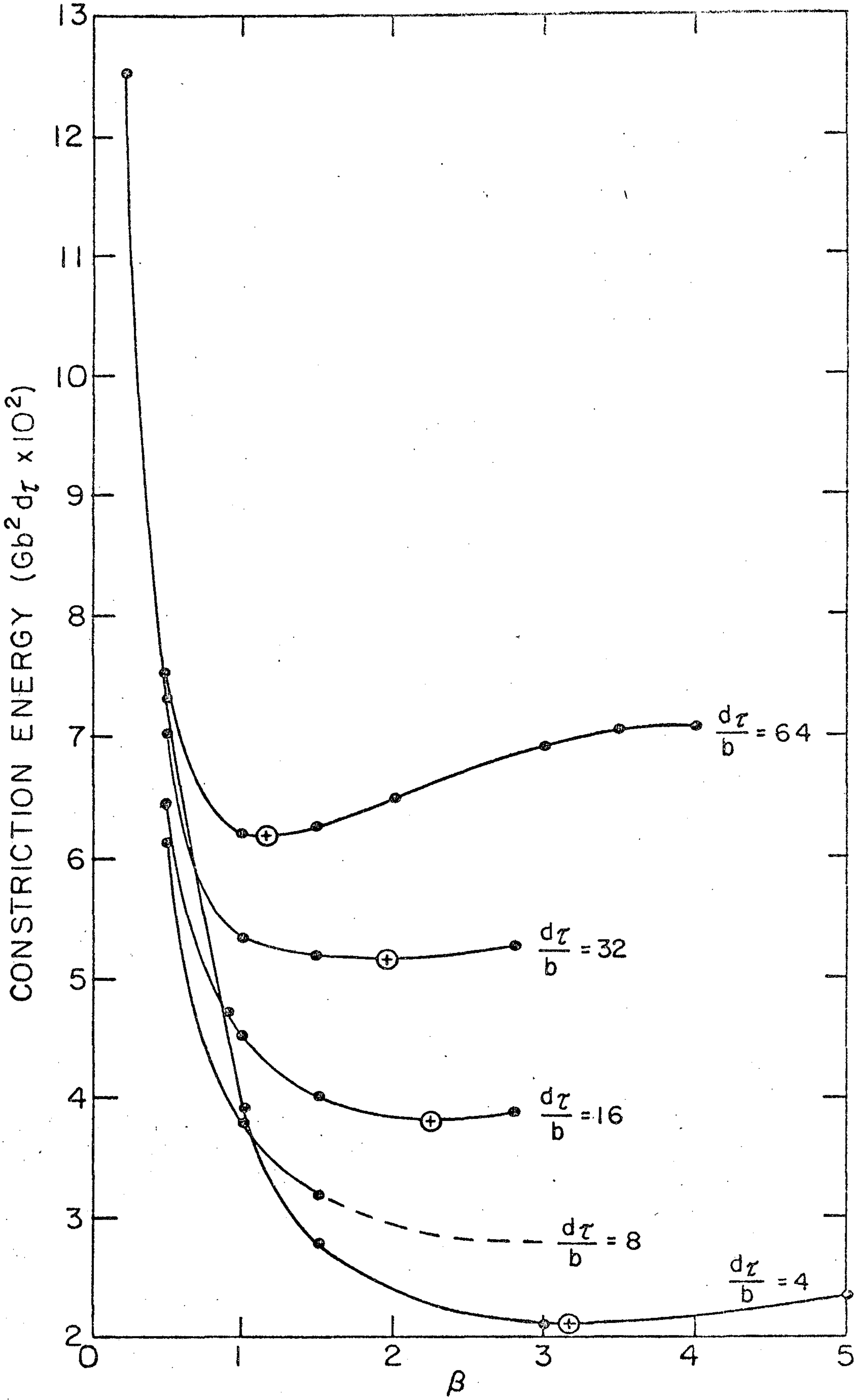


FIG. VII - I CONSTRICTION ENERGY vs. β PARAMETER.
EDGE CONSTRICTION $\alpha_c = 1.5$, $f = 0.3$.

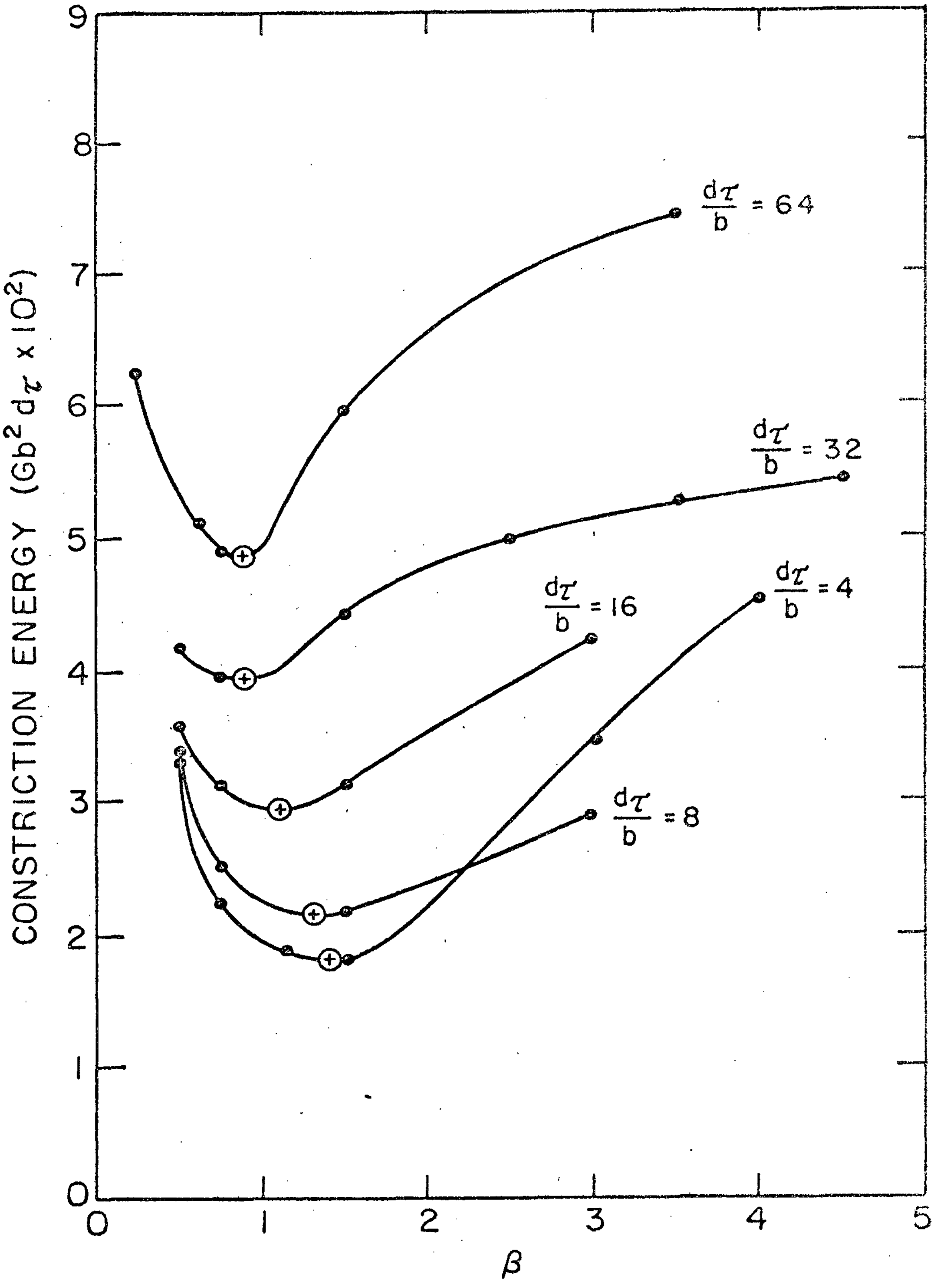


FIG. VII-2 CONSTRICTION ENERGY vs. β PARAMETER.
SCREW CONSTRICTION α_c=1.5, f=0.3.

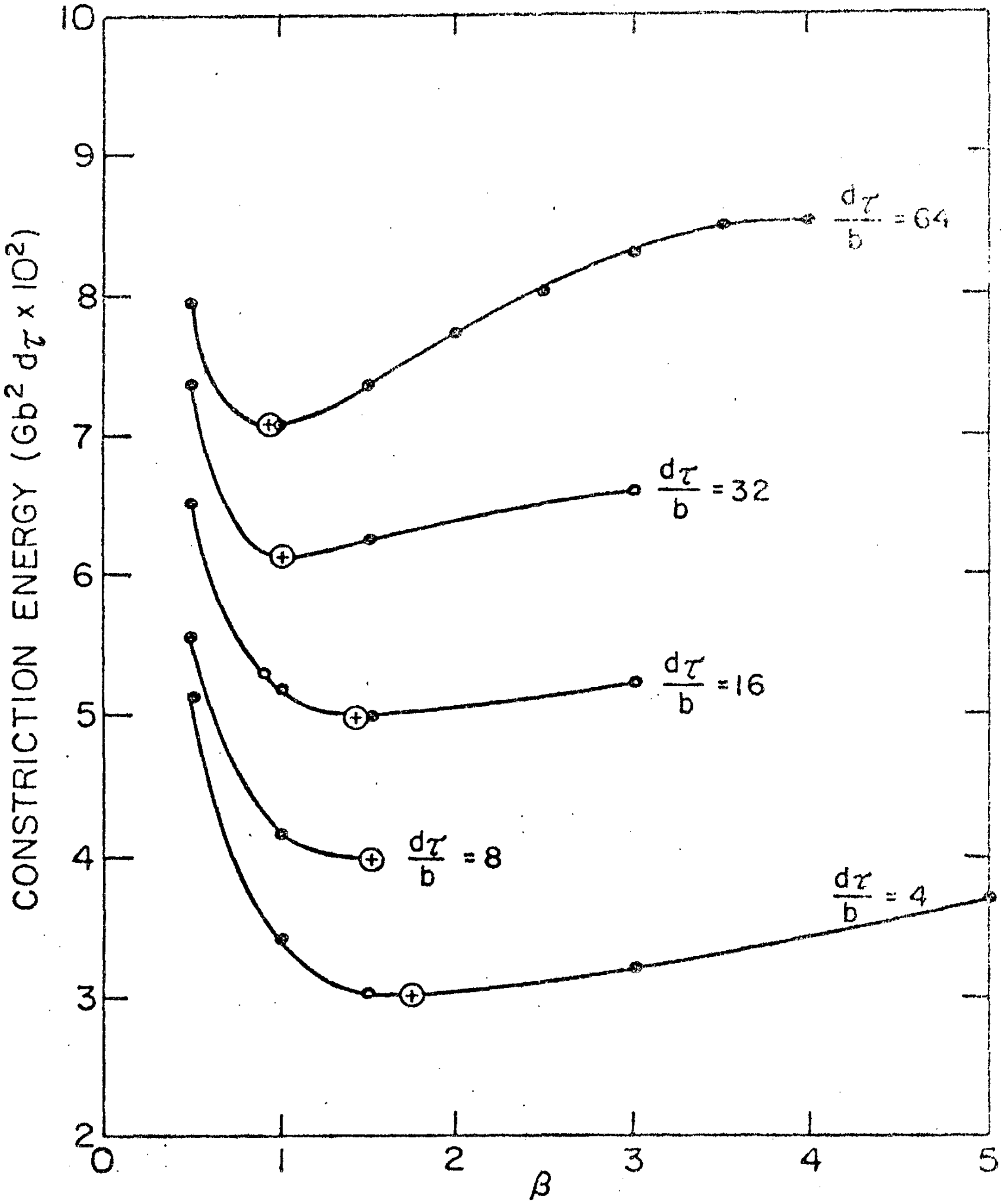


FIG. VII-3 CONSTRICTION ENERGY vs. β PARAMETER.
EDGE CONSTRICTION α_c=1.0, f=1.0

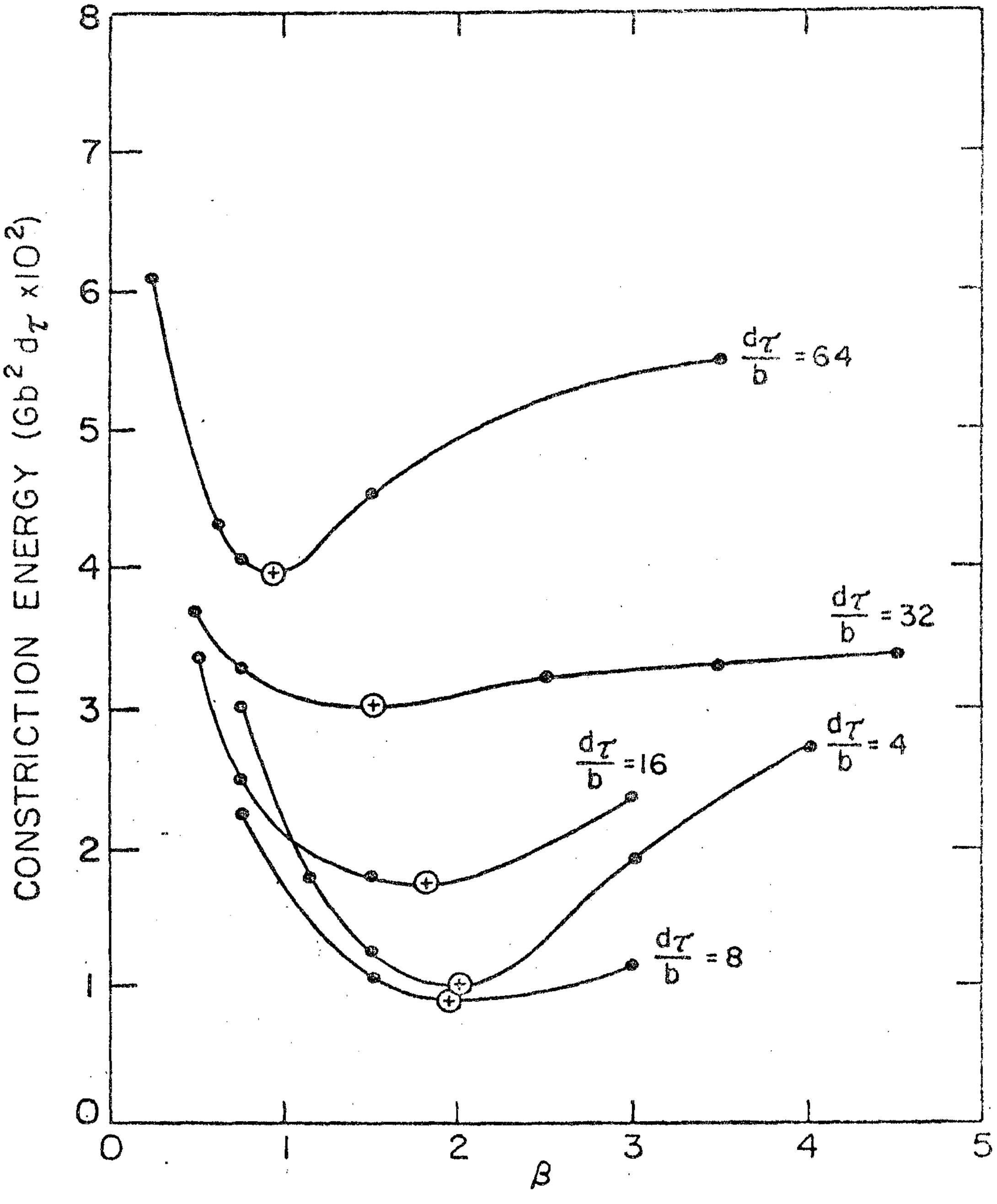


FIG. VII-4 CONSTRICTION ENERGY vs. β PARAMETER.
SCREW CONSTRICTION α_c = 1.0, f = 1.0.

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