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CORE TRACTION CONTRIBUTION TO JOG STRAIN ENERGIES

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CORE TRACTION CONTRIBUTION TO JOG STRAIN ENERGIES

In a previous calculation[1] based on the method of Kröner[2] we determined the energy of jogs in several types of undissociated dislocations. Through the work of Bullough and Foreman[3] it has come to our attention that a correction neglected in the Kröner formulation should be made to account for an additional core traction energy. This correction has been made as described below and the results are given in Table 1. The reader will notice that the α factors in the suggested core energy forms have been defined in a slightly different manner here than in our previous work in order to preserve the simple forms of the total jog energy expressions.

Kröner's method of determining the energy of a dislocation loop involves the evaluation of a double line integral. The line integral arises out of the volume integral for the energy of an elastically strained body

$$* \qquad E = \frac{1}{2} \int_v \sigma_{ij} \, \varepsilon_{ij} \, dv \qquad (1)$$

where E is the energy of the elastic material contained in volume v, an element dv being subject to the stress σ_{ij} and strain ε_{ij}. The above integral can be converted to an area integral through the relations

$$\varepsilon_{ij} = \frac{1}{2} \; \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \qquad (2)$$

*The convention of summing on repeated indices is used throughout this paper.

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

plus the divergence theorem giving

$$E = \frac{1}{2} \int_A \sigma_{ij} u_j dA_i \tag{4}$$

where A represents the area of a cut in the body on which elemental forces $dF_j = \sigma_{ij} dA_i$ act over local displacements u_j. By making a plane cut over a surface A, displacing the surfaces relatively by $u_j = b_j$, and rewelding the surfaces, a dislocation loop is produced. To avoid infinite stresses (and infinite E) in the theoretical body, a core region similar to a wormhole following the boundary of A must be cut out. If the surface of the core volume, A_c, is stress free, one can ignore this surface and integrate only over the surface area A in Eq. (4) to obtain the integral

$$E = \frac{1}{2} b_j \int_{A_i} \sigma_{ij} dA_i \tag{5}$$

for the energy of a hollow-cored dislocation loop. Next for σ_{ij} is inserted an expression

$$\sigma_{ij} = -2G\epsilon_{ikl} \epsilon_{jmn} \frac{\partial^2}{\partial x_k \partial x_m} (\chi_{ln} + \frac{\nu}{1-\nu} \chi_{pp} \delta_{ln}) \tag{6}$$

where 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 then

$$\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = 1$$
$$\epsilon_{132} = \epsilon_{321} = \epsilon_{213} = -1$$

δ_{ln} is a Kronecker delta defined such that it is one when $l = n$ and zero when $l \neq n$, G and ν are the shear modulus and Poisson's ratio for the material, and χ_{ln} is a stress function, a generalization of the scalar potential, chosen by Kröner for convenience. Kröner, and here is his unique contribution, expresses the stress function in terms of a dislocation density

$$\chi_{ln} = \frac{1}{8\pi} \left(\int_{v'} \epsilon_{nrs} \, \alpha_{ls} \, (r') \, \frac{\partial R}{\partial x_r} \, dv' \right)^S \tag{7}$$

where R is the distance $\sqrt{x'^2 + y'^2 + z'^2}$ from the coordinate origin at which we are evaluating χ_{ln}, α_{ls} (r') is a dislocation density such that upon completing a Burgers' circuit about a local area element dA_l the closure failure is $db_s = \alpha_{ls} \, dA_l$ and the $(\ )^S$ means that only the symmetrical part of the tensor is to be taken. If the energy of a dislocation loop is to be calculated one can write

$$\alpha_{ls} \, (r') \, dv' = [\alpha_{ks}(r') dA'_k] \, dl'_l$$

*

$$= b'_s \, dl'_l \tag{8}$$

where in essence the core volume is expressed as a core area dA'_k normal to the dislocation line times a length element dl'_l along the dislocation, and the Burgers' vector of the dislocation, b'_s, is obtained through integration of the dislocation density over the core area. One of the line integrations is due to this term involving dl'_l.

When Eqs. (6), (7) and (8) are inserted into Eq. (5), it should be noted that a product of three permutation symbols results under the area

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*$\alpha_{ks}(r')$ is regarded as so large in the core so that its product with the infinitesimal core area dA'_k is finite.

integral. Two can be eliminated by the relation

$$\varepsilon_{jmn}\,\varepsilon_{nrs} = \delta_{jr}\,\delta_{ms} - \delta_{mr}\,\delta_{js} \tag{9}$$

and the third vanishes by application of Stokes' theorem:

$$\int_{A_i} \varepsilon_{ikl}\,\frac{\partial T}{\partial x_k}\,dA_i = \oint_l T dl_l \tag{10}$$

The end result is the energy of a dislocation loop

$$* \quad E = -\frac{G}{8\pi}\,b_i b_j' \oint_l \oint_{l'} \frac{\partial}{\partial x_k}\frac{\partial R}{\partial x_k}\,[dl_j\;dl_i + \frac{2\nu}{1-\nu}\,dl_i'\;dl_j] +$$

$$\frac{2\nu}{1-\nu}\,[\frac{\partial}{\partial x_j}\frac{\partial R}{\partial x_i} - \delta_{ij}\,\frac{\partial}{\partial x_i}]\;dl_k'\;dl_k \tag{11}$$

where $R^2 = (x_i' - x_i)(x_i' - x_i)$. To get the above expression the relation

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

was used. Equation (11) was used alone to evaluate jog energies in the previous work of the authors.

If one wishes now to treat a dislocation containing core material instead of a hollow dislocation, it is not sufficient merely to add the energy contained in the core. The effect of the core tractions on the

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*The summation convention applies to derivatives as well as products, so

$$\frac{\partial}{\partial x_i}\left(\frac{\partial R}{\partial x_i}\right) = \frac{\partial^2 R}{\partial x_1^2} + \frac{\partial^2 R}{\partial x_2^2} + \frac{\partial^2 R}{\partial x_3^2}, \text{ etc.}$$

core surface which were ignored in the previous analysis, must be included in the calculation of the elastic energy of the material around the dislocation. An exact calculation of the effect of core tractions requires a knowledge of the core stress-deformation relation, but the core traction energy may be approximated by calculating the energy difference for the material outside the core of a cylindrical dislocation with and without a stress function that eliminates the tractions on the core surface. The stress functions to which we refer are treated by Cottrell.[4] It is assumed that the energy is so localized near the core that it is the same per unit length of dislocation for a curved dislocation. The resultant core traction energy is

$$E_{CT} = \frac{G}{16\pi(1-\nu)^2} \int_l b^2_{edge} \; d(\text{length of edge dislocation}) \qquad (13)$$

It is noteworthy that there is no core traction energy associated with a screw type dislocation. Addition of the results of Eq. (13) to those of Eq. (11) constitutes the core traction while Eq. (13) is our equation for the core traction energy. This correction is calculated somewhat differently by Bullough and Foreman due to their different integration technique, which involves integrating over slightly separated lines and depends upon the relative position of the lines chosen. Our technique is to integrate twice over the same line eliminating "self-interaction" of segments by putting appropriate limits on the integrals.

Even when the Kröner calculation is supplemented by the core traction energy term further uncertainty exists in the energy calculation when the change in energy of a deformed loop is to be calculated. The calculation of the elastic energy involves only the energy of elastically deformed material outside the core. If the loop is deformed the core volume changes, and a rise in core volume acts to reduce the energy of the material outside the core by removing initially strained material. It is to this phenomenon that the negative èlastic energy for a screw jog (see Table I) with $\zeta = a = b$ is atrributed. When the core energy (i.e. the energy of the contents of the core) is included none of the energies listed should be negative.

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TABLE I. JOG SELF ENERGIES

Dislocation Type	Frank	Edge	Screw
Elastic Energy*	$\frac{Gb_1^2}{4\pi(1-\nu)} [\ln \frac{a}{\zeta} + 2 (\frac{\zeta}{a}-1) + \frac{1}{4(1-\nu)}]$	$\frac{Gb_2^2 a}{4\pi} [\ln \frac{a}{\zeta} + \frac{(2\frac{\zeta}{a}-1)-\nu(\frac{\zeta}{a}-1)}{1-\nu}]$	$\frac{Gb_3^2 a}{4\pi(1-\nu)} [\ln \frac{a}{\zeta} + (2-\nu)(\frac{\zeta}{a}-1) - \frac{3-4\nu}{4(1-\nu)}]$
Suggested Core Energy Form	$\frac{Gb_1^2 a}{4\pi(1-\nu)} [\ln \frac{\zeta}{b}-2 (\frac{\zeta}{a}-1) - \frac{1}{4(1-\nu)} + \alpha_F]$	$\frac{Gb_2^2 a}{4\pi} [\ln \frac{\zeta}{b} - \frac{(2\frac{\zeta}{a}-1) - \nu (\frac{\zeta}{a}-1)}{(1-\nu)} + \alpha_E]$	$\frac{Gb_3^2 a}{4\pi} [\ln \frac{\zeta}{b} - (2-\nu)(\frac{\zeta}{a}-1) + \frac{3-4\nu}{4(1-\nu)} + \alpha_S]$
Core Traction Energy	$\frac{Gb_1^2 a}{16\pi(1-\nu)^2}$	0	$\frac{Gb_3^2 a}{16\pi(1-\nu)^2}$
Total Jog Energy	$\frac{Gb_1^2 a}{4\pi(1-\nu)} \ln (\frac{a}{b} e^{\alpha_F})$	$\frac{Gb_2^2 a}{4\pi} \ln (\frac{a}{b} e^{\alpha_E})$	$\frac{Gb_3^2 a}{4\pi(1-\nu)} \ln (\frac{a}{b} e^{\alpha_S})$

*ζ is of the order of magnitude of b.