Thermal Disorder in a Dislocation Core and its Effect on Damping*

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It is postulated that, at elevated temperatures, the core of a dislocation consists of a thermally disordered quasiliquid region, whose size increases with temperature. Calculations based on the effect of the disordering in relieving elastic stresses indicate that a flat strip core should be favored. A moving dislocation of this form will experience two distinct damping forces. One is thermodynamic, caused by the heat of disordering, and is analogous to the thermoelastic damping produced by the dislocation stress field; while the other is viscous, caused by the shear between the two sides of the strip. The calculated magnitudes of both of these damping forces in covalent and metallic crystals are comparable with those required to explain internal friction observations, although a positive demonstration of the validity of the mechanisms cannot be made on the basis of present data.

INTRODUCTION

A DISLOCATION moving through a crystal experiences a damping force, the magnitude of which depends on the dislocation velocity. Measurements of this damping force must be made indirectly and interpretation of the experiments is often open to doubt. It is generally supposed, however, that for small velocities, corresponding to values of the applied shear stress that are small compared to the shear modulus, the damping force is proportional to the velocity. This is the region which will be of interest in this paper.

Theoretically it is found that the nature of the damping force depends very strongly on the type of model assumed for the dislocation. This dependence is particularly sensitive to the structure of the dislocation core, where the Hooke's law approximation breaks down. The simplest model considers the core to be of very small radius and to move as an approximately straight cylinder. If the remainder of the crystal is treated as a continuum exhibiting linear elastic behavior, the only forces are those acting through the long-range stress field of the dislocation. Thermoelastic damping was treated by Eshelby[1] using this model in conjunction with a classical macroscopic thermodynamic method of calculation. If, in addition, nonlinear elastic effects occur near the core, interaction with thermal vibrations will occur. The periodic nature of the crystal can be taken into account by considering the dislocation core to be affected by a periodic Peierls stress field. Leibfried[2] and Nabarro[3] considered such a model, assuming that acoustic waves were scattered by a straight dislocation moving through the lattice without change of form.

A further improvement in the model is made by considering that the dislocation core does not move in the Peierls field as a straight segment, but rather proceeds by the formation and lateral motion of kinks.[4] The main sources of damping are then the energy losses experienced in thermal activation of kinks and the damping of the individual kinks. At low temperatures the damping is caused by the diffusion of built-in kinks (kinks necessitated by the geometry of the dislocation[5]); as the temperature is raised a little the thermal activation of kinks becomes important.[6–10] It appears logical to use discrete kink models at these moderately low temperatures. As the temperature becomes higher, however, the kink density becomes large and kink interactions become frequent. Eventually so much interaction occurs that one can no longer identify individual kinks. In this situation it is better to treat the entire region of the dislocation occupied by kinks as a disordered region of the crystal, and to consider this region as the dislocation core.

Such a model of the dislocation is discussed in this paper. It is assumed that the disorder in the dislocation core is very similar to that found in the liquid state, while the crystal outside the core is treated as a solid isotropic elastic continuum. There are then two separate sources of energy loss which originate at the core of the moving dislocation; one thermodynamic, due to the heat of disordering of the material passing through the dislocation core, and the other viscous, due to the shear rate of the disordered material. In the next section we calculate the size of the disordered region. Following sections then contain calculations of the magnitudes of the two types of damping, and a discussion of the applicability of the theory to experiment.

EQUILIBRIUM SIZE OF DISORDERED CORE

An immediate indication that disordering must occur in the core of a dislocation near the melting point is

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[1] J. D. Eshelby, Proc. Roy. Soc. (London) **A197**, 396 (1949).
[2] G. Leibfried, Z. Physik **127**, 344 (1950).
[3] F. R. N. Nabarro, Proc. Roy. Soc. (London) **A209**, 278 (1951).
[4] W. T. Read, Jr., *Dislocations in Crystals* (McGraw-Hill Book Company, Inc., New York, 1953), p. 46.
[5] A. D. Brailsford, Phys. Rev. **122**, 778 (1961).
[6] J. Lothe and J. P. Hirth, Phys. Rev. **115**, 543 (1959).
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obtained by considering the lowering of the melting point of the material as a consequence of hydrostatic pressure produced by the stress field of an edge dislocation. In a purely elastic and isotropic material, the pressure within an off-axis cylinder of diameter r will exceed $Gb/2\pi r(1-\nu)$, where G is the shear modulus, b the Burgers vector, and ν Poisson's ratio. The sign depends on whether the cylinder lies above or below the glide plane. If one now applies the Clapeyron equation for melting of bulk material, the melting point will be depressed in the positive pressure region for a material that contracts on melting, or in the tension region if the material expands. For example, in silicon, a material which has geometrically well-defined dislocations at low temperatures, a region of diameter of the order 10 Å will have its melting point suppressed more than 10% (170°C). In this paper we will refer to the region which becomes melted or disordered as the "core." In reality the core will not retain a cylindrical shape, since the material there will not be able to support shear stresses, and hence redistribution of the general stress pattern will occur, favoring a different core shape.

The exact method of calculating the core size would be to consider the free energy of the whole dislocation and then minimize this. Such a calculation would be very elaborate, involving a continuously decreasing disorder at increasing distances from the center. A more limited model is considered here, in which the core is taken to be a single phase, uniformly disordered, immediately surrounded by ideally elastic material. The core size may now be derived in a manner analogous to that employed for the standard Clapeyron equation.

Consider the core to have fixed, but arbitrary, shape and variable size. Denote the core size by a parameter ρ, having dimensions of length. The independent thermodynamic variables are then ρ and the temperature T. Initially it is supposed that the core is acted upon by an arbitrary stress field, whose net effect will be represented by a parameter p, conjugate to ρ, which may be thought as of analogous to a pressure which produces melting point depression. Take a boundary immediately surrounding the core, of dimension ρ_0, and let the internal energy of the total material within the boundary be $U(\rho,T)$. Then the heat entering through the boundary, in any general change, will be

$$dQ=dU+dW=(\partial U/\partial T)dT+(\partial U/\partial\rho)d\rho+pd\rho. \quad (1)$$

If these changes take place reversibly, the entropy change dQ/T will be a perfect differential. Hence,

$$(\partial U/\partial\rho)+p=T(\partial p/\partial T). \quad (2)$$

A change $d\rho$ involves the disordering of a volume $f(\rho)d\rho$ of material, with latent heat of solidification L. In an isothermal change, this heat all passes through the boundary. A change of temperature will require transfer of specific heat also; so, in general,

$$dQ=cdT+Lf(\rho)d\rho. \quad (3)$$

Comparing (1) and (3) and noting that $c=\partial U/\partial T$, yields

$$\begin{aligned} f(\rho)L&=(\partial U/\partial\rho)+p \\ &=T(\partial p/\partial T) \text{ from (3)}. \end{aligned} \quad (4)$$

In fact the material transforming is in a state of strain in the ordered phase, and in addition the total interface area may be changed during transformation. The effective latent heat is hence that for unstrained material, L_0, less the strain energy and surface energy contributions $L_s(\rho)$.

At this point we restrict consideration to equilibrium conditions only, with the fixed dislocation stress field as the source of p. Now ρ and p are functions of T only, and the partial differential in (4) may be replaced by a total. Integrating, and inserting the sum in place of L, gives

$$p/(L_0-L_s)f(\rho)=\ln T+\text{const}. \quad (5)$$

If now the elastic strain energy outside the boundary is $U_0(\rho,T)$, the parameter p is given by

$$p=\partial U_0/\partial\rho,$$

since all changes of elastic energy appear as work done on the core.

The constant in (5) may be evaluated by considering the dislocation at the melting point. Here the core remains melted in the absence of any peripheral forces, and hence the elastic system should be in a state of static equilibrium. The stress-field energy will continuously reduce as the core size increases, while the surface energy of the solid-liquid interface will increase. The latter is also of the nature of an elastic energy, and so the equilibrium core size ρ_m at T_m may be obtained by minimizing the total stress-field plus surface energy.

Two possible configurations of the disordered core, representing extreme cases, have been considered. They are the flat strip, lying in the glide plane (or some minimum energy plane such as the most closely packed, for a screw dislocation), and the cylinder. It is shown in the Appendix that the rate of change of elastic energy outside a fixed contour close to the core, as the core size changes, is finite for the strip, and zero for the cylindrical configuration. It is probable that the strip represents the most efficient configuration for the relief of stress energy by the core disordering mechanism, and it will be assumed from now on that the core takes this form.

Let q be the thickness and 2ρ the width of the strip, and suppose that only ρ varies with temperature. This constraint will affect the final answer only slightly, and is introduced as a simplifying approximation. The total elastic and surface energy (see Appendix) is

$$(G\beta b^2/4\pi)\ln(kR/\rho)+4\rho s,$$

where s is the energy per unit area of liquid-solid interface, and the constant β varies from $1/(1-\nu)$ for an edge dislocation to unity for a screw. Minimizing this gives

$$\rho_m = Gb^2\beta/16\pi s.$$

Noting that the shape function $f(\rho)$ will be $2q$, and substituting in Eq. (5) yields

$$\rho = \frac{Gb^2\beta}{8\pi([L_0 - L_s]q \ln(T_m/T) + 2s)} \tag{6}$$

for the equilibrium core size in the flat strip configuration.

The approximate stress distribution discussed in the Appendix gives a shear strain in the solidifying material at the strip edges of $b\beta/2\pi q$, and hence the strain energy modification to L is

$$Gb^2\beta^2/8\pi^2\rho^2.$$

This turns out usually to be only a small fraction of L_0, and so it may be introduced into (6) as a second-order correction. The magnitude of the surface energy correction is not certain, but it is assumed that this also is fairly small.

DAMPING FORCE

We now calculate the magnitudes of the thermodynamic and viscous damping forces mentioned in the Introduction, again assuming that in most respects the situation may be treated as macroscopic. Both sources of damping are additional to any which may act on the dislocation stress field.

The thermodynamic damping is derived from the rate of entropy gain due to the temperature difference between the leading and trailing edges of the core. If the core were sufficiently wide, the temperature difference would be proportional to the normal thermal resistivity as well as the rate of latent heat release. However, the width is usually comparable with the mean free path of the thermal phonons, and in this situation the heat-transfer mechanism becomes one of phonon radiation rather than diffusion. The phonons may be considered to travel with an effective group velocity v_s, rather less than that of lower frequency acoustic waves. If the rate of heat generation per unit length of dislocation at the solidifying edge is Qq, the excess heat density near the source will be Q/v_s. The temperature difference between leading and trailing edges is therefore

$$\delta T = 2Q/av_sc_v,$$

where c_v is the specific heat per unit volume, and a is an effective radius, of the order of one atom distance, of the material which may be considered to have its temperature changed.

The entropy gain rate, treating the system macroscopically, is

$$\frac{dS}{dt} = Q\left(\frac{1}{T_1} - \frac{1}{T_2}\right) = \frac{Q\delta T}{T^2},$$

if δT is small. If the configuration of the dislocation core remains constant as it moves, the rate of change of internal energy of the system will be

$$dU/dt = T(dS/dt) = Q\delta T/T, \tag{7}$$

which may be represented by a damping force coefficient B_t:

$$dU/dt = B_tV^2, \tag{8}$$

where V is the dislocation velocity. The heat-generation rate will be

$$Q = (L_0 - L_s)qV, \tag{9}$$

where $L_0 - L_s$ is the effective latent heat of solidfication. Thus, from (7), (8), and (9), the damping coefficient becomes

$$B_t = 2(L_0 - L_s)^2q^2/aTv_sc_v. \tag{10}$$

Viscous damping may be calculated very simply for a strip-shaped core by assuming that the shear flow pattern is laminar. The relative displacement of the two faces as the core passes by is b; since it takes time $2\rho/V$ to pass, the shear rate is

$$\dot{\theta} = (b/q)(V/2\rho).$$

The total power dissipation is $2\rho q\eta\dot{\theta}^2 = B_vV^2$, giving

$$B_v = \eta b^2/2\rho q. \tag{11}$$

In the case of a core which has a shape closer to the cylindrical, the flow pattern might become more complex. There will be a tendency for the core to "roll" as the dislocation progresses, lessening the frictional force. However, estimates of the flow pattern have been made for a cylinder, allowing the formation of four main eddies, which show that the viscous damping differs from Eq. (11) by a factor of the order of unity. It is supposed that this effect will be unimportant in the case of a nearly flat strip.

APPLICATION OF MODEL

The theory developed in the previous sections should apply to dislocations in crystals which have a low-impurity content so that interactions between impurities and dislocations are not significant, and in which dislocation motion is over such short distances that they do not actually intersect other dislocations in the course of their motion. Internal friction measurements, or microscopic studies of the motion of identifiable dislocations, are two ways in which such a situation may be studied. Unfortunately there is a scarcity of experimental data, the tendency having been to con-

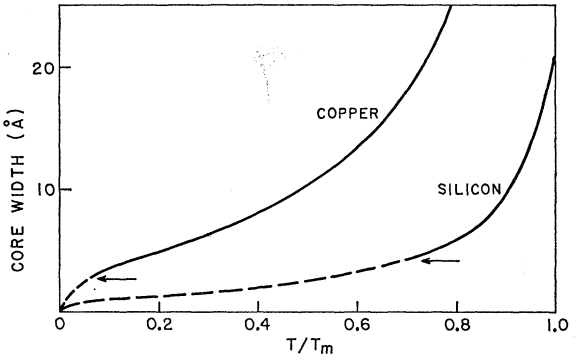

FIG. 1. Widths of disordered cores computed for copper and silicon. Arrows denote Burgers vector of dislocation, below which size the width loses its significance.

centrate on the behavior of dislocations at lower temperatures where appreciable dislocation broadening is not expected. We will take the case of two materials, for which there is some published information: silicon and copper. These form fairly typical covalent and metallic crystals. Ionic crystals are expected to behave in a similar manner to metallic, since the parameters involved have similar values.

The most significant factor in the theory is the heat of disorder. As a first approximation, this could be equated to the heat of fusion of the material and in copper we will assume this is the value. In silicon, melting involves not only disordering but also a change from essentially covalent to essentially metallic bonding,[11] which change presumably is exothermic. If we assume that in the core the disorder is sufficiently localized so that the covalent bonding is retained, and that one bond per atom is broken on the average, requiring about 1.5 eV, a heat of disorder is derived which is approximately twice that of melting; this will be used.

The second factor involved is the surface energy of the interface, and the value of this is very uncertain. No direct measurements exist, and such values as are quoted are derived from observations of supercooling of solidifying melts, using nucleation theory.[12] It is not clear whether the surface energy of significance under these conditions is the same as that at the dislocation core. We shall therefore guess a value for the surface energy of one-tenth the disorder energy, per atom. The core width will be sensitive to error in this approximation only near the melting point.

TABLE I. Values used in computing core widths.

	Silicon	Copper
Latent heat L (ergs cm^{-3})	1.2×10^{11}	1.6×10^{10}
Shear modulus G (dyne cm^{-2})	8×10^{11}	7.5×10^{11}
Burgers vector b (Å)	4.0	2.55
Strip width q (Å)	6.0	4.0
Melting point (°K)	1685	1356

Figure 1 shows the variation of core width to be expected for silicon and copper as a function of temperature. The dislocations considered are simple 60° dislocations in the (111) glide plane in both cases; Table I lists the values of parameters used. An isotropic average shear modulus is taken. It can be seen that as the temperature reduces to the Bordoni peak region in copper, below 110°K, and the region below 1200°K in silicon, the dislocation becomes less than one Burgers vector wide and it may be expected that the Peierls force should attain its full value. Above these temperatures, a smearing-out effect will occur. In both materials, dislocation behavior below these temperatures has been explained in terms of kink mechanisms, which require a large Peierls force; hence, the disordered-core theory is consistent with the kink hypothesis.

The thermodynamic component of damping may be computed from Eq. (10), the assumption being made that the effective phonon velocity is of the order 10^5 cm/sec. In silicon, B_t is then 2.5 dyn-sec-cm^{-2} at 1000°K and in copper 10^{-2} dyn-sec-cm^{-2}. These values are considerably larger than those obtained from the other models in which the Peierls force is not important, such as the thermoelastic theory of Eshelby ($B\sim10^{-5}$) or the interaction of thermal vibrations via nonlinear behavior near the core ($B\sim10^{-4}$), and hence will always dominate these other mechanisms.

Viscous damping is more difficult to evaluate, since a considerable extrapolation of viscosity data to the supercooled case is required. We assume that the viscosity is a thermally activated process, with the coefficient of viscosity $\eta\sim10^{-4}\exp(H/kT)$. In copper, the activation energy is assumed similar to that in other metals,[13] about 0.1 eV. In silicon, a higher activation energy is taken, corresponding to a bond-breaking process; the value of 1.4 eV gives a good match to the experimental observations. The viscous damping exceeds the thermodynamic damping below 0.1 T_m in copper and 0.85 T_m in silicon. It appears, therefore, that in copper (and presumably many other metals also) the viscous mechanism is never important, since below 0.1 T_m the kink description of dislocation motion becomes valid. In silicon, on the other hand, it is anticipated that it forms a good description between 0.7 T_m and 0.85 T_m.

At the present time, comparison with experiment cannot do more than indicate support for the theory as applied to silicon. A major difficulty is the extraction of a damping coefficient from the measurements of

[11] D. R. Hamilton and R. L. Seidensticker, J. Appl. Phys. **34**, 2697 (1963).

[12] J. H. Holloman and D. Turnbull, in *Progress in Metal Physics*, edited by B. Chalmers (Interscience Publishers, Inc., New York, 1953), Vol. 4, p. 333.

[13] C. J. Smithells, *Metals Reference Book* (Butterworths Scientific Publications, Ltd., Washington, 1962), Vol. II, p. 698.

internal friction, since the free length of dislocation is an important, and frequently unknown, factor. The Koehler-Granato-Lucke[14,15] stretched-string model of dislocation damping gives for the logarithmic decrement δ of a crystal, at low oscillation amplitudes,

$$\delta=\frac{\alpha 8Eb^2NL^2}{\pi^3 C}\frac{\omega\tau}{1+\omega^2\tau^2},$$

with relaxation time

$$\tau=L^2B/\pi^2C,$$

where E is Young's modulus, N the dislocation density, L the free length of the dislocation, C its line tension, and α an orientation factor of the order 0.25. Now if $\omega\tau\gg1$, both L and C vanish from the expression, and B can be computed readily from δ and N. For silicon, where the disordered-core theory predicts B always greater than unity, the inequality will hold for measurements at 10 kc/sec as long as $L>4\times10^{-4}$ cm, which will be the case in pure material with dislocation densities of less than 10^7 cm^{-2}. Figure 2 gives a curve for B derived from measurements of δ on a silicon crystal bar oscillating at 8 kc/sec and containing a dislocation density of approximately 10^6 cm^{-2}. The form of the curve is very similar to that obtained by summing B_t and B_v from the theory; the factor of 2 or so difference in magnitude is not significant as it could easily arise from a nonuniform orientation distribution of a portion of the dislocation.

In the case of copper, the situation is more complex as the damping coefficient is expected to be lower, and hence the dislocation length will become important. For most measurements reported, it is probable that $\omega\tau<1$. The internal friction will then be proportional to the damping coefficient, which itself varies inversely as the temperature. Such behavior is not observed, increases with temperature always being reported above about 200°K, sometimes gradual,[16] sometimes rapid.[17] Two additional effects, which would influence the temperature dependence of the logarithmic decrement, might be mentioned here. The first is the possible release of dislocation pinning points as the temperature increases. This could cause an increase of decrement with temperature, either by increasing the free dislocation lengths, or by allowing some less limited motion at the pinning points. Secondly, dislocations in the (111) plane of face-centered cubic metals split into two half-dislocations. Changes with temperature in the spacing of these half-dislocations, particularly the possibility of their recombining at higher temperatures,

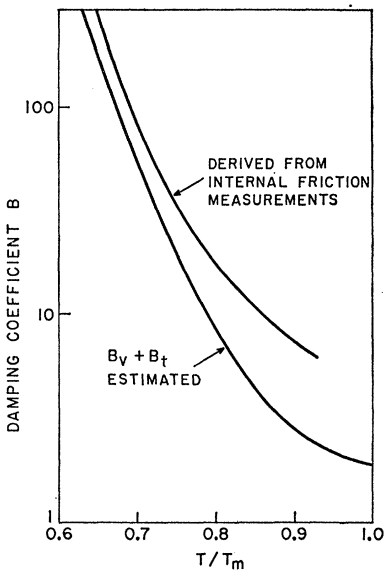

FIG. 2. Dislocation damping coefficient in silicon derived from the disordered-core model, compared with that derived from internal friction measurements by assuming a uniform dislocation distribution and free length greater than 10^{-3} cm.

could affect the temperature dependence of the logarithmic decrement. It is not clear what sort of effect this might be, although it is not expected to modify the behavior drastically. It is evident that further theoretical and experimental investigation is required.

DISCUSSION

A thermally disordered dislocation is a complicated system whose behavior can only be specified accurately in terms of the motions of a large number of atoms. The situation lies midway between a macroscopic and microscopic system; too small for the averaging processes implicit in the treatment of macroscopic systems to be used with complete rigor, and yet so large that analysis in terms of microscopic variables such as local phonon modes, or the statistics of some disorder parameter such as the kink density, would become immensely complex. The model which has been presented here uses the macroscopic approximation, modified at the points where it obviously breaks down, such as in the thermal conductivity. However, the validity of this approximation is purely intuitive, since the treatment is, strictly speaking, inconsistent; neither can it be said at present to be supported by any good fit to experimental data. In its defense, it may be argued that the dislocation is at least of macroscopic length, so that although thermal fluctuations, for instance, may exceed the systematic difference due to dislocation motion over a very short length of line, over the total length they will be averaged out.

One prediction of the theory is that even in an isotropic material, a screw dislocation will lose its radial symmetry at high temperatures. In a real crystal, the anisotropy will give preferred glide planes, and presumably the strip core would form in one of these planes.

[14] J. S. Koehler, in *Imperfections in Nearly Perfect Crystals*, edited by W. Shockley (John Wiley & Sons, Inc., New York, 1952), p. 197.
[15] A. Granato and K. Lucke, J. Appl. Phys. **27**, 583 (1956).
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[17] A. S. Darling, J. Inst. Metals **85**, 489 (1956).

The disordered-core theory modifies to some extent the concepts of interaction between impurities and the dislocation in several ways, which we will now briefly enumerate. Impurities which condense onto the dislocation will not only form a Cottrell atmosphere, but will also become incorporated in the core, the ratio of the equilibrium concentration in the core to that immediately surrounding it being of the order of the segregation coefficient for normal solidification. A core containing impurities will have a higher thermodynamic potential, and hence in order to minimize this by dilution, a further increase of core width will occur. Motion of the dislocation away from the impurities will require the dissipation of a pinning energy, but this will be less than for the small-core dislocation normally considered. In addition, an oscillation of the dislocation with amplitude less than the dislocation width will not involve the same pinning energy, and the impurities will act as "soft" pinning points in that case. If a dislocation moves sufficiently slowly for impurities to follow, there will be a significant frictional force, the relaxation time of the process being of the order of the time for an impurity to diffuse across the core. All these points require further exposition, and it is intended to do this in a later paper.

A further effect of the disordered core will be seen in the "pipe diffusion" of defects. Diffusion coefficients for this process are high[18,19] and special structures, such as that of a hollow core, have been postulated to explain their magnitude. Queisser *et al.*[18] derive an activation energy for dislocation diffusion of phosphorous in silicon which is about 1.5 eV less than that of bulk diffusion. This difference was interpreted in terms of excess concentration of vacancies and impurities near the dislocation due to the formation of Cottrell atmospheres. However, the disordered-strip model shows that in the 1050 to 1200°C region where the measurements were made, there is appreciable broadening, which significantly lowers the Cottrell binding energy. Excess vacancy concentrations outside the core will therefore not be so large, and this mechanism of enhanced diffusion becomes less important. The alternative explanation is that the lower activation energy is associ- with the disordered-core material itself, which presumably would have an energy closer to that of the liquid state. Such a theory is being developed, taking into account possible changes of core size with impurity concentration in the core and the ratio of this to the concentration in the surrounding solid.

SUMMARY

The model presented here attempts to deal with the very complex problem of dislocation configuration and damping force by applying macroscopic thermodynamics to a microscopic situation. Although not strictly correct, the model has the advantage of involving a relatively simple conceptual picture of the dislocation at high temperatures, that of the thermally disordered core. The disordered material is considered to be quasi-liquid, so that appeal may be made to the concepts of latent heat of disorder, and of viscosity, in the calculations. "Melting" of the core relieves the stresses in the vicinity. It seems to be a reasonable assumption that a flat strip configuration does this most efficiently, in both edge and screw dislocations, although this has not been proven. A cylindrical disordered-core coaxial with the dislocation does not relieve stresses. The core width increases considerably as the melting point is approached, and will be greater than several atomic spacings over a significant temperature range in many crystals. Near the melting temperature, the surface energy of the order-disorder interface is a controlling factor in the size, and uncertainty in the value of the surface energy is reflected in an uncertainty in the width here.

Two separate contributions to the dislocation damping coefficient are derived: thermodynamic and viscous. The thermodynamic damping originates in the heat required to produce disorder in the forward edge of the moving dislocation and the entropy changes in transferring this heat from the solidifying trailing edge. It varies inversely as the temperature, but disappears when the dislocation narrows to only one or two atoms wide. Viscous damping decreases with temperature due to both the increase of dislocation width and decrease in viscosity of the disordered core. Both mechanisms appear to give damping coefficients of a significantly large order of magnitude; although good estimates of the viscosity of the disordered core are difficult to make.

Application of the theory to silicon shows that the damping will be large and will predominate near the melting point, while at lower temperatures, it is reasonable to suppose that viscous damping becomes important. The magnitudes are consistent with those derived from experiment. In the case of copper, the thermodynamic damping is expected to dominate the viscous over a wide temperature range, but the form of the temperature dependence deviates considerably from the experimentally observed variation. When the temperature becomes so low that the core is only two or three atoms wide, the disorder is better described as an assembly of kinks, and the more complex theories of kink generation and diffusion may then be used in place of the viscosity approximation.

A disordered core is expected to modify dislocation interactions with impurities, and to lead to a higher equilibrium concentration of impurities in the core, "soft" pinning effects, additional dislocation drag mechanisms, and enhanced impurity diffusion along the dislocation.

[18] H. J. Queisser, K. Hubner, and W. Shockley, Phys. Rev. **123**, 1245 (1961).

[19] R. Tucker, A. Lasker, and R. Thomson, J. Appl. Phys. **34**, 445 (1963).

APPENDIX: DEPENDENCE OF STRESS-FIELD ENERGY ON CORE SIZE

1. Cylindrical Core

The dislocation core is considered to be a cylinder of radius ρ. We wish to calculate the stress-field energy per unit length, U_0, in the region outside a larger cylinder of radius ρ_0, and to obtain

$$\lim_{\rho_0 \to \rho} (\partial U_0/\partial \rho).$$

Consider a straight dislocation lying along the z axis and let σ^{ij} and e_{ij} be components of the stress and strain produced by this dislocation. Then

$$U_0 = \frac{1}{2}\int \sigma^{ij} e_{ij} dS, \tag{A1}$$

where the upper and lower indices denote contravariant and covariant components,[20] and the usual summation convention has been used. The integration is taken over the region of the xy plane between circles of radius ρ_0 and R (large). For an isotropic medium the stress and strain components are related by [21]

$$e_{ij} = \frac{1}{2G}\left[\sigma_{ij} - \frac{\nu}{\nu+1} g_{ij} g^{mn} \sigma_{mn}\right], \tag{A2}$$

where the g_{ij} are the components of the metric tensor.

The physical stress components[20] for a screw dislocation are given in Eq. (2.16) of Cottrell.[22] They are independent of ρ; hence U_0 will also be independent, and

$$\lim_{\rho_0 \to \rho} (\partial U_0/\partial \rho) = 0.$$

For an edge dislocation one cannot take the stress components directly from Eq. (2.10) of Cottrell. It is necessary to correct the components so that the stresses across the surface of the core vanish. Following the method outlined by Cottrell one obtains the corrected covariant stress components:

$$\begin{aligned}
\sigma_{rr} &= -\frac{Gb\sin\theta}{2\pi(1-\nu)r}\left[1-\frac{\rho^2}{r^2}\right], \\
\sigma_{\theta\theta} &= -\frac{Gbr\sin\theta}{2\pi(1-\nu)}\left[1+\frac{\rho^2}{r^2}\right], \\
\sigma_{\theta r} &= \sigma_{r\theta} = \frac{Gb\cos\theta}{2\pi(1-\nu)}\left[1-\frac{\rho^2}{r^2}\right], \\
\sigma_{zz} &= \nu(\sigma_{rr} + (r^2)^{-1}\sigma_{\theta\theta}).
\end{aligned} \tag{A3}$$

Now, using the relation $\sigma^{ij} = g^{ik} g^{jl} \sigma_{kl}$ to obtain the contravariant stress components, and neglecting terms in $1/R^2$ and $1/R^4$, we derive

$$U_0 = \frac{Gb^2}{4(1-\nu)}\left[\ln\frac{R}{\rho_0} - \frac{\rho^2}{2(1-\nu)\rho_0^2} + \frac{\rho^4}{4(1-\nu)\rho_0^4}\right], \tag{A4}$$

and again

$$\lim_{\rho_0 \to \rho} (\partial U_0/\partial \rho) = 0.$$

We might note that $\lim_{\rho_0 \to \rho} U_0$ does not agree with the expression given by Cottrell [the right side of Eq. (2.22b) of Ref. 22]. Cottrell calculates the energy by considering a half-plane cut made in the unstressed material and determining the work done in displacing the two sides of the cut by the Burgers vector. However, this procedure ignores the work done in changing the shape of the core during the displacement, and it is apparent that this work is of the same order as the correction terms.

2. Flat Strip Core

Let the dislocation core be a strip of variable width 2ρ in the glide plane and fixed thickness q. Take a fixed boundary outside the core, width $2\rho_0$, and thickness q; U_0 is the elastic energy outside this boundary. We are interested in the case $q \ll \rho$ and hence, for simplicity, will calculate U_0 in the limit $q \to 0$. Suppose U' is the energy outside the strip of width 2ρ. As $q \to 0$, the volume between the two strips becomes vanishingly small and hence $U' \to U_0$. Since the limits involved in calculating the partial derivatives are independent of q, they will also become equal as $q \to 0$.

A convenient way of deriving U_0 is the use of the analogy between the magnetostatic field energy of a current and the elastic field energy of a dislocation.[23] The analogy is effected in this case by substituting the elastic modulus $G\beta$ for the permeability μ_0, and the Burgers vector b for the current I. We regard the strip as having a uniform distribution of Burgers vector between $-\rho$ and $+\rho$, and hence take a uniform current distribution for the analogous case. The magnetostatic energy is related to the inductance L by

$$U_m = \tfrac{1}{2} L I^2,$$

while L is readily obtained from the formulas of Oberhettinger and Magnus[24] for the characteristic impedance of a transmission line consisting of a flat strip surrounded by a large outer conductor. If the outer conductor is sufficiently large, a good approximation is

$$L = (\mu_0/2\pi)\ln(kR/\rho),$$

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[20] See, for example, G. E. Hay, *Vector and Tensor Analysis* (Dover Publications Inc., New York, 1953), Chap VI.

[21] This can be obtained by generalizing Eq. (12.3) of Ref. 24, which is given in Cartesian coordinates. The m in this equation is the reciprocal of Poisson's ratio ($m = 1/\nu$).

[22] A. H. Cottrell, *Dislocations and Plastic Flow in Crystals* (Oxford University Press, London, 1953).

[23] R. de Wit, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1960), Vol. 10, p. 249.

[24] F. Oberhettinger und W. Magnus, *Anwendung der Elliptischen Functionen in Physik und Technik* (Springer-Verlag, Berlin, 1949), p. 63.

where k is of the order of 2.5 and depends on the geometry of the outer conductor, and mks units are used. Therefore

$$U_0=(G\beta b^2/4\pi)\ln(kR/\rho)$$

and

$$\partial U_0/\partial\rho=-(G\beta b^2/4\pi\rho).$$

The same expression is obtained by an approximation in which the material within a circle of radius ρ is taken to be uniformly stressed, in tension above and in compression below the strip, while outside the circle it is stressed just as if the strip were of infinitesimal width. This relatively simple stress distribution appears to be a good approximation to the exact situation.

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Surface Effect in Secondary and Photoelectric Emission

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The secondary emission yield of metals by the surface effect δ is expressed in terms of the surface photoelectric yield $y(\omega)$ for a radiation of frequency ω and angle of incidence of $\cos^{-1}\frac{1}{2}(5^{\frac{1}{2}}-1)$ which is about 52°. It is shown that $\delta\sim(2\pi\alpha E_p)^{-1}\int_{\omega_1}^{\omega_2} y(\omega)d\omega/\omega$, where E_p is the primary energy in atomic units, $\alpha=1/137$, ω_1 is the threshold frequency, and ω_2 depends on the energy of the primary and may be replaced by ∞. For a square-well potential model for a metal, $\delta\sim10^{-3}/E_p$ with a relative error of order $(E_F/E_p)\ln(E_p/E_F)$, where E_F is the Fermi energy.

1. INTRODUCTION

THE purpose of this paper is to establish a general and simple relation between the surface effect in secondary electron emission[1] (SSE) from metals and the surface photoelectric effect[2,3] (SPE), and to use this relation to show clearly why the SSE is so small that it can be neglected in explaining the experimental facts. Such a relation is of interest for its own sake, and in addition a new examination of the problem is desirable since most of the published papers on the SSE, are incorrect.[4,5]

[1] For a review of secondary emission see O. Hachenberg and W. Brauer, in *Advances in Electronics and Electron Physics* (Academic Press Inc., New York, 1959), Vol. XI, p. 413; A. J. Dekker, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1958), Vol. 6, p. 251.

[2] K. Mitchell, Proc. Roy. Soc. (London) **A146**, 442 (1934).

[3] I. Adawi, Phys. Rev. **134**, A788 (1964). This paper will be denoted by I.

[4] A. Viatskin, Zh. Eksperim. i Teor. Fiz. **9**, 826 (1939) treated a semi-infinite square-well potential model. The basic formulation is correct but the final integrations and conclusions are obscure and incorrect.

[5] W. Brauer and W. Klose, Ann. Physik **19**, 116 (1956). This paper has been assumed correct in the two review articles cited in Ref. 1, but it contains unfortunately basic errors. They treat a finite square well of width $2a$ in the limit that $a\to\infty$. The correct final state which should be used in the transition matrix element is the function v^* used here. Using the notation and Eq. (4.5) of I we have that the incoming wave v is given by $v=\frac{1}{2}(\phi^s/\Lambda_s^*+\phi^a/\Lambda_a^*)$. When the correct limiting procedure is applied as $a\to\infty$, the results of the finite and the semi-infinite square well become identical as has been discussed in general in I. With this in mind, and for a primary electron incident normal to the metal surface, none of the four delta functions obtained by Brauer and Klose and on which essentially all their discussion is based should arise; and the effect is precisely determined by terms similar to those they ignored. The yield by the surface effect in secondary emission as in photoelectric emission is independent of the dimensions of the model analyzed, and there is no need to introduce an *ad hoc* depth d_s for calculating the effect.

We shall use for convenience Hartree's atomic units in which $\hbar$, the electron mass m, the Bohr radius a_B, and the electron charge e are unity, and the speed of light c is 137. As was done in discussing the surface photoelectric effect in I, we treat the conduction electrons as independent noninteracting particles. The motion of a single electron in the y and z directions is free and can be described by the plane-wave $L^{-1}\exp i(k_y y+k_z z)$ obeying cyclic boundary conditions and normalized to unity in a square area of side L. The x motion is bound by a general surface potential $V(x)$ which is the same for all electrons and varies only in the direction x which is normal to the metal surface. This motion is described by the wave function $L^{-1/2}\phi_0(x)$ normalized to unity. The length L is the thickness of the metal plate which extends from $x=-L$ to $x=0$. The function $\phi_0(x)$ satisfies the wave equation,

$$H_1\phi_0=E_0\phi_0, \tag{1.1}$$

where

$$H_1(x)=-\tfrac{1}{2}\partial^2/\partial x^2+V(x). \tag{1.2}$$

Inside the metal, $V(x)$ is a constant equal to $-V_0$, and we can write $\phi_0(x)=2^{1/2}\sin(k_x x+\gamma)$ where γ is a phase factor depending on $V(x)$, and $\frac{1}{2}k_x^2=E_0+V_0$. The potential $V(x)$ rises to zero in the surface barrier regions near $x=0$ and $x=-L$ in a distance much less than L, and $\phi_0(x)$ behaves as $\exp(-px)$ for large x, where $-\frac{1}{2}p^2=E_0$. We ignore thermal effects and assume that all energy states below the Fermi energy E_F are occupied, and all energy states above the Fermi energy are empty. The conduction electrons in this model assume $\mathbf{k}$ values which fill "a Fermi hemisphere" given by $k^2=k_F^2$ and $k_x>0$, where k_F is the Fermi momentum,