Frictional Stress Acting on a Moving Dislocation in an Otherwise Perfect Crystal

DORIS KUHLMANN-WILSDORF
School of Metallurgical Engineering, University of Pennsylvania, Philadelphia, Pennsylvania
(Received June 27, 1960)

The problem of the frictional stress suffered by moving dislocations in otherwise perfect crystals is investigated. This is done without calculating the core energies of dislocations, but by considering stresses and strains on the slip plane. The level of frictional stresses obtained is much higher than reported previously. Since common glide dislocations in metals with close packed structures apparently do not suffer significant frictional stresses, mechanisms are discussed which tend to reduce their effect. A new such mechanism is discovered. It is based on the idea that the positions of dislocation axes are not defined with precision, but only within one to a few times the average displacement of the oscillating atoms. The expected result of this is a depression of the frictional stress for close packed metals even at very low temperatures, almost no effect on dislocations in crystals with diamond structures, and a temperature dependence proportional to $e^{-\text{const}T/T_M}$ for NaCl type salts and, probably, for bcc metals.

1. INTRODUCTION

THE question as to the magnitude of the frictional force with which an otherwise ideal crystal resists the motion of a dislocation has already been treated in several papers.[1–8] Most of these are based on a paper by Peierls,[1] and its clarification and development by Nabarro.[2] They approached the problem as follows: Imagine that an otherwise ideal crystal, containing one straight dislocation, is split along its slip plane, but that the original stresses and strains are maintained in the two resulting crystal halves by applying suitable tangential forces to the cut. These are the same forces with which the two atomic planes, which were facing each other across the slip plane before the cut was made, have interacted due to their misalignment. It is now assumed that the two crystal halves with the applied surface forces behave according to simple elastic theory. Obviously, the internal stresses tend to spread out the strain, i.e., tend to spread out the dislocation, while the tangential surface forces tend to contract the region of serious misalignment, i.e., tend to contract the dislocation. Equilibrium is reached when the tangential forces just balance the elastic stresses in the two crystal halves.

Depending on the exact law which is assumed to connect the forces of interaction with the relative misfit between the two crystal planes, different solutions may be found, for the equilibrium distribution of the displacements as well as the tangential forces.

As a next step, it is assumed that every atomic row parallel to the dislocation axis in one crystal half interacts only with the corresponding atomic row in the other crystal half, which is facing it across the slip plane; and that the forces of interaction act only through these atomic rows, and with the magnitude which is appropriate to their exact position. The energy of misfit of every pair of atomic rows can then be expressed as a function of the distance between the dislocation axis and the pair. This energy is a function of the exact position of the dislocation axis with respect to the crystal lattice. Summing over the misfit energies of all the pairs of atomic rows from minus infinity to plus infinity renders an expression for the total energy of misfit. This, again, depends on the exact position of the dislocation axis. The corresponding periodic force, acting on the dislocation because of the atomistic structure of the crystal, and commonly called the "Peierls-Nabarro force," is then found through differentiation.

The result of the calculation and its various refinements has been that $\tau_{D\,\max}$, the maximum value of this force, which has the character of a frictional stress on any moving dislocation, is about $10^{-4}\mu$ and smaller, where μ is the modulus of rigidity. Moreover $\tau_{D\,\max}$ was found to depend exponentially both on the "width" of the dislocation and on Poisson's ratio, ν, becoming the smaller the wider the dislocation and the smaller Poisson's ratio. Only Huntington,[8] although finding the same type of function for the frictional stress, arrives at much higher numerical values, namely $1.7\times10^{-2}\mu$ and $3.2\times10^{-3}\mu$.

2. CRITICISM OF PREVIOUS THEORIES

The Peierls-Nabarro calculation and its various refinements require a high level of mathematical competence, but while the elegant treatments of this difficult problem must be greatly admired, one should realistically concede that the numerical answers gained are unreliable. Two considerations make this amply clear:

(i) The physical reason why lattice friction exists at all—and which has been recognized all along—is the fact that the dislocation core energy is bound to vary

[1] R. E. Peierls, Proc. Phys. Soc. (London) **52**, 34 (1940).
[2] F. R. N. Nabarro, Proc. Phys. Soc. (London) **59**, 256 (1947).
[3] F. R. N. Nabarro, in *Advances in Physics*, edited by N. F. Mott (Taylor and Francis, Ltd., London, 1952), Vol. 1, p. 269.
[4] J. D. Eshelby, Phil. Mag. **40**, 903 (1949).
[5] G. Leibfried and H.-D. Dietze, Z. Physik **126**, 790 (1949); **131**, 113 (1951).
[6] H.-D. Dietze, Z. Physik **131**, 156 (1952); **132**, 107 (1952).
[7] A. J. Foreman, M. A. Jaswon, and J. K. Wood, Proc. Phys. Soc. (London) **A64**, 156 (1951).
[8] H. B. Huntington, Proc. Phys. Soc. (London) **B68**, 1043 (1955).

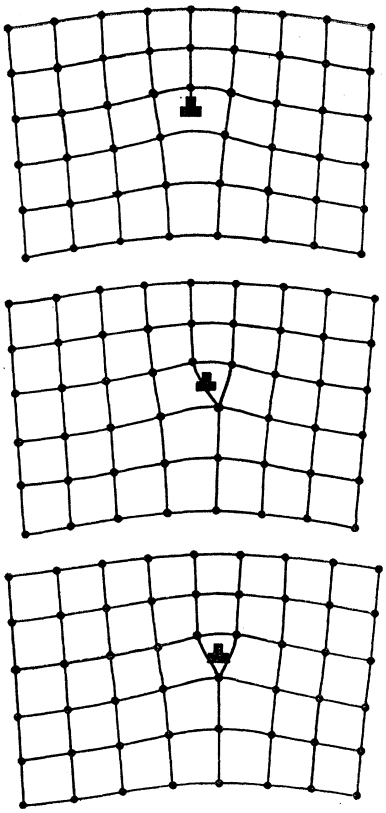

FIG. 1. Atomic displacements as a ⟨100⟩, {100} edge dislocation moves through a cubic primitive lattice by a distance $b/2$.

with the precise position of the dislocation axis, since the atomistic configuration in the core changes periodically. Nabarro[3] has illustrated this point by representing three different positions for an edge dislocation in a simple cubic lattice. His figure has been redrawn as Fig. 1.

Let us evaluate what is the percentage change of core energy which corresponds to a frictional stress of $10^{-4}\mu$ or less. We assume that the core energy is given by

$$U_c = U_0 + \tfrac{1}{2}\Delta U_c \cos(2\pi s/p + \varphi), \tag{1a}$$

with ΔU_c the total fluctuation of core energy during one cycle, s the coordinate perpendicular to the dislocation axis in the slip plane, p the distance between the "Peierls-Nabarro crests" in the direction of s, and φ an arbitrary phase angle. For a ⟨100⟩, {100} edge dislocation in a cubic primitive lattice p is equal to b, the Burgers vector, but in other lattices and for other dislocations p may very well be smaller than b. The frictional stress acting on the dislocation then becomes

$$\tau_D = -\frac{1}{b}\frac{dU_c}{ds} = \frac{\pi}{bp}\Delta U_c \sin\left(\frac{2\pi}{p}s + \varphi\right). \tag{2}$$

Consequently, a minimum resolved shear stress of

$$\tau_{D\,\max} = (\pi/bp)\Delta U_c \tag{2a}$$

is required for the sustained movement of the dislocation. For a typical metal with $p=b=2.8$ A and $\mu = 5\times10^{11}$ dynes/cm^2 we find $\Delta U_c = 1.2\times10^{-8}$ erg/cm $\cong 2\times10^{-4}$ ev/atomic plane, if $\tau_{D\,\max}$ is chosen as $10^{-4}\mu$.

This is an unbelievably low value, representing only two to four hundredths percent of typical core energies. Surely, core energy calculations with their unavoidable approximations and simplifications do not by far reach this accuracy, let alone that corresponding to the still much lower estimates of $\tau_{D\,\max}$ which may be found in the literature.

(ii) Nabarro[9] states that "On account of the approximate method of calculation employed, the two symmetrical configurations of the dislocation (see Fig. 1) have the same energy."

This remark amplifies the argument under (i). The conclusion is inescapable that the first-order effect in the periodic change of core energy has been lost completely.

3. LATTICE FRICTIONAL STRESS CALCULATED FROM AN APPROXIMATE METHOD

For the above reasons a new approach to the problem of lattice friction seemed to be needed. One most simple and unsophisticated method is to estimate the fractional change in core energy. This will be in the nature of an order of magnitude calculation, but crystal structure and atomic or ionic properties could be taken into consideration, and the numerical results could be more reliable than those available so far. In the cases of diamond, germanium, and silicon, for example, electrical energy contributes roughly as much to core energy as strain energy does, and since the former will fluctuate very much while the latter will stay more nearly constant, we expect the variation of core energy to be in the order of one third. Conversely, typical fcc metals have wide cores. Still, it would be surprising if their core energy fluctuated by much less than 0.1%.

By combining an expression for the elastic part of core energy per unit length, $U_c \cong \mu b^2/4\pi(1-\nu)$, with Eq. (2) one finds

$$\tau_{D\,\max} \cong (b/3p)\beta\mu, \tag{2b}$$

where $\beta = \Delta U_c/U_c$. According to the argument above, $10^{-3} \lesssim \beta \lesssim 0.5$, and thus the frictional stress becomes rather larger than assumed previously.

4. LATTICE FRICTIONAL STRESS CALCULATED BY A MORE REFINED METHOD

A second, more refined but still quite simple, calculation gives similarly high values for the frictional stress acting on a moving dislocation. It follows the Peierls-Nabarro method to some extent, but circumvents entirely the calculation of core energies:

Consider unit length of an arbitrary but straight dislocation, the axis and slip plane of which coincide

[9] See reference 3, p. 370.

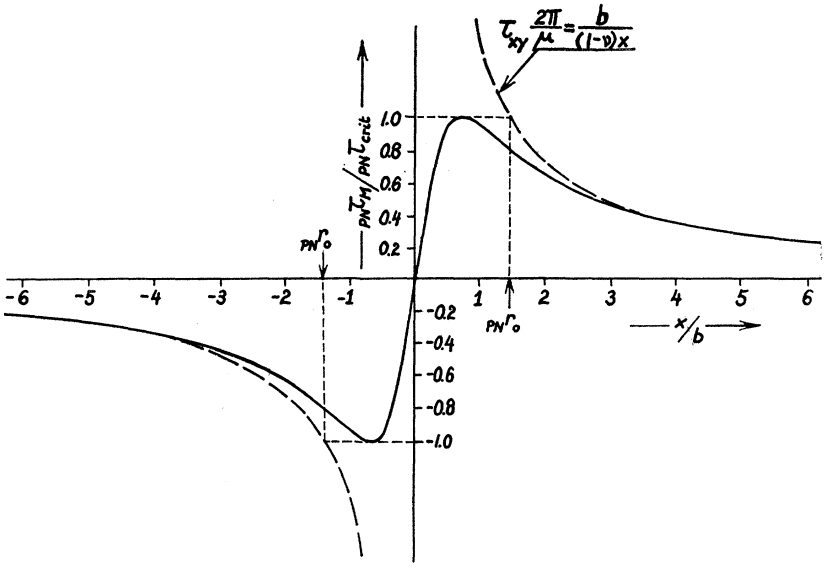

FIG. 2. Peierls' and Nabarro's solution for τ_M, the resolved shear stress acting on the slip plane due to the presence of a ⟨100⟩, {100} edge dislocation in a cubic primitive lattice, Eq. (6). Poisson's ratio has been taken as $\nu=0.3$.

with the z axis and the plane $y=0$, respectively. Let $\tau_M(x)$ be the shear stress which is set up due to the misfit between the two planes bordering the slip plane. For $x\gg b$ this must be equal to $\tau_M(x\gg b)=\tau_{xy}=A/x$, where A for an edge dislocation is given by $A_\perp=\mu b/2\pi(1-\nu)$ and for a screw dislocation by $A_s=\mu b/2\pi$, which is the shear stress set up by a dislocation on its own slip plane as it is calculated from elasticity theory. The detailed behavior of the function $\tau_M(x)$ for x comparable to or smaller than b is unknown, but it must vanish for $x=0$, it must be antisymmetrical in x so that $\tau_M(x)=-\tau_M(-x)$, and the function must have just one extremum on either side of the z axis. These deductions are qualitatively obvious, and are in full agreement with the particular solution derived by Nabarro[3] for an edge dislocation in a cubic primitive structure (Fig. 2).

No lattice force will act on the dislocation if it happens to be in a symmetrical position, as for instance those represented in Fig. 1, because for each row of atoms at $+x_j$, experiencing the force $b\tau_M(x_j)$, there will be one at $-x_j$, experiencing the force $b\tau_M(-x_j)=-b\tau_M(x_j)$. Different conditions obtain if the dislocation is in an arbitrary position with respect to the lattice. Let the jth atomic row be situated at x_j and be subject to the displacement $u(x_j)$. If the dislocation moved through the infinitesimally small distance ds, the jth atomic row would change its displacement from the value $u(x_j)$ to the displacement appropriate to its new relative distance from the dislocation axis, which is $u(x_j-ds)$, i.e., the jth row would move through the distance $-ds(du/dx)_{x_j}$. Since it is subject to the tangential force $b\tau_M(x_j)$ the work done thereby is $w_j=-dsb\tau_M(x_j)(du/dx)_x$ while the work done by all the rows of atoms equals the work done on the dislocation, so that

$$-\sum_{x_j=-\infty}^{+\infty} dsb\tau_M(x_j)\left(\frac{du}{dx}\right)_{x_j}=dsb\tau_D, \tag{3}$$

the sum to be taken over all rows of atoms in both crystal halves.

Equation (3) represents the same relationship which was used by Nabarro in connection with barrier problems as Eq. (24) in part III of reference 3. Equation (3) is exact, but in order to evaluate it, several approximations and assumptions are introduced. Our first assumption is that the work done by all atomic rows in the upper half will be closely similar to that done in the lower half, so that the sum may be multiplied by 2 and then taken over just one crystal half. It is further assumed that the lattice force has its highest value when the dislocation is midway between the two symmetrical positions (see Fig. 1), and that in a cubic primitive lattice the atoms then are at or close to $\cdots$, $-7b/4$, $-3b/4$, $+b/4$, $+5b/4$, $+9b/4\cdots$. In that case, and if the terms are rearranged as $+b/4$, $-3b/4$, $+5b/4$, $-7b/4$, $\cdots$, the sum consists of terms of alternating sign and with, in average, the greatest possible differences in magnitude from term to term. Hence,

$$\tau_{D\,\max}\cong 2\sum_{n=-\infty}^{+\infty}\tau_M\left(\frac{4n+1}{4}b\right)\left(\frac{du}{dx}\right)_{[(4n+1)/4]b}. \tag{4}$$

If the terms are taken in the order indicated above, the sum in Eq. (4) is bound to converge rapidly since, for $x\gtrsim 5b$, du/dx must already be close to zero, and $\tau_M(x\gtrsim 5b)\cong A/x$ as stated above. That the sum should converge so very rapidly is entirely logical from a physical standpoint, since the frictional force is due to the periodic changes in the core energy and, hence, is determined by the behavior of the atomic rows which

constitute the core. Also it must be expected that, within very large limits, lattice friction does not depend on the size of the specimen.

Fortunately it is possible to estimate the value of the sum without making any detailed assumptions about the functions τ_M and du/dx. Because the terms of the sum vary very rapidly, because only the first few terms determine the value of the sum, and because the terms have alternating signs, it is obvious that the value of the sum cannot be too different in magnitude from one half its largest term. This, in turn, is estimated as $\frac{1}{2}\tau_{crit}(\frac{1}{4}b/r_0)$ since, on the one hand, the shear stress in the core must reach its highest possible value for an undisturbed crystal,—which is τ_{crit}—, and since outside of r_0, the radius of the core, the displacement is close to $b/4$, while the factor $\frac{1}{2}$ is introduced to take account of the fact that du/dx has its largest value at the axis, where τ_M vanishes. Thus

$$\tau_{D\ max}\cong(b/8r_0)\tau_{crit}. \tag{5}$$

5. APPLICATIONS OF THE METHOD TO THE PEIERLS-NABARRO DISLOCATION AND TO DISLOCATIONS IN CLOSE PACKED LATTICES

In order to test this latter result, Eq. (4) was evaluated numerically for the particular functions ${}_{PN}\tau_M$ and u_{PN} derived by Peierls and Nabarro for the edge dislocation in a simple cubic lattice. These are, for $b=a$,

$${}_{PN}\tau_M(x)=-{}_{PN}\tau_{crit}\sin(-2\tan^{-1}\psi), \tag{6}$$

and

$$u_{PN}=-(b/2\pi)\tan^{-1}\psi, \tag{7}$$

where $\psi=2(1-\nu)x/b$ and ${}_{PN}\tau_{crit}=\mu/2\pi$. For $(du/dx)_{PN}$ we get

$$\left(\frac{du}{dx}\right)_{PN}=-\frac{(1-\nu)}{\pi(1+\psi^2)}, \tag{8}$$

so that

$${}_{PN}\tau_{D\ max}=\frac{(1-\nu)\mu}{\pi^2}\sum_{\substack{\psi=\frac{1}{2}(1-\nu)(4n+1)\\ n=-\infty}}^{+\infty}\frac{\sin(-2\tan^{-1}\psi)}{(1+\psi^2)}=\frac{(1-\nu)\mu}{\pi^2}S. \tag{9}$$

The functions (6), (7), and (8) together with the function $[\tau_M(du/dx)]_{PN}$ are represented in Figs. 2 and 3.

Summing, as indicated before, in the order $n=0,-1,+1,-2,+2,\cdots$, the sum S in (9) converges as rapidly as expected, and, for $\nu=0.3$, is close to 0.225. This renders

$$\begin{aligned}{}_{PN}\tau_{D\ max}&=[2(1-\nu)/\pi]0.225\,{}_{PN}\tau_{crit}\\&=0.143(1-\nu)\,{}_{PN}\tau_{crit}\cong0.1\,{}_{PN}\tau_{crit}\cong0.016\mu,\end{aligned} \tag{10}$$

and, with Eq. (2b), $(\Delta U_c/U_c)_{PN}=4.8\%$.

The value of ${}_{PN}\tau_{D\ max}\cong0.143(1-\nu)\,{}_{PN}\tau_{crit}$, Eq. (10), gained from Eq. (4), may be compared with Eq. (5) if r_0 is defined more precisely. Probably the most logical and simple definition for this parameter is

$$r_0=\frac{A}{\tau_{crit}},\quad\text{with } A \text{ equal to } A_\perp=\frac{\mu b}{2\pi(1-\nu)}\quad\text{or}\quad A_s=\frac{\mu b}{2\pi}, \tag{11}$$

depending on whether an edge or a screw dislocation is being considered. For the Peierls-Nabarro dislocation

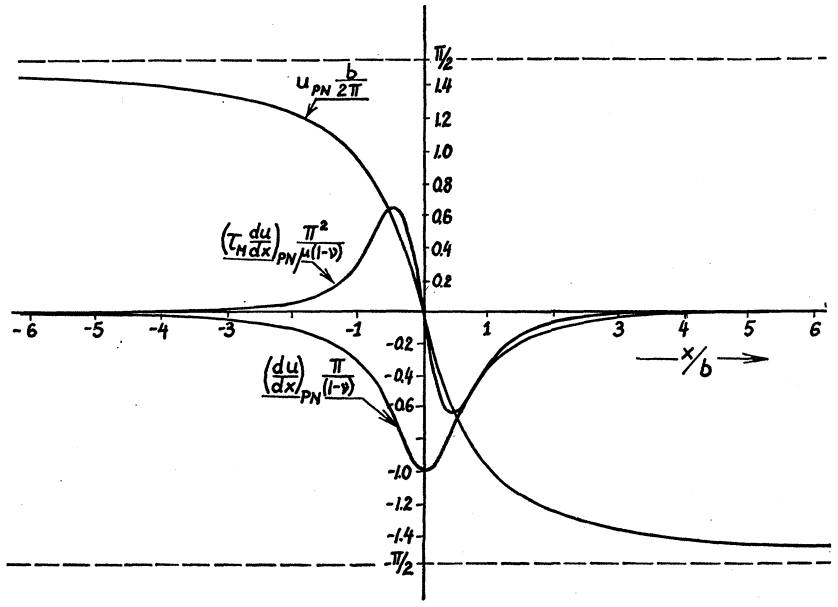

FIG. 3. Peierls' and Nabarro's solution for u, the displacements on either side of the slip plane of a ⟨100⟩, {100} edge dislocation in a cubic primitive lattice, Eq. (7), and the functions $(du/dx)_{PN}$ [Eq. (8)] and $[\tau_M(du/dx)]_{PN}$; ($\nu=0.3$).

this becomes, with $\nu=0.3$, ${}_{PN}r_0=b/(1-\nu)\cong 1.4b$, and ${}_{PN}\tau_{D\,max}\cong[(1-\nu)/8]_{PN}\tau_{crit}=0.125(1-\nu)_{PN}\tau_{crit}$. Thus, agreement within 12.5% exists between the two answers, a result which greatly strengthens our confidence in the accuracy of Eq. (5), and leads us to believe that it probably is reliable within a factor of 2 or so. Therefore we shall study it a little further and rewrite it into

$$ {}_{\perp}\tau_{D\,max}\cong\frac{\pi(1-\nu)}{4\mu}\tau_{crit}{}^2=\frac{\pi(1-\nu)}{4q^2}\mu \qquad (5a)$$

for an edge dislocation, respectively,

$$ {}_{s}\tau_{D\,max}\cong\frac{\pi}{4\mu}\tau_{crit}{}^2=\frac{\pi}{4q^2}\mu \qquad (5b)$$

for a screw. Here q has been introduced as the ratio μ/τ_{crit}.

Since, for typical glide dislocations in fcc and hcp metals, $q\cong 30$,[10] and with $\nu=0.3$, we obtain from Eqs. (5a and b) frictional stresses of about $6\times10^{-4}\mu$ and $9\times10^{-4}\mu$, acting on moving edge and screw dislocations in the close packed lattices; corresponding, according to Eq. (2b), to $\beta\cong 0.2\%$ if we assume $b=p$. Note that the frictional stress obtained for a screw dislocation is higher than that for an edge dislocation. This is due to the fact that the stresses around a screw dislocation are somewhat lower than those for an edge dislocation, leading to a smaller r_0.

At this point the question arises which feature in the Peierls-Nabarro calculation caused the great error in the final result for $\tau_{D\,max}$. Huntington,[8] who has considered the various assumptions, explicit or implicit, contained in the Peierls-Nabarro calculation, concludes that the model of Peierls and Nabarro has a "peculiar symmetry." Namely, comparing the atomic positions above and below the slip plane, "One configuration can be obtained from the other by reflection in the slip plane and reversal of the signs of all displacements" and further, "The model does not distinguish between the directions of u in determining p_{xy} (our τ_M) . . . ." When disturbing this symmetry, Huntington did indeed get a value for ${}_{PN}\tau_{D\,max}$ of 0.017μ, quite similar to the value derived above.

While it has been shown above that the frictional stress on a dislocation moving in a mathematically precise crystal lattice has been greatly underestimated in previous papers, even these much too small values for $\tau_{D\,max}$ have seemed to be too *high*, in view of the fact that, at least in certain crystals, dislocations move at stress levels of $10^{-5}\mu$ or $10^{-6}\mu$.

Various reasons were given why the frictional stress might have been overestimated or why a dislocation would move at stresses below $\tau_{D\,max}$. Foreman, Jaswon, and Wood,[7] for example, showed that the dislocation width in actual crystals should mostly be larger than that derived from the Peierls-Nabarro calculation. This conclusion doubtlessly is correct, but it would hardly affect our result very greatly since $\tau_{D\,max}$ is only inversely proportional to the diameter of the dislocation core. Dietze[6] has discussed the effect of temperature motion, and of the changes resulting in the calculations if it is recognized that the forces of misfit are not actually transmitted through point atoms. Again, although such considerations have a strong effect in the framework of the Peierls-Nabarro calculation, they do not affect our result materially.

On the other hand, several effects which may reduce lattice friction seem just as important now as previously. For example, Shockley[11] has pointed out that a dislocation would not normally lie in a "Peierls-Nabarro trough," and that parts which move first could pull the rest of the dislocation along. Also the geometry of actual crystal lattices can greatly modify the level of the frictional stress; and thermal activation helps dislocations to overcome the "Peierls-Nabarro hills." Whether the latter effects listed, however important they may be from case to case, hold the complete answer is problematic, though; particularly now that we find the frictional stress so much higher.

6. UNCERTAINTY IN THE POSITION OF A DISLOCATION AXIS DUE TO UNCORRELATED ATOMIC OSCILLATIONS

Contemplating this problem, one aspect presented itself which seems to have been overlooked in the past, namely that the position of a dislocation axis is not defined with absolute accuracy but only within certain limits. Instinctively, one may feel that these limits should be very narrow, since so very many atoms are involved and since their positions in turn are rather well defined. However, a simple calculation shows that this is not necessarily so.

As the result cannot depend much on the angle between the dislocation axis and the Burgers vector let us consider a screw dislocation first: The displacements of the crystal atoms due to the presence of a screw dislocation parallel to the z axis of a Cartesian coordinate system are given as $u_z=(b/2\pi)\theta$, where θ is the angle included between the radius vector and an arbitrary direction in the x-y plane. If the position of any given atom was known with point accuracy u_z would be known exactly, and observations on only two atoms would be sufficient to determine the exact position of the dislocation axis. In reality the atoms vibrate with a root mean square displacement $\bar{u}$, and measurements carried out by an observer positioned on, say, the jth atom in the crystal could determine the coordinates of the dislocation axis only to an ex-

[10] A. H. Cottrell, *Dislocations and Plastic Flow in Crystals* (Clarendon Press, Oxford, 1953), p. 10.

[11] W. Shockley, oral communication, quoted by N. F. Mott and F. R. N. Nabarro, *Report on Strength of Solids* (Physical Society, London, 1948), p. 1.

pected accuracy of $\Delta s_j' = (2\pi r_j/b)\bar{u}$, if r_j denotes the distance between the jth atom and the dislocation axis.

We assume that the dislocation is sufficiently flexible so that only the atoms in a plane perpendicular to the dislocation axis will determine the position of the dislocation axis in that plane. This is a quite reasonable assumption for small axis displacements and, moreover, the final result will hardly be affected even if the atoms in the neighboring planes should exert some influence. We may then conclude that all atoms in a ring of width dr_j define the position of the dislocation core with an expected accuracy of

$$\Delta s_j = \frac{2\pi r_j \bar{u}}{b(2\pi r_j dr_j/\alpha)^{\frac{1}{2}}} = \frac{\bar{u}}{b}\left(\frac{2\pi r_j \alpha}{dr_j}\right)^{\frac{1}{2}}$$

(where α is the area per atom in the plane considered), because the n-fold repetition of a measurement diminishes the expected error by the factor $1/\sqrt{n}$.

From the theory of errors[12] the average error M of a result gained from several series of measurements, each with its individual average error m_j, is known to be $M = \{\sum_j (1/m_j^2)\}^{-\frac{1}{2}}$. Hence, the root-mean-square deviation with which the position of the dislocation axis may be determined by observing all atoms outside of the dislocation core is given by

$$\delta_A'' = \left\{\sum_i \frac{1}{\Delta s_j^2}\right\}^{-\frac{1}{2}} = \frac{\bar{u}}{b}(2\pi\alpha)^{\frac{1}{2}}\left(\int_{r_0}^{R}\frac{dr}{r}\right)^{-\frac{1}{2}} = \frac{\bar{u}}{b}\left[\frac{2\pi\alpha}{\ln(R/r_0)}\right]^{\frac{1}{2}}. \quad (12)$$

With reasonable values for r_0, R and α/b^2 this is $\delta_A'' \simeq \bar{u}$.

Hence, from the displacements of all atoms outside of the core, the position of a dislocation axis cannot be determined with an accuracy better than about the amplitude of the atomic vibrations, even if observations were continued for any desired length of time.

Important though this result may be it is not the complete answer to our problem, since the center of the core may still be defined with greater or lesser accuracy than δ_A'', depending on the atomic arrangement in the core. This second part of the problem is treated more easily for an edge dislocation.

We refer back to the beginning of the paper where it was stated that the width of a dislocation is determined by the balance between the forces of misfit and the elastic stresses in the two crystal halves. Also we remember that the highest shear stress which can be supported by any given crystal plane in the absence of dislocations is $\tau_{\text{crit}} = A/r_0$. From this it seems a reasonable model to consider a cross section of the core of a positive edge dislocation as represented by two rows of uniformly spaced atoms, facing each other across the slip plane. The spacing in the upper row will be $a_u = [2r_0/(n+\frac{1}{2})]$ and that in the lower half $a_l = [2r_0/(n-\frac{1}{2})]$, with $n = 2r_0/p$ and $r_0 = \mu b/2\pi(1-\nu)\tau_{\text{crit}}$. The parameter p stands for the period of the lattice perpendicular to the dislocation axis, which is presumed to be equal to the distance between the "Peierls-Nabarro hills" in the direction normal to the crystal axis.

Due to the uncorrelated vibrations of the atoms, the position of either of the two rows of atoms will be uncertain within $\delta_R \cong \pm\bar{u}/\sqrt{n}$, and the relative position of the two rows by $\pm 2\delta_R/\sqrt{2}$.

A relative displacement Δx between the two rows of atoms causes the shift $\Delta s = [p/(a_l - a_u)]\Delta x$ of the dislocation axis, and, consequently,

$$\delta_A' = \frac{p}{a_l - a_u}\frac{\bar{u}}{(n/2)^{\frac{1}{2}}} \quad (13a)$$

may be taken as the root mean square uncertainty in the position of the dislocation axis.

From $a_u = pn/(n+\frac{1}{2})$ and $a_l = pn/(n-\frac{1}{2})$ follows $a_l - a_u \cong p/n = p^2/2r_0$, so that

$$\delta_A' \cong 2\left(\frac{r_0}{p}\right)^{\frac{1}{2}}\bar{u} = \bar{u}\left\{\frac{\mu b/p}{\pi(1-\nu)\tau_{\text{crit}}}\right\}^{\frac{1}{2}}. \quad (13b)$$

For a screw dislocation the factor $(1-\nu)$ is exchanged for 1.

This then is the *diffuseness* of the axis of a dislocation, and is quite distinct from thermal activation which may *shift* the axis of a dislocation: As a consequence of their vibrations, the atoms in a crystal containing a dislocation deviate from the ideal, mathematical pattern which would constitute a dislocation, so that physically the position of the dislocation axis is not defined precisely. δ_A' is a measure of the resulting uncertainty. This uncertainty is very similar in concept to that in Heisenberg's uncertainty relationship. It is meaningless to state the position of a dislocation more accurately than within this limit.

Equation (13b) probably is an underestimate. For one thing $\bar{u}$, the root mean square displacement, must be considerably larger for the loosely bound atoms in a dislocation core than the value appropriate to a perfect crystal. Also, it is not necessary for the complete rows of atoms to shift in order to shift the dislocation axis as measured from the atoms nearest to the center of the core, the region on which our interest is focused. Hence n in Eq. (13a) is overestimated, and is smaller than the value $2r_0/p$ which was used to gain Eq. (13b). To some extent these two errors are balanced by the fact that $(a_l - a_u)$ is larger at the center of the core than the average over the complete core which was used in Eq. (13b). We shall try to compensate for these uncertainties by multiplying δ_A' with a factor of 2. However we should keep in mind that the final value

$$\delta_A = 2\delta_A' = 4(r_0/p)^{\frac{1}{2}}\bar{u} \quad (13c)$$

[12] See, for example, F. Kohlrausch, *Praktische Physik* (B. G. Teubner, Berlin, 1943), Vol. 1, p. 16.

is uncertain by at least a factor 2, particularly as $\bar{u}$ itself is not well known, nor even well defined.

7. ESTIMATE OF THE AVERAGE DISPLACEMENTS OF OSCILLATING CRYSTAL ATOMS

For low temperatures the value of $\bar{u}$ may be estimated as follows: Consider all the atoms in a crystal as uncorrelated oscillators for which $m\ddot{x}=-Kx$ so that $x=A\sin[(K/m)^{\frac{1}{2}}t+\rho]$ with $K=4\pi^2\nu^2 mA^2$, where m is the atomic mass and ν the vibrational frequency of the atoms. For 0°K, the energy, $E=2\pi^2\nu^2 mA^2$, becomes the zero-point energy $E_0=h\nu_0\cong k\theta_D$, where θ_D is the Debye temperature, $h=6.6\times10^{-27}$ erg cm is Planck's constant, and $k=1.4\times10^{-16}$ erg/°K is Boltzmann's constant. Thus, A_0, the magnitude of the vibrational amplitude at absolute zero, becomes

$$A_0=(h/\pi)(2mk\theta_D)^{-\frac{1}{2}}. \tag{14a}$$

To this, $\bar{u}_0$, the root-mean-square displacement of the atoms at 0°K, is connected as $\bar{u}_0=A_0/\sqrt{2}$, so that

$$\bar{u}_0=(h/2\pi)(mk\theta_D)^{-\frac{1}{2}}. \tag{14b}$$

For temperatures T higher than θ_D the Einstein model would yield[13]

$$\bar{u}=(h/2\pi)\{mk\theta_E(e^{\theta_E/T}-1)\}^{-\frac{1}{2}}, \tag{14c}$$

with θ_E, the Einstein temperature, related to θ_D as $\theta_E=\frac{3}{4}\theta_D$. For $T\gg\theta_E$ this becomes

$$\bar{u}=(h/2\pi)(mk\theta_E)^{-\frac{1}{2}}(T/\theta_E)^{\frac{1}{2}}=\tfrac{4}{3}\bar{u}_0(T/\theta_D)^{\frac{1}{2}}. \tag{14d}$$

8. FRICTIONAL STRESS ON A DISLOCATION WHEN TAKING INTO ACCOUNT THE UNCERTAINTY IN THE AXIS POSITION

In the previous section it was shown that a dislocation axis is diffuse with a root mean square deviation of δ_A. Assuming a Gaussian distribution, we therefore find the energy of a dislocation core as

$$E_c=\frac{1}{\delta_A\sqrt{\pi}}\int_{-\infty}^{+\infty}U_c(x,s)\exp[-(x/\delta_A)^2]dx. \tag{15}$$

Following Eq. (1a), we assume U_c to vary sinusoidally with respect to x, the coordinate fixed with respect to the lattice, as well as s, the position of the dislocation axis, i.e., we introduce

$$\varphi=(2\pi/p)x+\varphi_0 \tag{1b}$$

to get

$$U_c=U_0+\tfrac{1}{2}\Delta U_c\cos\left(\frac{2\pi}{p}s+\frac{2\pi}{p}x+\varphi_0\right). \tag{1c}$$

[13] N. F. Mott and H. Jones, *The Theory of the Properties of Metals and Alloys* (Dover Publications, Inc., New York, 1936).

The lattice force on the dislocation then becomes

$$T\tau_D=\frac{1}{b}\frac{dE_c}{ds}=\frac{\Delta U_c}{2(\pi)^{\frac{1}{2}}\delta_A b}\left\{\frac{d}{ds}\int_{-\infty}^{+\infty}\exp[-(x/\delta_A)^2]\times\cos\left(\frac{2\pi}{p}x+\varphi(s)\right)dx\right\}, \tag{15a}$$

where $\varphi(s)=(2\pi/p)s+\varphi_0$, and the suffix T is meant to remind the reader that the diffuseness of the dislocation axis due to thermal motion is taken into account.

Equation (15a) can be solved by substituting

$$\cos[(2\pi/p)x+\varphi(s)]=\cos[(2\pi/p)x]\cos\varphi(s)-\sin[(2\pi/p)x]\sin\varphi(s).$$

The second of the resulting two integrals vanishes because the function $\exp[-(x/\delta_A)^2]\sin(2\pi/p)x$ is symmetrical in x, while the value of the first integral is given in the appropriate tables as

$$\int_{-\infty}^{+\infty}\exp[-(ax)^2]\cos Bx=\frac{\sqrt{\pi}}{a}\exp[-(B/2a)^2].$$

Finally, from Eq. (2a), we have $\Delta U_c/b=(p/\pi)\tau_{D\,\max}$ and thus, Eq. (15a) becomes

$$T\tau_D=\tau_{D\,\max}\frac{p}{2\pi}\exp[-(\pi\delta_A/p)^2]\frac{d}{ds}\times\left\{\cos\left(\frac{2\pi}{p}s+\varphi_0\right)\right\}. \tag{16}$$

$T\tau_{D\,\max}$, the smallest stress required for the continued motion of a dislocation, taking into account the uncorrelated vibrations of the atoms, then is given by

$$T\tau_{D\,\max}=\tau_{D\,\max}\exp[-(\pi\delta_A/p)^2]=\tau_{D\,\max}e^{-r_0/R_0} \tag{17}$$

if δ_A is expressed according to Eqs. (13c) and (11), and a critical radius R_0 is defined as

$$R_0(T)=(p/4\pi\bar{u})^2 p. \tag{17a}$$

For core radii larger than R_0, $T\tau_{D\,\max}$ is substantially smaller than $\tau_{D\,\max}$, the frictional stress calculated for a dislocation in a mathematically defined crystal lattice, while for r_0 smaller than R_0 it is $T\tau_{D\,\max}\cong\tau_{D\,\max}$.

We thus find a new type of temperature dependence for the frictional stress, which is *not* due to thermal activation. Thermal activation is caused by the *correlated* thermal motion of the atoms, while the present effect is due to the "uncertainty relationship" which is found for dislocations due to the *uncorrelated* atomic vibrations.

In order to gain some numerical result, let us take $p=b=2.8$ A and $\bar{u}_0=0.1$ A, a value probably appropriate for typical crystals at absolute zero temperature. Then $R_0\cong5b$. Actual dislocation core radii for almost

all substances and slip planes, with the exception of the common glide dislocations on the close packed planes in fcc and hcp structures, are smaller than this limiting value, since, according to Eq. (11), it corresponds to a critical stress amounting to only 4 or 5% of the modulus of rigidity. It would seem, then, that for glide dislocations on {111} in fcc crystals and {0001} in hcp crystals lattice friction becomes very small, even at the lowest temperatures.

Another numerical example may be linked to the measurements made of $\bar{u}$ for the cases of NaCl, KCl, and NaF.[14–17] At room temperature $\bar{u}$ was found uniformly at about $b/18$, and a measurement made for KCl at 86°K rendered $\bar{u}\cong b/30$. We again assume that $p=b$ and find $(R_0)_{\text{R.T.}}\cong 2b$, and $(R_0)_{86°\text{K}}\cong 5.5b$. With $r_0/b\cong\mu/5\tau_{\text{crit}}$ [see Eq. (11)] this means that a marked temperature dependence due to the cause under discussion is expected already at 86°K if, for the relevant slip planes in these substances, $\tau_{\text{crit}}\lesssim\mu/25$. If, on the other hand, $\tau_{\text{crit}}\cong\mu/10$, a much more likely value,[10] then the temperature effect would become marked at and above room temperature.

Finally, for diamond, germanium, and silicon, r_0, the core radius, is probably only about equal to the Burgers vector, corresponding to a large critical stress, and the present temperature effect in these materials can be expected to operate at very high temperatures only, if at all below their melting point.

In order to express the exponent $(\pi\delta_A/p)^2$ in terms of more obvious parameters we introduce $b/p=g\geq 1$, apply Eq. (14d) for $\bar{u}$, and make use of Lindemann's relationship that $\theta_D=C(T_M/AV^{\frac{2}{3}})^{\frac{1}{2}}$. In this latter equation T_M represents the melting temperature, A the atomic weight, V the atomic volume, and C a constant which is equal to 115 when cgs units are used.[13] After rearranging the terms and expressing $\tau_{D\,\max}$ and r_0 according to Eqs. (5a) and (11), we obtain, for an edge dislocation,

$$T\tau_{D\,\max}=\frac{\pi(1-\nu)}{4\mu}\tau_{\text{crit}}^2\exp\left[-f\frac{\mu g^3}{(1-\nu)\tau_{\text{crit}}}\frac{T}{T_M}\right], \quad (18)$$

while for a screw dislocation the factors $(1-\nu)$ are missing in the expression for $\tau_{D\,\max}$ as well as in the exponent.

The factor in the exponent varies somewhat with the crystal structure. It is given by

$$f=\frac{32h^2N^{5/3}}{9\pi kC^2}\left(\frac{a}{bw^{1/3}}\right)^2, \quad (18a)$$

with $g=b/p$, a the lattice constant, and w the number of atoms per unit cell. All the other symbols have the same meaning as before, namely, h=Planck's constant, N=Avogadro's number, k=Boltzmann's constant, C=Lindemann's constant, and b=Burgers vector. f is a dimensionless constant. For common crystal structures and lattice constants, f has a value close to 9×10^{-2}, but at best it is expected to be reliable only within the factor 2 or 3. Moreover, since Eq. (14d) was used, Eq. (18) will be fulfilled approximately for $T\gtrsim 2\theta_D$ but not for lower temperatures.

At the present moment it is doubtful how strongly the exponential factor in Eq. (18) will influence the frictional stress acting on glide dislocations in bcc metals. First, it will be necessary to make a more reliable determination of the critical parameter f. Furthermore, τ_{crit} must be evaluated as well as the parameter $g=b/p$, which, as pointed out already, may be different even for different dislocations on the same slip plane.

Actually, Eq. (18) is less suited for making numerical estimates about the level of the frictional stress than Eq. (17), mainly because Eq. (14d) is only very approximate. It was, however, introduced to show the expected dependence of $T\tau_{D\,\max}$ on the various parameters. Since the crystal structure probably determines the value of μ/τ_{crit} within fairly narrow limits, Eq. (18) shows that $T\tau_{D\,\max}/\mu$ depends only on T/T_M when comparing substances of the same type and crystal structure, as for example the bcc metals. We might understand, then, why sodium and potassium are so very soft at room temperature, whereas iron is of intermediate hardness, and tungsten, molybdenum and other high-melting bcc metals are quite strong up to several hundred degrees centigrade.

9. SUMMARY AND CONCLUSIONS

The contents and conclusions of the preceding investigation may be summed up into ten points.

(i) Most previous calculations of the frictional stress acting on moving dislocations in otherwise perfect crystals are unreliable. In them, the core energy of dislocations has been calculated by approximate methods and the frictional stress was gained through the differentiation of expressions for the core energies. The core energy fluctuations which correspond to typical frictional stresses derived in the past are in the order of one in two thousand to one in millions and less. It is clear that the accuracy of the approximate calculations of core energy could not possibly have reached the levels claimed for them implicitly.

(ii) By circumventing evaluations of the core energy, and instead considering the stresses and strains in the two atomic planes bordering the slip plane from either side, a general expression is obtained for the force acting on a dislocation in an arbitrary position.

(iii) Two fairly obvious assumptions are made to transform this general expression into an equation for

[14] I. Waller and R. W. James, Proc. Roy. Soc. (London) **117**, 214 (1927).
[15] R. W. James and E. M. Firth, Proc. Roy. Soc. (London) **117**, 62 (1927).
[16] R. W. James and G. W. Brindley, Proc. Roy. Soc. (London) **121**, 155 (1928).
[17] J. J. Schonka, Phys. Rev. **43**, 947 (1933).

$\tau_{D\,\max}$, the minimum stress which must be applied externally for the sustained motion of a dislocation in an otherwise perfect lattice. A trick is then used to rewrite the equation into a very simple form, which is $\tau_{D\,\max}=(b/8r_0)\tau_{\text{crit}}$, with r_0 the radius of the dislocation core, and with τ_{crit} the critical shear stress of the slip plane if no dislocations are present.

(iv) The equation $\tau_{D\,\max}=(b/8r_0)\tau_{\text{crit}}$ is tested by applying it to the Peierls-Nabarro dislocation and comparing that result with the numerical answer obtained from the relationship before simplification. Since the two answers differ by only 12.5% it is assumed that the simplified equation is adequate.

(v) The above equation for $\tau_{D\,\max}$ is used to determine the magnitude of the frictional stress for common glide dislocations in typical close packed lattices, as well as the corresponding fluctuations in core energy. These are found as $6\times10^{-4}\mu$ for edge dislocations, $9\times10^{-4}\mu$ for screw dislocations, and a fractional change of about 0.2% in core energy. The frictional stresses acting on dislocations in other structures are substantially higher.

(vi) Knowing that dislocations in close packed metals, like Zn or Al, move at very much lower stress levels than those calculated, a reason is sought why the frictional stress does not necessarily operate. Several such reasons have been discussed in the past. Some of them including thermal activation, are probably most important in nature, while other effects are found to be insignificant in the framework of the calculations given.

(vii) One effect, which the author believes to be very important, apparently was overlooked in previous investigations. It may be called the "uncertainty relationship for dislocations." Due to the fact that atoms are not mathematical points, but vibrate, their positions do not ideally conform to the pattern of a dislocation with a precisely defined axis. An uncertainty in the position of the dislocation axis exists which is similar to, or several times larger than, $\bar{u}$, the root mean square displacement of the crystal atoms.

(viii) Unfortunately, only a very few measurements of $\bar{u}$ are available, and no reliable simple relationships exist to connect it to other known parameters. However, the best estimates which can be made at this time indicate that the uncertainty in the position of dislocation axes is effective to reduce the level of the frictional stress on common glide dislocations in crystals with close packed lattices, even at the lowest temperatures. They further indicate that no great reduction in $\tau_{D\,\max}$ may be expected from this effect for dislocations in materials with a diamond structure. Salts of the NaCl type, and perhaps bcc metals, represent intermediate cases.

(ix) With the help of Einstein's formula for $\bar{u}$, on the one hand, and Lindemann's relationship, $\theta_D=C(T_M/AV^{\frac{2}{3}})^{\frac{1}{2}}$, on the other, the following formula for the frictional stress is found:

$$\tau\tau_{D\,\max}=\frac{\pi(1-\nu)}{4\mu}\tau_{\text{crit}}^{2}\exp\left(-f\frac{\mu g}{(1-\nu)\tau_{\text{crit}}}\frac{T}{T_M}\right).$$

Although the numerical value of f is somewhat uncertain, the type of dependence of the frictional stress on the critical stress, τ_{crit}, and on T_M, the temperature of melting, is interesting and seems to fit the observations on bcc metals.

(x) From the level of the frictional stresses, it is possible to calculate the fluctuations of core energy. This should be helpful in future calculations on the role of thermal activation in this field of effective lattice friction. On the basis of the formulas developed it is also possible to treat the case of changes in core energy which are not simply sinusoidal. For this, two or more solutions will be superimposed on each other.

ACKNOWLEDGMENTS

It is a pleasure to acknowledge stimulating discussions with my colleagues, Dr. N. Brown and Dr. J. N. Hobstetter, with Dr. K. Atkins, Department of Physics of the University of Pennsylvania, and with Dr. J. Bursk and Dr. R. Clelland, Department of Economics and Social Statistics of the University of Pennsylvania. Special thanks are due to my husband, Dr. H. G. F. Wilsdorf, of the Franklin Institute, Philadelphia, for many valuable suggestions and criticisms.

The financial support of the Office of Scientific Research of the Air Force is gratefully acknowledged.