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Abstract

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PHYSICS

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ON THE STRUCTURE OF A DISLOCATION IN A CRYSTAL LATTICE AND THE MECHANISM OF DISLOCATION MULTIPLICATION

(Presented by Academician I. V. Obreimov, 5 X 1965)

The properties of a dislocation in a crystal are determined by its atomic structure and depend on the physical nature of the violations of periodicity created by the dislocation in the lattice. At large distances from the dislocation axis the violation of periodicity can be described by small displacements of the lattice nodes. But the physical properties of a dislocation in a crystal depend extremely strongly on the disturbances it produces at small distances from its axis, where these disturbances are maximal. If it is assumed that here these disturbances can likewise be reduced only to displacements of the lattice nodes (as at large distances), then, naturally, the problem arises of finding the positions of the particles of the crystal in the region immediately adjacent to the dislocation axis. Such a problem has been considered many times with the use of various microscopic models and under various assumptions concerning the law of the forces of interatomic interaction (see, for example, ([1], [2])). In doing so, such a property of the crystal as the periodicity of its structure ([3]) was taken into account, while another very important property of the crystal—the finiteness of the disordering energy of its structure (the heat of fusion)—was usually left aside. It was always assumed *a priori* that a stable equilibrium configuration of the particles near the axis, corresponding to the minimum of the energy of the crystal with a dislocation, exists, and that equilibrium is attained by realizing such a configuration through static displacements, independently of the magnitude of the latter. This means that the atomic structure of the dislocation was considered, in essence, in a crystal with an infinitely large disordering energy (and with thermal motion neglected). However, the finite magnitude of this energy (the threshold properties of the medium) excludes the possibility of the existence of arbitrarily large displacements of particles in the crystal without its losing stability. Therefore a static equilibrium configuration of particles near the dislocation axis may be excluded by the stability conditions of the crystal.

1. Thermal fluctuations cannot lead to the nucleation in a perfect crystal of *stable*, i.e. noncollapsing spontaneously, dislocation loops (at temperatures far from the melting point) until an external tangential stress of

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order $G/30$ ([4]) is applied to the crystal. Meanwhile, an estimate (in the approximation of a Debye continuum) of the tangential stresses due to thermal fluctuations and arising at an individual point of the crystal shows that such "thermal" stresses reach the magnitude of the theoretical shear strength of the crystal ([5]). At points of the crystal where critical strains are reached by fluctuation, the stability of the lattice with respect to shear is lost and dislocation loops are nucleated. However, since a "favorable" fluctuation in a perfect crystal cannot encompass a large volume of the crystal ($\sim 2b^3$, where b is the Burgers vector) ([5]), the sizes of the dislocation loops formed by fluctuation turn out to be smaller than the critical ones ($R_{\text{cr}} \sim 10^4 b$ ([4])), necessary for stability.

loops. Such fluctuational, unstable dislocation loops exist in the crystal for a time which apparently does not exceed the period of thermal vibrations (the lifetime of the loops is $\sim \nu_D^{-1} \sim 10^{-13}$ sec, ν_D being the Debye frequency), and collapse. Only if an external shear stress of the order of $G/30$ (G is the shear modulus) [(4)] is applied to the crystal and the critical shear deformations ($\sim 1/30$) are reached, does the crystal lattice become unstable with respect to shear—the dislocation loops arising by fluctuation in a perfect crystal

[Fig. 1 and Fig. 2 diagrams]

Fig. 1. Scheme of the process of fluctuational nucleation and annihilation of statistical dislocation loops in the region of the physical core of a dislocation. AB is the dislocation axis. Dashed lines conventionally outline the region of the physical core

Fig. 2. Scheme of nucleation of secondary statistical loops and the true size of the double kink

turn out to be stable, i.e., they do not collapse, but propagate through the crystal—shear arises.

2. Let us consider an infinitely extended crystal containing one rectilinear dislocation (for definiteness, an edge dislocation) along the z-axis of a rectangular coordinate system, whose slip plane is $y = 0$, and whose Burgers vector b is directed along the x-axis. The shear deformation e_{xy} which this dislocation produces at some point on the x-axis is

$$e_{xy}(x) = \frac{b}{2\pi(1-\nu)x} + o(b/x)$$

(the isotropic case), where ν is Poisson' s ratio [(6)]. If we move the point toward the origin of coordinates, the shear deformation at this point will increase and, at some distance x_k from the origin, will reach the critical value e_{xy}^k, corresponding to the theoretical strength of the crystal. Assuming that $e_{xy}^k \sim 1/30$, $\nu = 1/3$, we obtain the estimate

$$x_k \sim b/2\pi(1-\nu)e_{xy}^k \sim 7.5\,b.$$

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The deformations in the slip plane $y = 0$ caused by the dislocation in the crystal exceed the critical value at all points $x \leq x_k$. Thus the crystal lattice in an entire region of the crystal adjacent to the dislocation axis proves to be unstable with respect to shear—the dislocation loops arising there by fluctuation prove to be stable. The boundaries of this region, which we shall call the **physical core of the dislocation**, are determined by the equation $e_{xy}(x, y) = e_{xy}^k =$ const. The term "physical" is intended to emphasize the difference from the definition, accepted in the continuum theory of dislocations, of the elastic core of a dislocation as simply the region where the linear theory of elasticity [6], or the theory of elasticity in general [1,2], is invalid. The boundaries of the elastic core are to a large extent conventional, as is the division of the crystal into two regions (the elastic core and "not core"). The boundaries of the physical core, however, separate two regions of the crystal that differ in the physical state of the crystal lattice: it is unstable to shear in the core region and stable outside the core.

3. The instability of the crystal lattice to shear in the region of the physical core of a dislocation leads to the nucleation there, owing to thermal

···of new fluctuations, stable (and, consequently, expanding) dislocation loops. If the dimensions of such loops were much smaller than the dimensions of the region where the stresses responsible for the appearance of these loops are sufficiently large, then the appearance of the loops would have little effect on the state of the crystal in this region. However, the dimensions of the stable loops that arise (radius $R \sim 2b$ [4]) turn out to be comparable with the dimensions of the region under consideration (Fig. 1). Therefore the deformation (and stress) field of each such dislocation loop compensates the field of the original rectilinear dislocation that caused its nucleation and expansion (in a region $\sim R$). A peculiar local relaxation of the stress of the initial dislocation occurs in the vicinity of the nucleated loop. Since this thereby eliminates the cause that initiated the nucleation and ensures the stability of the given loop, it must collapse (its lifetime may be estimated as $t \geq 3x_k/c_t \sim 10^{-12}$ sec, i.e., it is a "long-lived" loop; c_t is the velocity of propagation of shear waves). At subsequent moments the whole process will be repeated from the beginning with a frequency determined by the probability of nucleation of dislocation loops. Relaxation thus has a statistical character. The process considered schematically in the slip plane can be illustrated by successive drawings for one nucleated loop (Fig. 1). It is seen that the interaction of the fluctuation-nucleated loop (let us call it statistical) with the initial dislocation may be described as the appearance of an unstable double kink on the dislocation axis. Its height is $a \sim 2x_k \sim 15b$. To determine correctly the shape of the kink, i.e., the ratio a/r (see Fig. 2), it is necessary to take into account the secondary processes occurring near the dislocation line after the fluctuation nucleation of one statistical loop.

Fig. 3. Shape of the physical core of a screw dislocation in alkali-halide crystals LiF and RbJ, described by the equation $e_{yz}(x, y) =$ const (allowing for elastic anisotropy according to [11]). b is the Burgers vector for the corresponding

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Fig. 3. Shape of the physical core of a screw dislocation in alkali-halide crystals LiF and RbJ, described by the equation $e_{yz}(x, y) = \text{const}$ (allowing for elastic anisotropy according to ([11])). b is the Burgers vector for the corresponding crystal.

Figure 1: Fig. 3. Shape of the physical core of a screw dislocation in alkali-halide crystals LiF and RbJ, described by the equation $e_{yz}(x, y) = \text{const}$ (allowing for elastic anisotropy according to ([11])). b is the Burgers vector for the corresponding crystal.

crystal.

In the region where the deformation fields of the initial dislocation and of the nucleated loop are superposed, there is practically activationless nucleation of new (secondary) statistical loops during a time $t_0 \sim 10^{-13}$ sec. Since the lifetime of these loops is an order of magnitude greater than t_0, about ten of them will nucleate around the primary loop before it collapses (see Fig. 2). Then for the double kink formed as a result of the interaction of all these loops, the ratio $a/r \sim 0.1$, and the length $r \sim 10^2 b$. The sequence of drawings $1a, d, e$ (without the intermediate stages b, c, g) very much recalls the scheme for the formation of a priori double kinks developed by Seeger ([7]) for the Peierls—Nabarro model. However, we see that the appearance of double kinks and their geometry are a consequence of rather general properties of a crystal lattice containing a dislocation and need not be considered a priori. The Peierls potential evidently has little influence on the process of nucleation of statistical loops, since the Peierls stress τ_p^0 ([8]) is much smaller than the critical stress $G/30$ corresponding to the boundary of the physical core. It is possible that the known difficulties that arise in Seeger' s scheme when it is compared with experiment ([9]) can be resolved within the framework of the model presented here.

4. Double kinks can become stable if a sufficient external shear stress is applied to the crystal. Its estimate according to ([10]) gives

$$\tau \sim \frac{Gb}{8\pi} \frac{1}{a} \left(\frac{a}{r}\right)^2 \sim G \cdot 10^{-5},$$

here $a = 15b,\ a/r = 0.1$. Under the action of such a stress, a double kink will propagate along the dislocation, moving it by the amount a, where a is the height of the kink. The elementary act of displacement of a dislocation during glide thus consists in moving it not by a distance equal to b, but by a quantity an order of magnitude larger ($a \sim 15b$).

5. Up to now the discussion has been limited to statistical dislocation loops that arise by fluctuation in the original glide plane containing the axis of the dislocation line. However, in parallel glide planes, separated from the original one, statistical dislocation loops also arise in the region of the

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Figure 4

Figure 2: Figure 4

physical core of the dislocation. If a tangential stress of sufficient magnitude is applied to the crystal, then such dislocation loops in glide planes parallel to the original one will propagate without limit in the crystal. But this will be nothing other than multiplication of the original dislocation. Multiplication may occur in any of the glide planes encompassed by the physical core of the dislocation. The number of such planes is determined by the size $2y_k$ of the physical core of the dislocation in the direction normal to the original glide plane. For example, for a screw dislocation in LiF, $2y_k \sim\sim 1/2x_k \sim 3b$, and in RbJ $2y_k \sim 4x_k \sim 20b$ (see Fig. 3).

Fig. 4. Scheme of the formation of a complex double kink on a dislocation. *a* —statistical loop in a glide plane parallel to the original one; *b* —complex double kink

The interaction of statistical loops from parallel glide planes with the original dislocation can be described as the formation of a complex double kink (Fig. 4). The stable propagation of such a kink under the action of an external tangential stress ensures the motion of the dislocation in a new glide plane. Since the phenomenon takes place simultaneously at many points of the initial dislocation line and encompasses glide planes at different distances, this means the beginning of the process of multiplication of the initial dislocation. We see that the propagation of shear in the original glide plane (motion of the dislocation) and the occurrence of shear in parallel planes (multiplication of the dislocation) are, in essence, phenomena of the same type, differing quantitatively rather than qualitatively.

The ability of a dislocation to multiply (multiplicativity) is as much an intrinsic property inherent in it as mobility, and is determined, evidently, by the properties of its physical core. Therefore, multiplication of dislocations may not require any special scheme, although the result of multiplication by means of such schemes (Frank—Read, double cross slip, etc.) can be described.

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