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MOBILITY OF DISLOCATIONS IN A LATTICE WITH LARGE PEIERLS BARRIERS

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The mobility of dislocations under the action of an applied stress is considered. The basic mechanism of motion is activation. The cases of small and large stresses are investigated in detail and also long and short dislocations. A comparison of the calculation with the experimentally observed power-law dependence of the dislocation velocity on the stress is made.

1. INTRODUCTION

IN substances with a large Peierls barrier (Ge, Si, Fe, and others) the motion of the dislocations depends upon an activation mechanism: a dislocation ejects a segment bounded by two kinks (a double kink, see Fig. 1) into a neighboring potential valley. The time for formation and expansion of such a segment determines the mobility of the dislocations.

Experimental investigations of the mobility of individual dislocations have been carried out on germanium[1,2] and silicon.[3] The results of articles[1,3] are described by an empirical formula of the form

$$v = \text{const}\cdot\sigma^m e^{-U/T}, \tag{1}$$

where v denotes the dislocation velocity, σ is the stress, and m and U are constants.[1)] Formula (1) confirms the activation character of the motion. Here the power-law dependence of v on σ is nontrivial. Apparently the stress in the indicated experiments is not too large so that U does not depend on σ. Such a dependence was observed in experiments on plastic flow in the transition metals (see the review[4]).

The goal of the present article is a theoretical investigation of the dependence of the dislocation velocity on the applied stress, when it is small in comparison with the Peierls stress σ_P, and also an investigation of the dependence on the length of the dislocation.

In a series of articles (see the review articles[4,5]) the activation energy $U(\sigma)$ was investigated in the case when the stress σ is comparable with σ_P. A simple model of a dislocation is usually used: a string positioned in potential profile. The quantity $U(\sigma)$ is found from a solution of the mechanical problem for a nonlinear string.[2)] Such a treatment is valid for sufficiently large stresses. Namely, it is necessary that the work σb^3 of the external forces over a lattice period b should be large in comparison with the fluctuation energy T. For the case of small stresses Lothe and Hirth[6] have proposed another treatment, which we shall follow below.

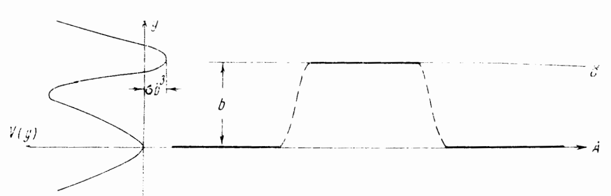

FIG. 1

2. MODEL OF STRAIGHT SEGMENTS

It is assumed that the dislocation segment which is ejected into a neighboring valley lies at the bottom (see Fig. 1). This means that it is found in a state of metastable equilibrium with the crystal. The free energy F of a sufficiently long dislocation segment is determined by the formula

$$\mathcal{F}(l) = 2U_0 - \sigma b^2 l - \alpha / l \quad (l \gg b). \tag{2}$$

Here l denotes the length of the segment, U_0 denotes the energy of one kink, the second term is equal to the gain in energy due to the applied stress, and the third term describes the attraction between kinks. By definition the force of linear attraction is given by

$$p = -\frac{\partial \mathcal{F}}{\partial l} = \sigma b^2 - \frac{\alpha}{l^2}. \tag{3}$$

This force tends to decrease small segments with length $l < l_c$ and to increase large ones with $l > l_c$ where $l_c = (\alpha/\sigma b^2)^{1/2}$ (see also[7]).

In such a formulation, the problem reduces to the well-known problem of the formation of a nucleation center in a metastable phase. A dislocation in trough A plays the role of the metastable phase, the stable phase corresponds to a dislocation in trough B (Fig. 1). The difference between our problem and the well-known problem of the formation of droplets in a supercooled gas (or bubbles in a superheated liquid) (see[8]) lies not only in the number of dimensions but primarily in the small difference between the phases. In the problem about the condensation of droplets, for example, the difference between the density of the liquid and the density of the gas is very important. Because of this a density gradient appears in the gas, and the growth of a droplet is determined by a diffusion current across its surface. In our case the density of the string's particles is identical in the different "phases". In such a situation diffusion growth of a segment is impossible. The motion of its boundaries due to a difference of the linear stresses p in the different phases (see Eq. (3)) is another simple mechanism for the growth of a segment.

We note that our treatment is correct upon fulfillment

[1)]The results of the measurements on Ge by Kabler [2] appear to be different. In this connection, however, see the criticism in articles [1,3].

[2)]We note that the critical size l_c of a double kink is determined incorrectly in [4]. In particular, for small values of σ one must have $l_c \sim |l n\sigma|$.

of the following conditions. The height of the Peierls barrier $U_0 \gg T$ so that transitions from one valley to another take place very slowly. In this case one can assume that long dislocation segments are able to reach a state of equilibrium with the medium and that the transition of a dislocation into a neighboring valley is a slow diffusion process.

3. DIFFUSION OF SEGMENTS ACCORDING TO SIZES

During the time of growth of a segment of critical dimensions (if it is large in comparison with b) the motion of the boundaries (kinks) is able to become steady. The velocity w of the steady-state motion is determined by a balance of the difference in stresses and the force of friction. Without going into a detailed investigation of the dissipative processes, let us introduce the mobility μ:

$$w = \mu p. \tag{4}$$

Equation (4) determines the change in the length l of the segment due to the difference in the stresses p. Thermal fluctuations lead to random changes of l. In order to describe the growth of a segment, we introduce a distribution function $f(l, t)$ which obeys the diffusion equation:

$$\frac{\partial f}{\partial t} + \frac{\partial j}{\partial l} = 0, \tag{5}$$

$$j = -D\frac{\partial f}{\partial l} + 2wf = -D\frac{\partial f}{\partial l} + 2\mu\left(\sigma b^2 - \frac{\alpha}{l^2}\right)f. \tag{6}$$

The diffusion coefficient D is related to the mobility μ by the Einstein relation so that j = 0 in the static case, and the distribution function f becomes a Boltzmann distribution:

$$f = Ae^{-\mathcal{F}(l)/T}. \tag{7}$$

It is assumed that in the initial state (t = 0) short segments of length smaller than a certain value $l_1 \ll l_c$ are able to reach thermodynamic equilibrium and are described by the functions (7), but for $l > l_1$ the function $f(l, 0)$ vanishes.

For large transition times τ in the quasisteady-state approximation one can regard the probability current j as constant in the initial stage of the process. From Eq. (5) it is seen that j is connected to τ by the relation $j = 1/\tau$. Using Eq. (6) we find

$$j = 2\mu TA \int e^{\mathcal{F}(l)/T}\, dl, \tag{8}$$

where the constant $A = e^{\mathcal{F}(0)/T}f(0, 0)$ (see Eq. (7)). Of course, $l = 0$ should not be understood literally. As the zero region of distances we admit distances which are smaller than l_1 but large in comparison with b. For us it is important that the constant A does not depend on the applied stress and does not contain an exponential dependence on 1/T. A has the dimensions of an inverse length. We shall regard the value of $A \sim b^{-1}$.

From Eq. (8) we find the following expression for τ:

$$\tau = \frac{b}{2\mu T}\int_0^\infty e^{\mathcal{F}(l)/T}\, dl. \tag{9}$$

Using Eq. (2) we reduce the expression for τ to the form

$$\tau = \frac{e^{2U_0/T}}{\mu T}\left(\frac{\alpha}{\sigma}\right)^{1/2} K_1\left(\frac{2b\sqrt{\alpha\sigma}}{T}\right), \tag{10}$$

where K_1 is the Macdonald function.

In the limiting case of large stresses ($\sigma \gg \sigma_0 = T^2/4\alpha b^2$) from Eq. (10) we obtain

$$\tau = \frac{\alpha^{1/4}\sigma^{-3/4}}{\mu\sqrt{2\pi bT}}\exp\left\{\frac{2(U_0 - b\sqrt{\alpha\sigma})}{T}\right\}. \tag{11}$$

This is a case customarily encountered in statistics, when nucleation centers with dimensions close to critical give the major contribution to the transition.

In the other limiting case of small values $\sigma \ll \sigma_0$, values of $l \sim T/\sigma b^2$ introduce the major contribution to the integral (9). This is associated with the fact that the fluctuations of the length in the region of an extremum of $\mathcal{F}(l)$ are large. In this connection

$$\tau = \frac{1}{2\mu\sigma b}e^{2U_0/T}. \tag{12}$$

In what follows we shall understand by l_c the characteristic values of the lengths of the segments, i.e., $l_c = \sqrt{\alpha/\sigma b^2}$ for $\sigma \gtrsim \sigma_0$ and $l_c = T/\sigma b^2$ for $\sigma \lesssim \sigma_0$. The limiting cases of small and large values of σ were first investigated by Lothe and Hirth.[9]

4. VELOCITY OF INDIVIDUAL DISLOCATIONS

Now let us consider a dislocation of total length L. In order of magnitude the average number of segments N(L, t) ejected into valley B during a time $t \ll \tau$ is given by

$$N(L, t) = \frac{L}{l_c}\frac{t}{\tau}. \tag{13}$$

In fact, τ is the time for the creation of a nucleation center of critical dimensions. The probability for the appearance of such a nucleation center in a dislocation segment of length l_c is equal, in order of magnitude, to t/τ. One can determine the number of nucleation centers appearing in a dislocation of length L during a time t by dividing it mentally into segments of length L_c and multiplying the number of such segments by the probability for the appearance of a nucleation in each of them. It is assumed that in regard to the attainment of critical dimensions by a nucleation, the kinks move rapidly so that the time, during which a dislocation goes from one valley to the other, is appreciably smaller than τ.

According to Eq. (13) the average number of nucleation centers appearing per unit time and per unit length is equal to $1/l_c\tau$. However, according to Lothe and Hirth,[9] this quantity is equal to $1/b\tau$ (in our notation). This leads to an essential difference in the dependence of the velocity on the stress: instead of $v \sim \sigma^{3/2}$ (formula (17)) $v \sim \sigma$ is obtained. The reason for the discrepancy consists in the fact that in[9] nucleation centers being formed at distances smaller than l_c from each other were actually assumed to be independent. In fact, one should identify them because they combine, not yet having achieved critical dimensions (before the stage of expansion with constant velocity $2w = 2\mu\sigma b^2$).

Let $N(L, t) \gg 1$. Then the average distance between segments is equal to $l_c\tau/t$. The nucleation centers enlarge with a constant velocity 2w so that after a time of order $t' = l_c\tau/wt$ the entire dislocation crosses into the neighboring valley.

We shall assume that the expansion takes place sufficiently rapidly so that $t' \ll \tau$. In this case the value of t' coincides with t in order of magnitude. From here we obtain

$$t=\sqrt{l_c\tau/w},\qquad l'\equiv wt=\sqrt{l_c w\tau}. \tag{14}$$

The velocity v of the dislocation is determined by the formula

$$v=b/t=b\sqrt{w/l_c\tau}. \tag{15}$$

Formula (15) is valid under the assumption $L \gg l'$. In the opposite case the time for a transition of the dislocation into the neighboring valley is equal to $\tau l_c/L$ and the dislocation velocity is given by

$$v=bL/\tau l_c. \tag{16}$$

Thus the velocity of dislocations linearly depends on their length for small $L < \sqrt{l_c w \tau}$ and does not depend on L for $L > \sqrt{l_c w\tau}$. This conclusion is evidently in qualitative agreement with experiment[3], in which the dependence of v on the radius of a dislocation loop was measured.

In the region $L > \sqrt{l_c w \tau}$ the velocity v depends on the stress in the following way:

$$v\sim\mu b^{7/2}T^{-1/2}\sigma^{3/2}e^{-U_0/T},\qquad \sigma\ll\sigma_0, \tag{17}$$

$$v\sim\mu b^{11/4}\alpha^{-3/8}T^{1/4}\sigma^{9/8}\exp\left\{-\frac{U_0-b\sqrt{\alpha\sigma}}{T}\right\},\qquad \sigma\gg\sigma_0. \tag{18}$$

In the region of a linear increase of the velocity with length, the coefficient associated with L in two limiting cases is given by

$$v/L\sim\mu b^4T^{-1}\sigma^2e^{-2U_0/T},\qquad \sigma\ll\sigma_0. \tag{19}$$

$$\frac{v}{L}\sim\mu b^{5/2}T^{1/2}\alpha^{-3/4}\sigma^{5/4}\exp\left\{-\frac{2(U_0-b\sqrt{\alpha\sigma})}{T}\right\},\qquad \sigma\gg\sigma_0. \tag{20}$$

Let us emphasize that an exponential dependence on 1/T may also be contained in μ (a Peierls barrier of the second kind). For very small stresses the kink moves so slowly that a segment of critical size is not able to "get started" during the time of its formation. Then, in order of magnitude τ agrees with the time for the advance of the dislocation by one lattice constant. In this case

$$(\sigma b^3\ll Te^{-2U_0/T}),\quad v=b/\tau. \tag{21}$$

We emphasize that the estimates obtained by us for the velocity of motion of dislocations only pertains to the case of sufficiently long dislocations, namely $L \gg l_c = T/\sigma b^2$. In this case the dislocation moves by ejecting a double kink of size l_c into the valley with a smaller value of the energy. In the opposite case, $L < l_c$, the whole dislocation undergoes random jumps. The time for a single jump is determined by formula (9), where the integration is carried out from 0 to L. A directed motion arises due to the small difference in the frequencies of jumps along and opposite to the direction of the acting forces. The corresponding value of the dislocation velocity is given by

$$v=2\mu\sigma b^2e^{-2U_0/T}=b/\tau. \tag{22}$$

Thus, for very small lengths L the velocity becomes a nonvanishing constant quantity. A schematic graph of the velocity as a function of the length is given in Fig. 2.

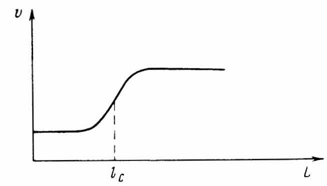

FIG. 2

The dependence of v on σ and on L is usually observed in an experiment. In this connection, it is not known beforehand to what range of parameters a given experiment refers. Therefore one can actually only talk about the exponent m in the empirical formula (1) or about the dependence of the activation energy on σ. In the case of long dislocations the different dependences of v on σ for small ($\sigma \ll \sigma_0$, formula (17)) and large ($\sigma \gg \sigma_0$, formula (18)) stresses correspond to the different dependences of v/L for short dislocations (formulas (19) and (20)).

The most detailed experiments with regard to measurements of the velocity of motion of individual dislocations were carried out on germanium and silicon.[1,3] Experiments on silicon give m = (3/2) ± 0.1, an activation energy which does not depend on σ, and a linear dependence of v on L for small lengths in complete agreement with our theory (the case of small stresses). Unfortunately the dependence of v/L on σ for small lengths was not measured.

The experiments on germanium[1] give values for m between the limits 1.0–1.2. It is possible that in this case the mobility of the kinks is small. There are no measurements of the dependence of the dislocation velocity in germanium on their length.

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