COMPARISON OF THEORY OF DISLOCATION MOBILITY WITH EXPERIMENTAL DATA FOR SILICON

V. N. EROFEEV and V. I. NIKITENKO

Institute of Solid State Physics, USSR Academy of Sciences

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Results are presented of an experimental study of the dependence of the velocity of individual dislocations on the stress, temperature, and length of the dislocation line in silicon single crystals. The obtained data are analyzed on the basis of the theories of dislocation mobility in crystals with high Peierls barriers. It is shown that in the investigated interval of stresses (1–50 kg/mm^2) and temperatures (500–800° C), they agree qualitatively with the diffusion theory of formation of a double kink. Discrepancies are noted between the experimental data and the predictions of the theory with respect to the critical dimension of the dislocation, which determines the dependence of the dislocation velocity on the length.

THEORIES have been recently developed (a review of the work performed prior to[1-2] is given in[3-6]), describing the laws of dislocation motion in crystals with high Peierls barriers both for the case of large applied stresses τ (comparable with the Peierls stresses τ_p) and for the case of small τ. In particular[1,5,7], a power-law dependence was obtained for the velocity of individual dislocations v on τ ($v \sim \tau^m$, $m \approx 1.2-1.5$), and this law describes the experimental data for Si single crystals[8,9], which are characterized, according to the unanimous opinion of the investigators, by high Peierls barriers.

So far, however, no comparison has been made of the theoretical and experimental results of investigations of dislocation mobility in these crystals in a wide stress interval. We present in this paper the results of an experimental study of the velocity of individual dislocations in silicon on the stresses and the temperature in wide ranges of their variation and compare the results with the corresponding theories.

EXPERIMENTAL RESULTS

The measurements were performed on samples cut from dislocation-free single crystals of undoped n-Si[1)] ($n = 1.8 \times 10^{14}$ cm^{-3}), using a previously described procedure[8,9]. The external load was applied with the aid of four-support flexure, and the dislocations were revealed by selective chemical etching. For experiments with high stresses (30–100 kg/mm^2), the samples were prepared with particular care, to prevent surface damage that causes premature failure of the crystal. After growing isolated dislocation half-loops with diameter $\sim 200\ \mu$ from a scoring mark (under the influence of small loads during the process of high-temperature flexure), the sample was chemically polished in a solution 1Hf : 7HNO$_3$ until the layer damaged in scoring was completely removed, and etched in a solution 1HF : 3HNO$_3$: 2CH$_3$COOH to reveal the initial placement of the dislocations. The sample was then placed on carefully polished cylindrical supports, the distance between which was such that the marks left by the supports of the preceding loading remain outside the stressed region. The load was applied smoothly. The rise time of the τ pulse did not exceed 5% of the pulse duration.

The samples were oriented so that their broad face was the {100} plane and their lateral faces the {110} planes. With such an orientation, the Burgers vector of the dislocation half-loops lying in two equivalent glide planes {111} was directed into the interior of the material along one of the two ⟨110⟩ directions and dislocations of different types, 60° and screw, emerged on the {100} surface of the sample. Some differences between the shapes of the etch pits belonging to one half-loop were observed, but no significant difference in the velocities of dislocations of different orientations were observed.

The results of the measurements of the velocities of individual dislocations v as functions of the tangential stresses τ at temperatures 500–800° C are shown in Fig. 1 in coordinates log v and log τ. We see from the figure that the $v(\tau)$ dependence can be described by the expression $v \sim \tau^m$. The exponent m changes insignificantly with changing temperature: when the latter increases from 500 to 800° C, the exponent decreases from 1.43 to 1.30.

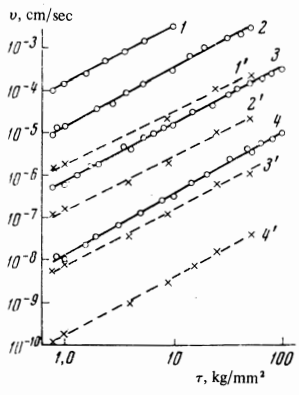

FIG. 1. Dependence of the velocity of individual dislocations v on the tangential stresses τ in undoped silicon at temperatures 800° (1, 1′) 700° (2, 2′), 600° (3, 3′) and 500° C (4, 4′). The solid lines (1–4) denote the experimental results: $m_1 = 1.30$, $m_2 = 1.33$, $m_3 = 1.35$, $m_4 = 1.43$. The dashed curves (1′–4′) describe the results of calculations by formula (7): $m_1' = 1.28$, $m_2' = 1.30$, $m_3' = 1.33$, $m_4' = 1.38$.

[1)] The sign of the charge and the carrier density were caused by the phosphorus impurity remaining in the initial raw material after zone purification.

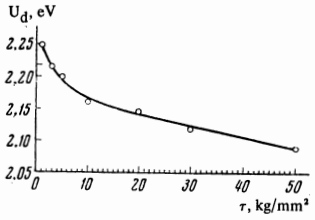

FIG. 2. Dependence of the activation energy of the dislocation motion U_d on the stress τ (experimental data).

The dependence of the velocity on the temperature at constant stress has a form typical of thermal-activation processes: $v \sim \exp\{-U_d(\tau)/kT\}$, where k is the Boltzmann constant and U_d is the effective activation energy of dislocation motion. A plot of the function $U_d(\tau)$ is shown in Fig. 2.

To study the influence of the dislocation length L on the velocity v, the dislocations were introduced by three-point flexure. In the center of the sample, under the central support, where the stresses were maximal, the dislocations extended over almost the entire width of the face (~ 2 mm). With decreasing distance to the end supports, the dimensions of the produced half-loops continuously decreased, in accordance with a linear decrease of the tangential stresses to zero. The sample was subsequently bent in accordance with a four-point scheme. A section of the sample with half-loops of different diameters (20—2000 μ) was in the zone of constant stresses.

No dependence of the dislocation velocity v on the diameter of the dislocation half-loops (on the length L) was observed. For the investigated half-loop dimensions, this agrees with the results of[8].

DISCUSSION OF RESULTS

The most important parameter determining the thermally-activated displacement of a dislocation in a field of Peierls forces is the energy of formation of a double kink of critical dimension U_k. At a low stress level $\tau \lesssim 0.1\ \tau_p$, the $U_k(\tau)$ dependence is given by[1]

$$U_k = 2(U_0 - \sqrt{\alpha a b \tau}) = 2(U_0 - \beta\sqrt{\tau}), \qquad (1)$$

where U_0 is the energy of one kink, a is the minimum distance between neighboring valleys of the potential relief, b is the modulus of the Burgers vector, α is a parameter determining the interaction of two kinks forming a pair, and $\beta = \sqrt{\alpha a b}$. The quantity α can be calculated from the results of[6] by means of the formula

$$\alpha = \frac{Ga^2b^2}{8\pi(1-\nu)}[(1+\nu)\cos^2\varphi + (1-2\nu)\sin^2\varphi],$$

where G is the shear modulus, ν the Poisson coefficient, and φ the angle between the direction of the dislocation line and the Burgers vector. For a 60° dislocation in silicon, $\alpha = 4.67 \times 10^{-20}$ dyne-cm^2 and $\beta = 7.72 \times 10^{-18}$ dyne$^{1/2}$ cm^2.

If we assume, as was done up to now[10-12], that the experimentally obtained activation energy of dislocation motion U_d is equal to the energy of formation of the double kink U_k, then the energy of one kink $U_0 = 1.175$ eV (1.88×10^{-12} erg) can be calculated from the value $U_d = 2.25$ eV at a low value of the stress, close to the starting value, $\tau = 1$ kg/mm^2, when formula (1) should be valid. On the other hand, the energy of one kink, determined by minimizing the linear energy of a dislocation with a kink[4], is equal to

$$U_0 = \frac{2E_0 a}{\pi}\left(\frac{2\tau_p' ab}{\pi E_0}\right)^{1/2} \qquad (2)$$

in the case of a sinusoidal relief and

$$U_0 = \frac{\pi^{3/2}E_0 a}{8}\left(\frac{2\tau_p' ab}{\pi E_0}\right)^{1/2} \qquad (3)$$

for a relief of quasiparabolic form.

After substituting the linear dislocation energy $E_0 \approx Gb^2/2$ and the value of U_0 obtained above from (2) and (3), we can determine the Peierls stresses. The calculated values $\tau_p^s = 160$ kg/mm^2 and $\tau_p^k = 140$ kg/mm^2 exceed by only a factor of three the maximum stresses in experiments on the measurement of $U_d(\tau)$. For such τ, the dependence of the energy of production of a double kink on the stresses should be determined not by Eq. (1), but by an equation obtained from a solution of the mechanical problem for a nonlinear string[13]

$$U_k = 2\int_{y_0}^{y_{max}} \{V(y)^2 - [\tau b(y - y_0) + V(y_0)]^2\}^{1/2}\, dy. \qquad (4)$$

Guyot and Dorn[4] carried out a numerical integration of (4) for different reliefs V(y) and plotted[2] $U_k(\tau/\tau_p)$. Using their plot, it is possible to show that the energy of formation of a double kink (and, as we have assumed, the energy of activation of the dislocation motion) should decrease by almost a factor of two in the investigated stress interval. This does not agree at all with the experimental data (Fig. 2).

Consequently, our assumption that the activation energy of dislocation motion is equal to the energy of formation of a double kink has been found to be incorrect. We assume then that the measured effective activation energy of dislocation motion corresponds to the energy of one kink. In this case the estimate of the Peierls stresses yields $\tau_p^s = 640$ kg/mm^2 and $\tau_p^k = 560$ kg/mm^2. The external stresses τ now fall in the interval where the formation of the double kink is described by the diffusion theory. We shall therefore from now on compare the experimental data with the results of[1,5,7].

According to the diffusion theory, the form of the dependence of the dislocation velocity on the stress and on the temperature is determined by the ratio of τ and τ_0, and also of L and l_0, where τ_0 and l_0 are the characteristic values of the stress and of the length of the dislocation segment; $\tau_0 = (kT)^2/4\alpha ab$ is the stress at which the subtrahend $2\beta\sqrt{\tau_0}$ in (1) is equal to the average thermal energy. When $\tau \gg \tau_0$, the $U_k(\tau)$ dependence becomes significant and must be taken into account. In the entire temperature interval, the employed stresses τ were larger than $\tau_0 = 0.48$—0.92 kg/mm^2.

The formula

$$l_0 = \frac{2b}{(8\pi)^{1/4}}\left(\frac{\tau b^3}{kT}\right)^{1/4}\left(\frac{G}{\tau}\right)^{1/8}\exp\left\{\frac{U_0 - \beta\sqrt{\tau}}{kT}\right\} \qquad (5)$$

determines the form of the v(L) dependence. If the dislocation length is $L < l_0$, then the dislocation velocity is

[2] For a sinusoidal Peierls relief, the plot of $U_k(\tau/\tau_p)$ was first constructed by Rozhanskii et al. [14] using the results of an investigation of Frenkel-Kontorova model by Indenbom and Orlov [3].

proportional to its length:

$$v = \frac{(8\pi)^{1/4}}{b^2} LD \left(\frac{\tau b^3}{kT}\right)^{1/2} \left(\frac{\tau}{G}\right)^{1/4} \exp\left\{-\frac{2U_0 - 2\beta\sqrt{\tau}}{kT}\right\}, \qquad (6)$$

where $D \approx \nu_D b^2$ is the diffusion coefficient and ν_D is the Debye frequency.

Different authors have calculated the frequency ν of formation of a double kink in different ways. The formula presented pertains to a case when $\nu \sim L/b$[7]. If it is assumed that $\nu \sim L/l_c$, where $l_c = (\alpha/\tau ab)^{1/2}$ is the critical width of the double kink, then we obtain a formula that differs from (5) by the amount $(G/\tau)^{1/4}$[1]. This increases l_0 insignificantly. The values of l_0 calculated from (5) exceed the length of the dislocation half-loops, on which the measurements were made, for almost the entire range of temperatures and stresses, even under the condition when the activation energy of the dislocation motion U_d correlates with the energy of one kink U_0, and not with $2U_0$ as obtained from (6). However, no dependence of v on the half-loop diameter was observed. One can only assume that allowance for the impurities present in the crystal can decrease l_0 to values $l_0 < L$, when in accordance with[1,5,7] there is no v(L) dependence and the equation for the dislocation velocity becomes

$$v = \frac{2(8\pi)^{1/8}}{b} D \left(\frac{\tau b^3}{kT}\right)^{3/4} \left(\frac{\tau}{G}\right)^{1/8} \exp\left\{-\frac{U_0 - \beta\sqrt{\tau}}{kT}\right\}. \qquad (7)$$

The calculation of v under the assumption that $\nu \sim L/l_c$ changes (7) by $(\tau/G)^{1/4}$, which hardly influences the form of the $v(\tau)$ dependence. As indicated by Kazantsev and Pokrovskiĭ[1], the difference between these two approaches results in noticeably different m only when $\tau < \tau_0$.

The dependence of the pre-exponential factor in (7) on τ is the result of taking into account the dependence of the kink velocity v_k on the stresses:

$$v_c = D\tau ab / kT. \qquad (8)$$

At certain τ and T, the kink velocity calculated from (8) exceeds the velocity of sound. In such cases, v was estimated with the pre-exponential factor in (7) taken at values of τ such that the velocity v_k still did not exceed the velocity of sound. This correction is equivalent to assuming that the velocity of the kink at high $\tau > 20-30$ kg/mm^2 ceases to be limited by the friction forces connected with the stimulated scattering of phophonons (the flutter effect), and the relativistic losses become decisive.

The experimental data were processed in accordance with (7). The dependence of the dislocation motion activation energy on the stresses was determined (with allowance for the pre-exponential factor), as shown in Fig. 3. Since the measurement error is $\Delta U_d \approx 0.08 \times 10^{-12}$ erg, the obtained dependence can be approximated by a straight line whose slope determines β. The value $\beta \approx 4 \times 10^{-18}$ dyne$^{1/2}$ dm^2 obtained in this manner is of the same order as the previously calculated $\beta = 7.72 \times 10^{-18}$ dyne$^{1/2}$ cm^2. The kink energy turned out to be $U_0 \approx 3.7 \times 10^{-12}$ erg (2.32 eV).

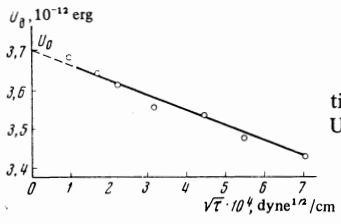

FIG. 3. Dislocation motion activation energy as the function $U_d(\sqrt{\tau})$.

The obtained β and U_0 were used to calculate, using (7), the dislocation velocities v for different stresses and temperatures. The results of the calculations are shown in Fig. 1. The obtained points fit on straight lines with slopes m = 1.28–1.38. The values of m agree with those obtained from experiment. However, the velocities v determined by experiment exceed the calculated values by two orders of magnitude[3]. This discrepancy can apparently be regarded as one more evidence that the kink velocity at the investigated stresses and temperatures is limited not only by the flutter effect, which determines (8).

CONCLUSION

1. A comparison of the experimental dependence of the dislocation motion activation energy in silicon on the stresses (1–50 kg/mm^2) with the results of the theory based on the string model[3,4,13] indicates that the measured value $U_d \approx 2.2$ eV corresponds to the energy of a single kink and not to the energy of formation of a double kink. This conclusion does not agree with the results of calculations of the energy of the double kink in silicon, performed by the Leibfried-Dietze and the pseudopotential methods[10,11]. The solutions obtained on the basis of the string model employed by us can apparently be reconciled with those obtained in[10,11] by using the modified linear-energy approximation[15] in calculating the equilibrium form of a dislocation with a kink in a field of large Peierls barriers.

2. The dislocation velocity in the interval $v \sim 10^{-8}-10^{-2}$ cm/sec at $\tau \sim 1-50$ kg/mm^2 and T = 500–800°C is controlled by diffusion processes of growth of the double kink produced by thermal fluctuation to the critical dimension. The diffusion theory[1,5,7] describes qualitatively the experimentally observed $v(\tau, T)$ dependence, but no exact quantitative agreement between the results is attained.

3. The experimental data do not agree with the prediction of the theory[1,5,7] with respect to the critical dimension of the dislocation length, beyond which the v(L) dependence vanishes. It is possible that allowance for the influence of point defects on the diffusion motion of the kink will eliminate this discrepancy. The degree to which such an influence is significant may be evidenced by the presence of starting stresses for the motion of dislocations in silicon[8,9].

Notice should be taken of one more possible conclusion that can be drawn from the aforementioned contradictions: the effective dislocation motion activation energy observed in the experiment may be the sum of the activation energy of the formation of the double kink and the activation energy of the motion of the kink in the field of Peierls forces of the second kind. No detailed theoretical analysis of such a situation has been performed as yet.

[3]The theoretical expression obtained for the dislocation velocity for the case $\nu \sim L/l_c$ [1] gives still lower values of v.

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