

Influence of electrically active impurities on the mobility of separate dislocations in germanium

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The dependence of the velocity of separate dislocations in germanium single crystals on the field strength (0.15–20 kgf/mm²), temperature (280–580°C) and density (10¹³–10¹⁹ at/cm³) of electrically active Ga, Sb and As impurities is investigated. The laws of dislocation motion are found to differ significantly in the low (up to 2–4 kgf/mm²) and high field strength regions. The data are compared with all existing theories of dislocation mobility in crystals with high Peierls barriers. It is shown that the experimental results can be explained qualitatively by theories in which the effect of point defects on the creation and motion of double kinks is taken into account by assuming that in all crystals the concentration of the dislocation point defects is very high. Some possible causes of a number of discrepancies between the theoretical predictions and the experimental data are discussed.

The existence of translational symmetry in a crystal lattice determines inevitably the periodic character of the function $W(x)$ that describes the dependence of the dislocation energy on the displacement in the slip plane along the direction of the displacement x . At absolute zero temperature, the classical¹¹ motion of a dislocation in the potential field of a crystal lattice can occur only at stresses τ exceeding the Peierls stresses $\tau_P = [\partial W(x)/\partial x]_{\max}$. At higher temperatures, thermally-activated surmounting of the Peierls barriers is possible at $\tau < \tau_P$, owing to the formation of double kinks on the dislocation. A theoretical analysis shows^[2-6] that the dependence of the dislocation velocity v on the applied stresses and on the temperature T is determined by the ratio of the external and Peierls stresses, and also by the length L of the dislocation.

A check^[7-9] of the developed concepts, performed on silicon single crystals, has revealed that in real crystals the quantitative rules describing dislocation mobility are radically altered under the influence of point defects. They result in the appearance of starting stresses for dislocation motion, and decreases the activation energy U of their displacement and the critical dimension of the dislocation line, starting with which the dependence of v on L begins. An analysis of the experimental data has shown that in Si single crystals, which have the highest Peierls barriers of all the investigated materials, the impurities cause an appreciable lowering of the energy of formation of a double kink of critical size. This phenomenon was subsequently treated theoretically^[10,11]. We must emphasize the following somewhat unexpected fact: When dislocations move in Si single crystals with most diverse types of impurities, the rules for the motion of point defects considered in^[12,13], which are naturally derived when the resistance of the defect to the broadening of the double kinks is theoretically taken into account, do not appear.

Investigations^[14-17] of the mobility of individual dislocations in germanium single crystals were performed only with weakly doped crystals at a relatively low level of external stresses. They have shown that in this case, in a certain interval of stresses and temperatures, there appear effects connected with the stopping of the kinks by the point defects, and this leads to an increase of the activation energy of dislocation motion. At the same time, the data^[18] on the mobility of the dislocation rows

offered evidence of the possible decrease of the value of U under the influence of the impurities. It was therefore to be hoped that in Ge crystals, which have a lower value of τ_P than Si, it would be possible to investigate the laws governing the effect of impurities both on the initiations of the double kinks and on the motion along the dislocations. The research described in this article was performed for this purpose.

It should be noted that the knowledge of these laws is also of practical interest, since dislocation motion through many high-melting-point BCC metals of importance in technology, which are characterized by not too high Peierls barriers, can be determined by the joint action of both effects.

EXPERIMENTAL PROCEDURE

The investigations were performed on single crystals of n- and p-type, grown by the Czochralski method and doped during the growth with Sb, As, and Ga. The density of the electrically-active impurities in each crystal is given in the table. We used prismatic samples of two orientations: "a"—with the faces {100}, {110}, and {110}, and "b" with the faces {111}, {112}, and {110} (the face symbols are given in order of decreasing area). The procedure for producing single dislocations in the samples was similar to that described earlier for Si^[19]. In the type "a" samples, the half-loop sections emerging to the surface had different orientations, some screw, and others 60°. In the samples of type "b" the half-loops and near surface sections of different orientations (screw and 60°) and of 60° orientation only were

Impurity density and values of the pre-exponential factor $\log v_0$ for the investigated crystal

| Doping impurity | Impurity density, cm ⁻³ | $\tau, \kappa T/mm^2$ | | | | | | |
|-----------------|------------------------------------|-------------------------------------|------------|-----------|-----------|-----------|-----------|-----------|
| | | 0.5 | 1 | 2 | 6 | 10 | 20 | |
| Ga | 6 · 10 ¹³ | 13.2 ± 1.2 | 10.0 ± 0.5 | 7.5 ± 0.5 | 7.5 ± 0.5 | — | — | |
| Ga | 2 · 10 ¹⁶ | 13.7 ± 0.9 | 10.5 ± 0.5 | 7.4 ± 0.5 | 6.9 ± 0.5 | 6.8 ± 0.5 | 6.8 ± 0.5 | |
| Ga | 10 ¹⁷ | 13.4 ± 1.0 | 10.7 ± 0.6 | 7.8 ± 0.5 | 7.8 ± 0.4 | 6.9 ± 0.5 | 6.6 ± 0.4 | |
| Ga | 10 ¹⁹ | 8.8 ± 1.0 | 8.2 ± 0.6 | 6.4 ± 0.6 | 6.8 ± 0.4 | 7.2 ± 0.4 | — | |
| Sb | 10 ¹³ | 12.7 ± 1.0 | 7.8 ± 0.8 | 6.5 ± 0.4 | 6.0 ± 0.4 | 6.2 ± 0.4 | — | |
| Sb | 1.3 · 10 ¹⁷ | 60° dislocations screw dislocations | 13.6 ± 1.1 | 7.5 ± 0.8 | 6.4 ± 0.4 | 6.5 ± 0.4 | 6.0 ± 0.4 | 5.6 ± 0.6 |
| | | | 4.4 ± 0.6 | 5.2 ± 0.5 | 6.3 ± 0.4 | 6.5 ± 0.4 | 6.4 ± 0.4 | 5.8 ± 0.5 |

equally probable. At small τ ($< 1 \text{ kgf/mm}^2$) and low T ($< 400^\circ\text{C}$) one of the sections of the half-loop in samples of type "a" and in some of the dislocations in the samples of type "b" had a higher velocity than the other. A comparison of the velocities of these sections with the velocities of half-loops that are known to have 60° orientation, which could easily be found in samples of type "b" on one side of the scratch^[9], and also the determination of the Burgers vector by x-ray topography, has shown that the half-loop section with the higher velocities had a screw orientation. This fact made it possible to separate distinctly the screw and the 60° dislocations after the subsequent deformation.

It was observed earlier^[20] that the dislocations half-loops in Ge can contract spontaneously as a result of self-action forces. Our experiments have shown that for samples oriented in accord with type "b" there is no contraction if the half-loop diameter exceeds 400μ . Therefore all the measurements were performed only on half-loops with large initial diameters. In samples of orientation "a" the contraction stresses are larger and amount to $0.15\text{--}0.1 \text{ kgf/mm}^2$ for half-loops of $400\text{--}600 \mu$ diameter. During the heating and subsequent deformation we therefore applied to these samples an additional "stabilizing" stress to balance the contraction stress. The dislocation velocities were investigated in the temperature interval $280\text{--}580^\circ\text{C}$ at stresses $0.15\text{--}20 \text{ kgf/mm}^2$.²⁾ The error in the determination of the velocity, due to the errors in the measurements of T , τ , and the test time, was on the average $\pm 5\%$. The spread in the velocities of dislocations of one type, observed in the experiment, exceeded as a rule this error. Figures 1a, 1b, and 4 (below) show the values of the dislocation velocities together with the measured spreads. Each point is the arithmetic mean of 25–30 measurements of the velocities of individual dislocations.

The doping-impurity content of the crystal was monitored by mass spectrometry and against the results of measurements of the electric characteristics. The comparison has shown that the investigated crystals differed significantly only in the content of the electrically active impurities. The concentrations of the electrically inactive impurities of the heavy elements (Si, Cu, etc.) were approximately the same and did not exceed $5 \times 10^{15} \text{ cm}^{-3}$.

The experimentally employed samples contained practically no growth dislocations. Exceptions were crystals with Ga contents 6×10^{13} and 10^{19} cm^{-3} . The dislocation velocities in these crystals were measured only up to 10 kgf/mm^2 , inasmuch as a strong multiplication of the dislocation rows near the local stress concentrators set in at higher τ .

EXPERIMENTAL RESULTS

We investigated the dependence of the velocity of individual 60° dislocations on the temperature and on the stresses in all the Ge crystals listed in the table. For the crystal containing 10^{17} cm^{-3} Sb, we measured also the velocities of the screw dislocations in the stress interval $0.5\text{--}20 \text{ kgf/mm}^2$. Figures 1a and 1b show typical plots of $v(1/T)$ at different τ for the crystal with Sb density 10^{17} cm^{-3} . When plotted in coordinates $\log v(1/T)$, the experimental results fit well straight lines whose slopes characterize the activation energy of the dislocation motion, i.e., the results are described by the formula

$$v = v_0(\tau) \exp[-U(\tau) / kT], \quad (1)$$

which is typical of the thermal-activation processes. Extrapolation of the straight lines to the ordinate axis yielded the values of $\log v_0(\tau)$, which are listed in the table together with the errors resulting from the observed scatter of the dislocation velocities. The quantity $\log v_0$ for 60° dislocations is a decreasing function of the stresses, it drops sharply with increasing τ in the region of small τ ($< 2 \text{ kgf/mm}^2$), and at $\tau > 2 \text{ kgf/mm}^2$ it decreases insignificantly (Fig. 2).

The activation energy of the motion of 60° dislocations (U^{60°) is also a function of the stress, decreasing rapidly with increasing τ from 0.5 to 2 kgf/mm^2 and varying little with further increase of τ . Figures 2 and 3 illustrate the $U(\tau)$ dependence for different crystals. The average error in the determination of U amounts to $\pm 0.05 \text{ eV}$ in the interval of high τ and to $\pm 0.12 \text{ eV}$ in the interval of low τ .

The activation energy of the motion of screw dislocations U^{screw} and $\log v^{\text{screw}}$, measured in the crystal

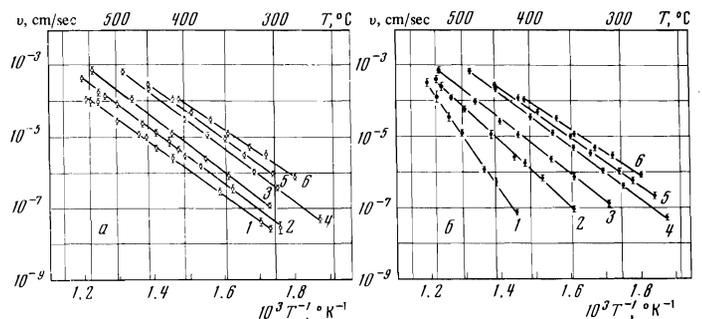


FIG. 1. Velocities of screw (a) and 60° (b) dislocations in Ge containing $1.3 \times 10^{17} \text{ cm}^{-3}$ Sb vs. the temperature for different τ : 1) 0.5 kgf/mm^2 , 2) 1 kgf/mm^2 , 3) 2 kgf/mm^2 , 4) 6 kgf/mm^2 , 5) 10 kgf/mm^2 , 6) 20 kgf/mm^2 .

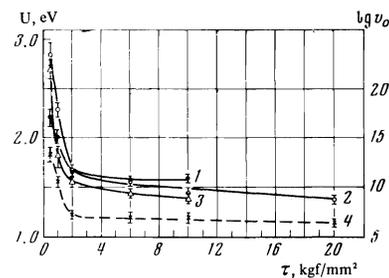


FIG. 2. Dependence of the activation energy of the motion of 60° dislocations (curves 1, 2, 3) on the stress for crystals doped with Ga: 1) 10^{19} cm^{-3} , 2) $2 \times 10^{16} \text{ cm}^{-3}$, and crystals doped with Sb: 3) 10^{13} cm^{-3} . The dashed curve 4 shows the dependence of the pre-exponential factor on the stresses for a crystal with Ga density $2 \times 10^{16} \text{ cm}^{-3}$.

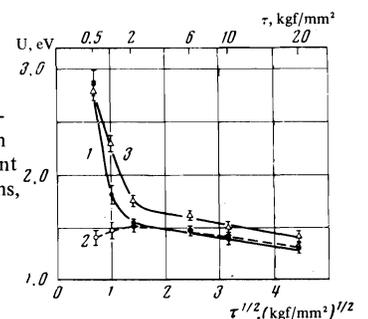


FIG. 3. Dependence of the activation energy of dislocation motion U on $\sqrt{\tau}$ for crystals with Sb content $1.3 \times 10^{17} \text{ cm}^{-3}$ (1— 60° dislocations, 2—screw dislocations) and with Ga content 10^{17} cm^{-3} (curve 3).

with the Sb density 10^{17} cm^{-3} , coincide at $\tau > 2 \text{ kgf/mm}^2$ with U^{60° and $\log v^{60^\circ}$ within the limits of the measurement error. At $\tau < 2 \text{ kgf/mm}^2$, their dependences on τ are entirely different than for 60° dislocations, and U^{scr} and $\log v_0^{\text{scr}}$ even decrease somewhat with decreasing τ (Fig. 3, table), and do not agree with those observed in [16].

The character of the influence of the impurities on the dislocation mobility in Ge depends on the type of impurity, its density, and the applied stress. An increase of the density of Sb to 10^{17} cm^{-3} does not change the dislocation mobility: in crystals with Sb impurity 10^{13} and 10^{17} cm^{-3} the values of v^{60° coincide³⁾ within the limits of measurement errors for all the investigated T and τ . A similar result is obtained by doping Ga to a density 10^{17} cm^{-3} : the activation energy U^{60° in a crystal with a Ga content $6 \times 10^{13} \text{ cm}^{-3}$ (which at $\tau = 0.5, 1, 2$, and 6 kgf/mm^2 are equal to $2.80 \pm 0.17, 21.7 \pm 0.08, 1.70 \pm 0.05$, and $1.58 \pm 0.04 \text{ eV}$, respectively) are close to the corresponding values of U^{60° for more highly doped p-type crystals.

At a higher degree of doping, however, n- and p-type impurities exert a noticeable influence on the dislocation mobility. Doping with 10^{19} cm^{-3} of arsenic, as in Si^[8], decreases U^{60° greatly to 1.05 eV and increases the dislocation velocity (Fig. 4). In addition, it leads to the appearance of high starting stresses for the dislocation motion, $\tau_{\text{st}} = 2 \text{ kgf/mm}^2$. In all the remaining crystals, the starting stresses in the investigated temperature region could not be observed, owing to the low dislocation mobility in the region of very low stresses, when the velocities drop below 10^{-8} cm/sec . The measurement of the dislocation mobility in the crystal with arsenic density 10^{19} cm^{-3} at $\tau > 6 \text{ kgf/mm}^2$ turned out to be difficult because of the multiplication of the dislocation rows, initiated by impurity clusters.

Doping with 10^{19} cm^{-3} gallium, to the contrary, decreases the dislocation velocities at all stresses, and increases somewhat U^{60° in the region of high τ , as was observed earlier by the authors of [18] in measurements of dislocation-row velocities. However, the activation energy values given in [18] are higher than those obtained by us. This character of the influence of a p-type impurity is the opposite of that observed in Si^[8,9]. At low τ , the influence of Ga on the dislocation mobility has an entirely different character, viz., $\log v^{60^\circ}$ and U^{60° in a crystal with a Ga density 10^{19} in-

crease with decreasing τ more slowly than in all the remaining crystals, and at $\tau = 0.5 \text{ kgf/mm}^2$ the value of U^{60° is lower by $0.5\text{--}0.6 \text{ eV}$ than in the remaining crystals.

The dependence of the dislocation velocity on τ is not described by the power-law function $v \sim \tau^n \times \exp(-U/kT)$ in the entire investigated stress interval. One can separate on the $\log v$ ($\log \tau$) curve a linear section at $\tau > 2 \text{ kgf/mm}^2$, with a slope n that ranges from 1.2 to 1.5 for different crystals. At $\tau < 2 \text{ kgf/mm}^2$ the $v(\tau)$ dependence is steeper and its approximation by a straight line yields $n \sim 3.5$. The theories [12,13] predict for small τ a relation of the type $v \sim \text{const} \cdot \exp(-\tau_1/\tau) \exp(-U/kT)$. Figure 1 shows the experimental plots of $\log v$ as functions of $(1/\tau)$. Small sections of these curves, from 0.5 to 2 kgf/mm^2 , can be described by a straight line, but below 0.5 kgf/mm^2 the velocities are higher than called for by this relation.

For the crystal with Sb content 10^{13} cm^{-3} , we investigated the dependence of the dislocation velocity on the diameter of the dislocation half-loop at $\tau = 1 \text{ kgf/mm}^2$ and 2 kgf/mm^2 , and respectively $T = 350$ and 300°C . When the half-loop diameter was increased from 400 to 1000μ , no change larger than the measurement error was observed in the velocities of the screw and 60° dislocations.

In addition, we investigated the effect of the heating conditions and of the thermal annealing on the dislocation velocities. It was found that an increase of the standard heating rate ($10\text{--}15 \text{ deg/min}$) by five or six times does not change the dislocation mobility at either high or low stresses. Only at very high heating rates ($120\text{--}200 \text{ deg/min}$) does the dislocation mobility in the interval of small τ increase by a factor $3\text{--}4$ in comparison with the usual heating conditions, and at $\tau = 6 \text{ kgf/mm}^2$ the change of the heating rate does not affect the dislocation rate. Annealing of the samples for six hours at 450°C did not change the dislocation velocity.

COMPARISON OF EXPERIMENTAL DATA WITH THEORIES OF DISLOCATION MOBILITY IN A FIELD OF PEIERLS FORCES

Dislocation motion in a field of Peierls forces satisfied relation (1), which represents the thermally-activated character of this process. The physical meaning and the values of the parameters v_0 and $U(\tau)$ in Eq. (1) depend essentially [2-6] on the mechanism whereby the dislocation moves from one groove of the potential relief to the neighboring one. If the dislocation length L is small (but larger than $kT/\tau ab$), then its velocity is limited only by the probability of production of a double kink of critical dimension l_c in the direction of action of the force:

$$v = aJL, \quad (2)$$

where a is the distance between the neighboring grooves of the relief, b is the value of the Burgers vector, and J is the probability of production of a double kink in a unit time per unit length. If the dislocation is long enough (many double kinks can be produced on it simultaneously, expand at a velocity $2v_b$, and annihilate after covering a distance L_{cr}), then the dislocation velocity ceases to depend on its length: $v = aJL_{\text{cr}}$. The value of L_{cr} is determined from the equality of the time $(1/JL_{\text{cr}})$ of double-kink production over a length L_{cr} to the time $(L_{\text{cr}}/2v_b)$ of the passage of the kinks over this segment: $L_{\text{cr}} = (2v_b/J)^{1/2}$. In this case the dislocation velocity is

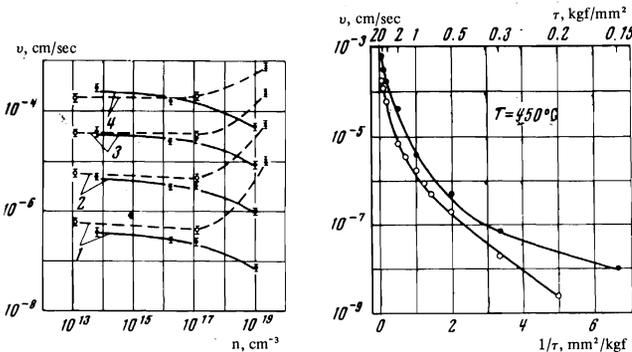


FIG. 4

FIG. 4. Dependence of the velocity of 60° dislocations on the densities of the Ga (\bullet), Sb (\circ), and As (\times) impurities at the temperatures 300° (1), 350° (2), 400° (3), and 450°C (4) at $\tau = 6 \text{ kgf/mm}^2$.

FIG. 5. Dependence of the dislocation velocity on $1/\tau$ for crystals with Ga content 10^{17} cm^{-3} (\bullet) and 10^{19} cm^{-3} (\circ).

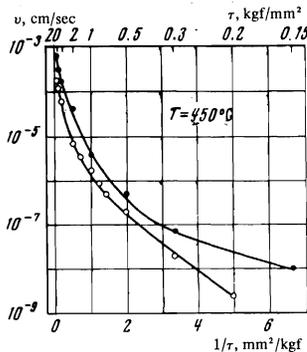


FIG. 5

$$v = a(2\nu_k J)^{1/2}. \quad (3)$$

In the discussed experiments we observed no dependence of the dislocation velocity on the dislocation length. It is therefore natural to assume that the experimental data should be described by formula (3). The form of the functions $J(T, \tau)$ and $\nu_k(T, \tau)$ depends on the mechanism that limits the mobility of the kink, and on the conditions under which the kink is produced, which, in turn, are determined by the ratio τ/τ_p .

As already mentioned, the $U(\tau)$ curve (Fig. 2) is distinctly divided into two sections. At $\tau < 2 \text{ kgf/mm}^2$ the value of the activation volume $\gamma = \partial U/\partial \ln \tau$ is approximately $600b^3$, whereas at $\tau > 2 \text{ kgf/mm}^2$ we have $\gamma \approx (5-10)b^3$. On the basis of [12-6, 12, 13] we can assume that at $\tau < 2 \text{ kgf/mm}^2$ the mobility of the bends is determined by their thermally-activated overcoming of the barriers E_{kp} , which are connected with the point defects, and at higher stresses, when $\tau ab \bar{l} > E_{kp}$ (\bar{l} is the average distance between defects), ν_k is limited by the phonon mechanisms, and J can be calculated from the diffusion theory of double-kink production [5, 6, 14].

We shall first analyze the experimental data for stresses $\tau > 2 \text{ kgf/mm}^2$ under the assumptions that if the impurity volume densities range from 10^{13} to 10^{17} cm^{-3} then the impurities change only insignificantly the energy of the double kink:

$$U_{dk} = 2U_k - \tau ab \bar{l} - \alpha/l, \quad (4)$$

where U_k is the energy of one kink, l is the width of the double kink, $\alpha = Ga^2b^2[(1+\nu)\cos^2\varphi + (1-2\nu)\sin^2\varphi]/8\pi(1-\nu)$ is a parameter that determines the attraction force (α/l^2) of the kinks, forming a pair, φ is the angle between the direction of the dislocation and the Burgers vector, ν is the Poisson coefficient, and G is the shear modulus.

Formula (4) is valid when l exceeds the width of the single kink $\omega = (a/2)\sqrt{E_0/W_P^0}$ (E_0 is the energy of the linear tension of the dislocation, and $W_P^0 = \tau_p ab/2\pi$ is the Peierls energy).

The shift of the entire dislocation from one groove of the potential relief to another can be caused only by those double kinks whose dimensions exceed the critical value

$$l_c = \sqrt{\alpha/\tau ab}, \quad (5)$$

determined from the equality of the force τab that pushes the kinks apart to the force of their mutual attraction. Some of them can collapse under the influence of the thermal fluctuations, if one of them is smaller than $l_c + l_g$, where $l_g = b[(bkT/\alpha)(l_c/b)^3]^{1/2}$. The quantity l_g is determined from the equality of the work of the forces $(2l_g^2(\partial^2 U/\partial l^2))_l = l_c$, that tend to broaden the kink to the average thermal energy kT .

The drift velocity of the kink in the field of the external stresses can be described by the formula $\nu_k = D_k(\tau ab/kT)$. In the limiting case the diffusion coefficient of the kink is $D_k = \nu_D b^2$, and then $\nu_k = \nu_s(\tau ab^2/kT)$ where ν_s is the speed of sound and ν_D is the Debye frequency.

Under the indicated assumptions, the probability of production of a double kink per unit length and per unit time is

$$J_0 = \nu_s \left(\frac{b}{l_g}\right) \frac{1}{b^2} \exp\left[-\frac{U_{dk}(\tau)}{kT}\right]. \quad (6)$$

The kink energy corresponding to l_c is

$$U_{dk}(\tau) = 2U_k - 2\beta\sqrt{\tau}, \quad \beta = (\alpha ab)^{1/2}. \quad (7)$$

For the case considered by us ($L > L_{cr}$) we have

$$v = \nu_s \left(\frac{b}{l_g}\right)^{1/2} \left(\frac{2\tau ab^2}{kT}\right)^{1/2} \exp\left(-\frac{U_k - \beta\sqrt{\tau}}{kT}\right) \quad (8)$$

and

$$L_{cr} = b \left(\frac{l_g}{b}\right)^{1/2} \left(\frac{2\tau ab^2}{kT}\right)^{1/2} \exp\left(\frac{U_k - \beta\sqrt{\tau}}{kT}\right). \quad (9)$$

Let us compare the experimental data with the predictions of the discussed theory.

A. Using for Ge the parameters $\nu_D = 6.04 \times 10^{12} \text{ sec}^{-1}$, $b = 4 \times 10^{-8} \text{ cm}$, $a = 3.48 \times 10^{-8} \text{ cm}$, and $C = 6.58 \times 10^{11} \text{ dyn/cm}^2$ we calculated the value $\beta = 8 \times 10^{-13} \text{ dyn}^{1/2} \text{ cm}^2$ ($5 \times 10^{-2} \text{ eV}/(\text{kgf/mm}^2)^{1/2}$). The experimental $U(\sqrt{\tau})$ dependence (Fig. 3) was used to determine the values of β_{exp} . For Ge with an impurity density $10^{13} - 10^{17} \text{ cm}^{-3}$ we have $\beta = (13-15) \times 10^{-18} \text{ dyn}^{1/2} \text{ cm}^2$, i.e., higher than the theoretical value of β . The possible explanation is the following. As already mentioned, formula (4), meaning also (7), is valid when $l_c \gtrsim \omega$. From the experimentally obtained values of U_k we can calculate the values of τ_p and ω . For a sinusoidal relief we have $\tau_p = \pi^3 U_k^2/4a^3 b^3 G = 300 \text{ kgf/mm}^2$ and $\omega = (\pi ab G/4\tau_p)^{1/2} = 5b$. We calculated the values of l_c for different values of τ in accordance with formula (5). It turned out that even at $\tau \approx 10 \text{ kgf/mm}^2$ the value of l_c becomes smaller than ω . For large $\tau > 0.1 \tau_p$, expression (7) should go over into

$$U_{dk}(\tau) = 2(2E_0)^{1/2} \int_{-\infty}^{\infty} \{ [W(x) - W(x_0) - \tau b(x - x_0)] \}^{1/2} dx$$

and, as shown in [4], it can be approximated at $\tau < 0.9 \times \tau_p$ by the function $U_{dk}(\tau) = 2U_k - \gamma\tau$, which ensures a stronger $U_{dk}(\tau)$ dependence. It can be assumed that the large value of β is due precisely to this sharper decrease of U at high $\tau \approx 20 \text{ kgf/mm}^2$. Another more probable explanation of this fact will be considered below.

B. Let us compare the pre-exponential quantity in (8), which we shall denote by ν_0^T , with the experimental values of ν_0 (see the table). An analysis shows that at all the investigated stresses ν_0 cannot exceed the speed of sound since l_c and l_g are quantities of the same order and $(\tau ab/kT) < 1$. However, the experimental values of ν_0 greatly exceed $\nu_s \approx 2 \times 10^5 \text{ cm/sec}$.

C. The calculation of L_{cr} in accordance with (9) yielded values from 15 to $2 \times 10^6 \text{ cm}$, which greatly exceed the diameters of the dislocation half-loops employed in the experiment. This means that ν should exhibit a dependence on L at all values of T and τ , but this is not confirmed by experiment.

The foregoing disparities between experiment and the theory based on the model of annihilating kinks shows that in Ge, just as in Si, the Peierls mechanism in pure form does not determine all the regularities of the dislocation motion even at $\tau > E_{kp}/ab\bar{l}$, and it is apparently necessary to take into account the influence of the point defects. In the high-stress interval, it can become manifest in a change of the frequency of production of double kinks of critical dimensions. The short-range field of the elastic stresses or else the long-range electrostatic field of the charged point defects can

locally alter the energy of the dislocation line by an amount E_{dp} , meaning also the energy of formation of the double kink^[10,11]. It must be emphasized that even for one defect, regardless of the sign of the quantity E_{dp} , the effective activation energy of dislocation motion should decrease. If the point defect increases the dislocation energy, then its transition to a neighboring groove of the potential relief is most likely to start at the point where it is located. If E_{dp} is of negative sign, the double kink will "run into" the point defect. The probability of double-kink production is in this case

$$J = J_0 [1 + (l_c/b)c \exp(E_{dp}/kT)],$$

where J_0 is the probability of double-kink production in the absence of defects (see (6)), and c is their concentration. Petukhov^[10] took into account also the probability of encountering a newly produced kink with a barrier from a cluster of m defects located at a distance $l \lesssim E_{dp}/\tau$ ab $\ll \bar{l}$, where the time required to overcome the barrier exceeds the time of production of a new double kink. The resultant expression for the dislocation velocity is

$$v = \frac{ab}{c} \left(\frac{\tau ab^2}{E_{dp} c} \right)^{m-1} \exp\left(m \ln \frac{E}{E_{dp}}\right) \left(1 + \frac{l_c}{b} c \exp \frac{E_{dp}}{kT}\right) J_0, \quad (10)$$

where

$$E = U_{dk} - kT \ln \left(1 + \frac{l_c}{b} c \exp \frac{E_{dp}}{kT}\right). \quad (11)$$

The minimal possible value of m is determined by the formula

$$m = \frac{E}{E_{dp}} \left(1 - \frac{kT}{E_{dp}} \ln \frac{E_{dp} c}{\tau ab^2}\right)^{-1}. \quad (12)$$

In this model, the dislocation velocity should cease to depend on the length at

$$L_{cr} \tau = \frac{b}{c} \left(\frac{\tau ab^2}{E_{dp} c} \right)^{m-1} \exp\left(m \ln \frac{E}{E_{dp}}\right). \quad (13)$$

An estimate of L_{cr}^T (using the value $U_{dk} = 1.75$ eV theoretically obtained in^[21] and an acceptable set of possible values of c and E_{dp}) shows that it increases rapidly with increasing m , and only when m is on the order of one or two dislocation-line lengths used in the experiment does it exceed L_{cr}^T . This means that at $m = 1$ the double kinks are produced practically on each defect, so that L_{cr}^T becomes a quantity of the order of the average distance between point defects. At $m = 1$, the solution of (12) with respect to E_{dp} yields a value $E_{dp} \approx 0.8$ eV, and expression (10) for the velocity takes the form:

$$v = a\bar{l} \frac{E}{E_{dp}} \left(1 + c \frac{l_c}{b} \exp \frac{E_{dp}}{kT}\right) J_0. \quad (14)$$

The effective dislocation-motion activation energy determined by it is equal to

$$U = 2U_k - 2\beta\bar{l}\tau - E_{dp}. \quad (15)$$

If E_{dp} is assumed to be independent of the stresses, then it follows from the presented experimental data and from (15) that $2U_k \approx 2.44$ eV. The Peierls stress, calculated at $U_k = 1.22$ eV, still admits of the use of the diffusion theory for the calculation of J_0 . Good agreement for this model is reached between the theoretical and experimental values of β (7.2×10^{-18} dyn^{1/2}/cm²). The values of the pre-exponential $v_0 \approx v_s(l_c/l_g)(E/E_{dp})$ calculated from the short-range-action theory, while of the same order of magnitude as those obtained in the experiment, still remain below the experimental values, even though if one takes into account the error in the determination of v_0 .

Since no dependence of v on L was observed at the experimentally employed dislocation lengths ($> 10^{-2}$ cm), this means in the short-range-action model that the average distance between the defects on the dislocation is $\bar{l} < 10^{-2}$ cm, and consequently their concentration is $c > 10^{-6}$. It appears that in fact c is much larger than this minimal estimate. This is evidenced by the presence of a break on the $U(\tau)$ curve at $\tau \approx 2$ kgf/mm². This break as already mentioned, may be due to the fact that at lower stresses the kink, owing to the work of the external forces, cannot overcome the barrier E_{kp} connected with the point defect. It is natural to assume that E_{kp} and E_{dp} are quantities of the same order. This leads to the estimate $\bar{l} \sim 100b$ and to the important conclusion that in all the investigated crystals the concentration of the point defects on the dislocation is very large ($\sim 10^{-2}$). It is obvious that it cannot be due to electrically active impurities. Such defects may be impurities of light elements (C, N, O), or vacancies which have large diffusion coefficients, so that during the time of heating and cooling a Cottrell atmosphere has time to be formed between the introduced dislocations. These times are short, as can be evidenced by the fact that the dislocation velocities in the region of small τ change only when the standard heating rate is increased to 120 deg/min.

Thus, allowance for the short-range-action defects (although their nature remains unclear) explains, in the case of weakly doped crystals, the contradictions between the predictions of the diffusion theory and the experimental data on the $v(L)$ dependence and on the values of β , and also make it possible to explain why the values of v_0 exceed those that follow from diffusion theory. However, the character of the variation of v and U with increasing concentration of the electrically active impurities cannot be interpreted by remaining only within the framework of the short-range-action theory. We therefore proceed to analyze the possible consequences of allowance for long-range Coulomb forces between charged defects and dislocations.

Petukhov and Pokrovskii^[11] have shown that the interaction between electrons captured by a dislocation and positively-charged donor impurities can decrease the energy of the double kink by an amount

$$\Delta E = - \frac{8\pi e^2}{15ea} \left(\frac{e^2}{kT \epsilon a \ln c^{-1}} \right)^{1/2}, \quad (16)$$

where ϵ is the dielectric constant in the crystal and e is the electron charge. The character of the variation of U in Ge doped with Sb and As when the density of the latter is increased agrees qualitatively with that called for by (16). However, quantitative agreement is obtained only for crystals strongly doped with arsenic (10^{19} cm⁻³). The expected decrease of U following doping with antimony to 10^{17} cm⁻³ is not observed. This model does not offer a direct explanation for the small increase of the activation energy of dislocation motion in Ge doped with acceptor impurities. It appears that effects that determine the strong growth of the activation energy of the motion as a result of the stopping of the kinks by the defects still manifest themselves in these crystals in the investigated stress interval.

At a low level of applied stresses ($\tau < E_{kp}/ab\bar{l}$), thermoactivation processes help the kinks overcome the barriers connected with the point defects. If we take into account only the first defect encountered after the appearance of the double kink, then the effective bend velocity is $v_k^{eff} = v_k^0 \exp(-E_{kp}/kT)$. A double kink whose

dimension exceeds the critical value ($l_c + l_g$), and whose expansion is stopped by obstacles, acquires a finite probability of collapsing. This decreases also the effective frequency of production of the double kinks that determine the velocity of dislocation motion. A theory that takes into account the noted distinguishing features was developed in^[12,13]. The expressions obtained in^[12] for J_{eff} and v take the form

$$J_{\text{eff}} = J_0 \left(1 + \frac{E_{\text{kp}}}{\tau ab\bar{l}} + \frac{l_c}{\bar{l}} \right) \exp \left(- \frac{E_{\text{kp}}}{\tau ab\bar{l}} - \frac{l_c}{\bar{l}} \right), \quad (17)$$

$$v = v_0 L \left(1 + \frac{E_{\text{kp}}}{\tau ab\bar{l}} + \frac{l_c}{\bar{l}} \right) \exp \left(- \frac{U_{\text{dk}}}{kT} - \frac{E_{\text{kp}}}{\tau ab\bar{l}} - \frac{l_c}{\bar{l}} \right) \quad (18)$$

at

$$L \leq (2\nu_k^{\text{eff}} J_{\text{eff}})^{1/2} = L_{\text{cr}}^{\text{eff}}$$

and

$$v = (2a\bar{l}\nu_0\nu_f^0)^{1/2} \left(1 + \frac{E_{\text{kp}}}{\tau ab\bar{l}} + \frac{l_c}{\bar{l}} \right)^{1/2} \times \exp \left(- \frac{U_{\text{dk}} + E_{\text{kp}}}{2kT} - \frac{E_{\text{kp}}}{2\tau ab\bar{l}} - \frac{l_c}{2\bar{l}} \right) \quad (19)$$

at $L \gg L_{\text{cr}}^{\text{eff}}$. Here ν_0^* and ν_f^0 are quantities defined in^[12].

As indicated in^[12], a $U(\tau)$ dependence that agrees with experiment can be obtained by assuming that the average distance between the point defects varies with temperature like $\bar{l} = \bar{l}_0 \exp(-\epsilon/kT)$. Formulas (18) and (19) determine the linear connection between $\log v$ and $1/\tau$ at small τ . The velocities obtained in our measurements can be described by this linear relation only in the stress interval $0.5 - 2 \text{ kgf/mm}^2$. In this interval of τ , the slope of the lines $\log v$ ($1/\tau$) gives the ratio $E_{\text{kp}}/ab\bar{l}$, from which, by specifying certain values of E_{kp} , it is possible to obtain \bar{l} and then make it more accurate by using an iteration method, as was done in^[13,16]. With such a reduction of the results for crystals with Sb and Ga densities 10^{13} and 10^{19} cm^{-3} , respectively, it turned out that \bar{l} has an exponential temperature dependence with an activation energy $\epsilon = 0.26 \text{ eV}$ for the first of the crystals and $\epsilon = 0.18 \text{ eV}$ for the second. In the temperature interval $400 - 550^\circ$, the value of \bar{l} increases from 50 to $130b$ in a crystal with Sb density 10^{13} at $E_{\text{kp}} = 1 \text{ eV}$ and from 80 to $140b$ in a crystal with Ga density 10^{19} cm^{-3} .

Using the obtained values of \bar{l} we calculated the dislocation velocities, and from the $v(1/T)$ dependence we determined the values of the effective activation energies for different τ . It turned out that the numerical $U(\tau)$ dependence agrees qualitatively with that observed in experiment, but the experimental values of U lie much lower than the theoretical ones. Variation of the parameter E_{kp} in the range from 0.1 to 2 eV has shown that the smallest differences, 0.3 to 0.5 eV , are reached at $E_{\text{kp}} = 1 \text{ eV}$, i.e., when E_{kp} and E_{dp} are close in value. The decrease of the activation energy of the motion of 60° dislocations when the content of the Ga impurity atoms is strongly increased in the crystal is determined, within the framework of the considered model, by a weaker $\bar{l}(T)$ dependence.

Thus, many experimental results at low stresses can be qualitatively explained by taking into account the interaction of a moving kink with barriers produced by point defects. However, no quantitative agreement between the predictions of the theory^[12,13] and experiment is obtained. Moreover, from the point of view of the theory some of the experimental data are surprising, namely the $U(\tau)$ dependence for screw dislocations and $v(\tau)$ for 60° dislocations at $\tau < 0.5 \text{ kgf/mm}^2$.

CONCLUSION

Single crystals of Si and Ge are regarded as classical objects with which to check the theory of dislocation mobility limited by thermally-activated overcoming of the proper potential barriers of the crystal lattice (the Peierls barriers). The experimental results described in this article for Ge and their subsequent comparison with the existing theories have shown that, just as in Si, the laws governing dislocation motion in real crystals cannot be understood without taking account the diverse effects of point defects. The spectrum of its manifestations becomes more complicated with lowering of the Peierls barriers. Unlike in Si, the interval of the investigated stresses is separated into two distinct parts in which the dislocation behaviors have different characters.

At high stresses ($\tau \gtrsim 2 \text{ kgf/mm}^2$) the results can be qualitatively described, as for Si, by the diffusion theory of production of double kinks on the dislocation, with account taken of the fact that the energy of the double kink decreases under the influence of both short-range (elastic) and long-range (electrostatic) fields of the point defects. To explain the low values of L_{cr} it must be proposed that the dislocation is always characterized by a very high concentration of surrounding point defects. They increase the probability of double-kink production in the field of the distortions associated with the defects, and hinder the runaway of the kinks. The theoretical estimates in^[10] do not contradict the experimental facts. Schaumburg, discussing the data of^[16], took into account the influence of only one of two possible limiting variants: subdivision of the dislocation into sections by unsurmountable obstacles. It should be noted that this should inevitably yield an unrealistically high density of very strong stops. The average distance between them should be smaller than $U_{\text{dk}}/\tau ab$, which amounts to $(25 - 100)b$ for the high investigated values of τ . It seems to us that if we attempt nevertheless to describe the dislocation mobility in semiconductors within the framework of the Peierls model, we must take into account the influence of point defects not only on the motion of the bands, but also on the generation of double kinks.

At low stresses ($\tau < 2 - 4 \text{ kgf/mm}^2$), for all crystals with acceptor impurity and for crystals slightly doped with donor impurities one observes a relatively strong dependence of v and U on τ . This dependence can be qualitatively explained by taking into account the influence of the weak obstacles on the motion of the kinks along the dislocation^[12,13]. In this case, too, estimates show a very high ($\sim 10^{-2}$) concentration of point defects on the dislocation. However, not all the experimental results in the range of low τ can be reconciled with the predictions of the theories. One of the causes of the discrepancy may be that at such high defect densities on the dislocation it is necessary to take into account that a thermal-fluctuation collapse of the double kink may result not only from the first defect-induced barrier encountered by the kink. It is necessary to take into account also the influence of the succeeding barriers.

For Ge with As density 10^{19} cm^{-3} , no region of sharp increase of the activation energy with decreasing τ is observed. In this crystal, as in Si, starting stresses are observed for the dislocation motion, and further-

more of rather large magnitude ($\sim 2 \text{ kgf/mm}^2$). It appears that this is due to the increased density of the stops for the kinks on the dislocation. One cannot exclude the possibility that in Si, too, this is precisely why no interval of rapid growth of U is observed with decreasing τ .

Thus, the aggregate of the experimental data obtained with Si and Ge offers convincing evidence that to describe the real laws governing the motion of dislocations within the framework of the Peierls model we need a more profound development of the theory, with allowance for the spatial inhomogeneity, due to the point defects, and of the crystal lattice potential reliefs that limit the motions of the dislocation and of the kinks. It is necessary in this case to analyze in detail the influence of various cases of statistical distribution of defects, of the values of the barriers associated with the defects, etc. From the experimental point of view, it is necessary to investigate the concrete state of the nucleus of the dislocations whose mobilities are measured, for the purpose of estimating the true concentration of the point defects and the degree of splitting of the dislocations. We consider these questions to be extremely important for the understanding of the nature of processes that limit the dislocation motion in the case when $\tau < \tau_p$, and for the development of methods for controlling the plasticity of brittle metals.

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- ¹In some papers, e.g., [1], it is indicated that quantum tunneling through the Peierls barrier is possible.
- ²In the stress interval $0.15\text{--}0.5 \text{ kgf/mm}^2$ the measurements were made only on crystals oriented in accord with type "b."
- ³It turned out that the tests of [17] were performed in a furnace with an increased axial temperature gradient, so that the temperature at the investigated section of the sample was $10\text{--}15^\circ$ higher than the measured one. This explains the higher values of the velocities, and the somewhat lower values of the activation energy of the dislocation motion, which are seen when the results of [17] are compared with those presented here.
- ⁴The results of [1], where a more general solution is given, practically coincide with those obtained in [5,6].
- ⁵For a relief of quasiparabolic shape, the values of τ_p and ω differ insignificantly from those written out for the sinusoidal relief.

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