SovietRxiv

Soviet-era science, translated into English

THE INFLUENCE OF IMPURITIES ON THE OVERCOMING OF HIGH PEIERLS BARRIERS BY DISLOCATIONS

PHYSICS

1969

SovietRxiv

View the original and related papers at https://sovietrxiv.org/items/ru-196901.24898

Source: Math-Net.Ru and CyberLeninka. Machine translation. Verify with the original.

SovietRxiv

Abstract

Full Text

UDC 539.4.019.3

PHYSICS

V. N. EROFEEV, V. I. NIKITENKO, V. B. OSVENSKII

THE INFLUENCE OF IMPURITIES ON THE OVERCOMING OF HIGH PEIERLS BARRIERS BY DISLOCATIONS

(Presented by Academician G. V. Kurdyumov, 16 IV 1969)

The interaction of dislocations with dissolved impurity atoms is one of the cardinal problems of the physics of strength, since alloying is the most widespread and effective method of altering the mechanical properties of crystals. In this connection, the elastic interaction of dislocations with impurities is usually considered; this interaction should inevitably lead to strengthening of the material. Such an approach is justified in the study of the plasticity of crystals with a relatively low value of the Peierls stress, for example f.c.c. metals and alkali-halide crystals, in which the mobility of dislocations is limited by interaction with point defects that are pinning centers. However, in crystals with high Peierls stresses, in particular in semiconductors with covalent bonding, the energy of elastic interaction of dislocations with impurities may turn out to be considerably smaller than the energy that must be expended in order to move dislocations in the field of Peierls forces, and the mobility of dislocations is limited by the resistance of the crystal matrix. In this case one cannot unambiguously expect strengthening of crystals upon alloying. The introduced impurity may substantially affect the efficiency of thermally activated overcoming of the potential Peierls barrier by dislocations. Indeed, the study of the macroscopic characteristics of plastic deformation of covalent semiconductors ([1–3]) has shown that, depending on the type and concentration of alloying impurities, both strengthening and softening of the material may occur. However, the macroscopic parameters of plastic deformation (for example, the yield point) are determined not only by the mobility of dislocations, but also by the regularities of their multiplication, which may change under strong alloying. Therefore, in order to elucidate the influence of impurities on the mechanism by which dislocations overcome high Peierls barriers, a direct study of the motion of individual dislocations is necessary.

In the present work we give the results of an investigation of the dependence of the velocity of motion of individual dislocations on stress and temperature in silicon single crystals with different contents of donor (As and Sb) and acceptor (B) impurities.

SovietRxiv

Figure 1

Figure 1: Figure 1

Figure 2

Figure 2: Figure 2

To determine dislocation velocities we used the well-known method of measuring the displacement of dislocation half-loops emerging at the surface by means of etch pits. The main source of these half-loops was a scratch made at room temperature on the {111} surface of the specimen. Loading of specimens, which had the form of a parallelepiped of dimensions $1.8 \times 2.5 \times 25$ mm, was carried out according to the four-point bending scheme. The resolved shear stresses along $\langle 110 \rangle$ in two slip planes {111}, symmetric with respect to the bending axis $\langle 112 \rangle$, were calculated from the formula $\tau = 0.41\, 3cP/dh^2$, where 0.41 is the orientation factor, c is the half-difference of the distances between the lower and upper bending supports, d is the width, h the thickness of the specimen, and P the external force.

To reveal dislocations a chromium etchant was used ($CrO_3 : H_2O : HF = 1 : 2 : 3$).

All measurements were carried out only on single isolated half-loops, which, upon introduction, were expanded from the scratch to distances of more than $15\,\mu$, since at smaller sizes the dislocation velocity depends on the half-loop diameter ([4]).

Fig. 1. Dependence of the activation energy of the motion of individual dislocations in silicon ($\tau = 12$ kg/mm^2) on impurity concentration: 1—B, 2—As, 3—Sb, 4—undoped (according to the data of ([4]))

Fig. 2. Dependence of the velocity of motion of 60-degree dislocations ($\tau = 12$ kg/mm^2) on impurity concentration at various temperatures in silicon doped with: 1—B, 2—As, 3—Sb, 4—undoped (according to the data of ([4]))

The study of dislocation velocities in doped silicon single crystals was carried out in the temperature range 450—800° at stresses from 0.2 to 35 kg/mm^2. The dependence of the velocity of motion of individual dislocations on stress and temperature for most single crystals is described by the expression

$$v = v_0 (\tau/\tau_0)^m \exp(-U/kT), \tag{1}$$

where $\tau_0 = 1$ kg/mm^2, U is the activation energy, and v_0 is a constant. The exponent m practically does not differ for screw and 60-degree dislocations and decreases insignificantly with doping (within the range 1.5—1.3). An increase in the concentration of acceptor (B) and donor (As, Sb) impurities leads to a

SovietRxiv

decrease in the activation energy U of dislocation motion. In this case donor impurities exert a considerably stronger influence (Fig. 1).

In work ([5]), in studying the motion of the leading dislocation of a row in silicon at 600°, it was found that the dislocation velocity in crystals with As ($n = 10^{19}$ cm^{-3}) is 6 times greater, and in crystals with Ga ($p = 6 \cdot 10^{17}$ cm^{-3}) is 2 times smaller, than in undoped silicon. Similar data were obtained in work ([2]) for Ge. However, the results of our experiments show that the character of the influence of doping impurities on dislocation mobility is more complex and depends on temperature (Fig. 2). At a relatively low temperature (450°), doping with both B and As leads to an increase in dislocation velocity compared with undoped silicon. With increasing temperature, the difference in dislocation velocities between undoped and doped n- and p-type crystals decreases. At 750 and 800°, the acceptor impurity already leads to a certain decrease in dislocation velocity, whereas the donor impurity still increases it. Such a change in the ratio of dislocation velocities for crystals with different impurity contents is due to the influence of doping on the activation energy of dislocation motion.

The results obtained in the present work are not consistent with the conclusions of the theory of Patel and Frisch ([6,7]), according to which an increase in the concentration of a donor impurity should lead to an acceleration of dislocation motion, while an acceptor impurity should decrease the dislocation velocity in Ge and Si.

According to existing theoretical concepts (for example, the reviews ([8,9])), the overcoming of high Peierls barriers in semiconductor single crystals occurs through the formation of thermally activated double kinks. In this case the quantity U in formula (1) should correspond to the activation energy for the formation of a double kink U_{dk}. The experimentally determined values of U ([4,10]) do indeed coincide with the value U_{dk}, calculated by Labusch ([11]) for Si and Ge.

The activation energy for the formation of a double kink in the approximation of constancy of the line energy E_0 of a dislocation is determined by the expression ([12])

$$U_{\text{dk}} = 2\sqrt{2E_0}\int_{x_0}^{x_{\max}} \sqrt{V(x) - V(x_0) - \tau b(x - x_0)}\,dx, \tag{2}$$

where $V(x)$ is a function describing the potential relief in which the dislocation moves, x_0 is the position of stable equilibrium of a straight dislocation in the field of external stresses, and b is the Burgers vector.

Analysis of expression (2), taking into account possible changes in the state of the crystal lattice during alloying, shows that the experimentally observed change in the energy of formation of a double kink cannot be explained by a local change in τ or b near impurity atoms, nor by a change in E_0 due to the influence of impurities on the elastic constants of the lattice. Most probably,

SovietRxiv

the observed effect is caused by a change in the potential relief of the lattice $V(x)$ during alloying, which facilitates the overcoming of the potential barrier by dislocations. In our opinion, the change in relief is associated with the electrical activity of impurities, which leads to a change in the electronic structure of the crystal.

In conclusion, we note that materials with high Peierls barriers are characterized by increased brittleness at relatively low temperatures. The formation of microcracks, which are sources of brittle fracture, is associated with the low mobility of dislocations. Therefore, for such materials, along with the macroscopic characteristics of plastic deformation, special importance is acquired by microplasticity, caused by the motion of individual dislocations or small dislocation groups. Undoubtedly, from the point of view of lowering the temperature threshold of brittle fracture in these materials, the possibility of increasing microplasticity, in particular by alloying, plays an important role.

The authors express their gratitude to V. L. Indenbom and V. L. Pokrovskii for useful discussion of the results.

Institute of Solid State Physics
Academy of Sciences of the USSR
Chernogolovka, Moscow Region

State Institute
of the Rare-Metals Industry
Moscow

Received
11 IV 1969

REFERENCES

1. M. G. Mil' vidskii, V. B. Osvenskii, O. G. Stolyarov, *Inorganic Materials*, **1**, 1449 (1965).

2. A. R. Chaudhuri, J. R. Patel, *Phys. Rev.*, **143**, 601 (1966).

3. V. B. Osvenskii, M. G. Mil' vidskii, O. G. Stolyarov, *Crystallography*, **13**, 831 (1968).

4. V. I. Nikitenko, V. N. Erofeev, N. M. Nagornaya, in: *Dynamics of Dislocations*, Kharkov, 1968, p. 84.

5. J. R. Patel, P. E. Freeland, *Phys. Rev. Letters*, **18**, 833 (1967).

6. J. R. Patel, H. L. Frisch, ibid., **18**, 784 (1967).

SovietRxiv

7. J. R. Patel, H. L. Frisch, *Appl. Phys. Letters*, **13**, 25 (1968).

8. V. I. Nikitenko, in: *Dislocations and Physical Properties of Semiconductors*, "Nauka," 1967, p. 30.

9. P. Haasen, *Dislocation dynamics*, Battelle Inst. Mater. Sci. Colloq., 1967, p. 701.

10. C. Schäfer, *Phys. Stat. Solidi*, **19**, 297 (1967).

11. R. Labusch, ibid., **10**, 645 (1965).

12. V. L. Indenbom, A. N. Orlov, in: *Dynamics of Dislocations*, Kharkov, 1968, p. 5.

Note: Figure translations are in progress. See original paper for figures.

Source: Math-Net.Ru and CyberLeninka. Machine translation. Verify with the original.