TEMPERATURE DEPENDENCES OF THE DEFORMATION AGEING OF SCREW AND EDGE DISLOCATIONS IN NaCl SINGLE CRYSTALS

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Temperature dependences of the deformation ageing of screw and edge dislocations in NaCl single crystals have been studied. It is found that the temperature strongly influences the process of ageing of screw dislocations, but weakly affects that of edge ones. It is shown that the centers of the strong pinning of screw dislocations arise in the regions of thermal kink formation. Basing on the experimental data, the energy of a kink formation and the concentration of thermal kinks in the temperature range 20—100 °C are determined. The results obtained are in good agreement with the theoretical calculations.

Introduction

Features of an interaction of dislocations with impurity atoms, peculiarities of a dislocation structure and a state of their cores are known to strongly influence the mechanical properties of crystalline materials. It is these topics that have been at the center of attention of a number of theoretical [1—3] and experimental works [4, 5]. However, a majority of the experimental papers devoted to studying the features of the dislocation movement in a material containing impurity atoms is concentrated on the characteristics of those dislocations which are not subjected to ageing. In the previous works, we have shown that the deformation ageing process strongly affects the mobility of both screw [6] and edge [7] dislocations. What is more, independent of a dislocation type, the following process should occur: impurity atoms, having fallen from the atmosphere on a dislocation and diffusing along it, have to accumulate at the points which pin down the movable dislocation segments, i. e. at obstacles. It has been shown experimentally that these obstacles appear not arbitrarily, but at a fixed distance from a crystal surface [8—9]. To explain such behavior of the centers of the strong pinning of dislocations, we have studied the temperature dependences of the deformation ageing of screw and edge dislocations.

Specimens and Procedure of Investigations

All the studies were performed on NaCl crystals with a yield stress $\tau_s = (3 \pm 0.2)5$ MPa. The motion of aged dislocations, both the screw and edge ones, was studied according to the procedure described in works [6, 7]. After the dislocations were driven to a starting position, they were subjected to ageing either in a desiccator at room temperature or in an electric oven at temperatures 50 and 100 °C. The ageing process was followed by a four-bearing bend loading for 2 s at room temperature. Calculation of a fraction of the displaced dislocations, $\Delta N/N$, was carried out as described in works [6, 7].

Experimental Results and Discussion

Figs. 1 and 2 show some examples of the dependence of $\Delta N/N$ vs applied stress τ for the edge and screw dislocations, respectively, after they were aged for 20 h. As can be seen from the figures, the temperature scarcely influences the unpinning stress for edge dislocations, but strongly affects it for screw ones.

Such a character of the temperature effect on $\Delta N/N(\sigma)$ curves can be explained basing on the assumption about a formation of the centers of strong pinning on the dislocation irregularities such as thermal kinks and jogs.

According to [10], the free energy of a kink formation is

$$F_k = U_k - T_k, \tag{1}$$

where $2U_k$ and $2S_k$ are the energy and entropy terms, respectively. In comparison with the elastic energy and the mismatch energy in a core ($2W_k$), other contributions to $2U_k$ are negligible. The latter term can be written as

$$W_k = W_f + W_{\text{in}}, \tag{2}$$

where W_f is the energy of the kink formation and W_{in} is that of the interaction between kinks. The corresponding

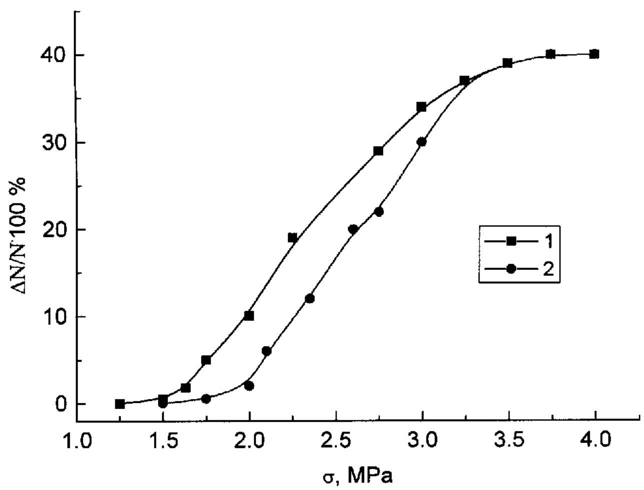

Fig. 1. Dependence of the percentage of displaced edge dislocations on the applied external stress at $T = 20$ (*1*) and 100 °C (*2*). The ageing time is 20 h

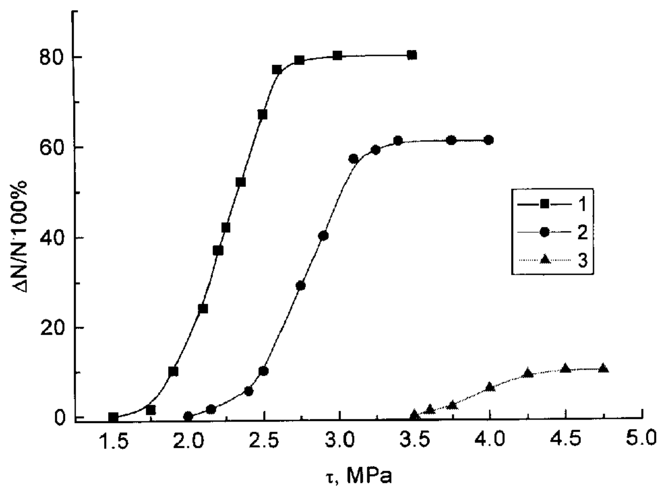

Fig. 2. Dependence of the percentage of displaced screw dislocations on the applied external stress at $T = 20$ (*1*), 50 (*2*), and 100 °C (*3*). The ageing time is 20 h

expressions for these terms are

$$W_f = \frac{\mu b^2 a}{4\pi(1-\nu)}\left[\ln\frac{a}{e\rho} - (1-\nu)\right], \tag{3}$$

and

$$W_{\rm in} = -\frac{\mu b^2 a^2}{2\pi L}\frac{1+\nu}{1-\nu}. \tag{4}$$

Here, μ is the shear modulus, b — Burgers vector, ν — Poisson coefficient, $e = 2.71$; $\rho - b/2\alpha$, $\alpha = 4$ for non-metals, L — the length of a dislocation segment, a — a distance between the points of the symmetry recurrence, taken along a dislocation.

When the distance between kinks is far greater than a kink width, $W_{\rm in}$ becomes negligible in comparison with W_f. Then

$$U_k \approx W_k = \text{const.} \tag{5}$$

Consider the case where all kinks are localized in a position which corresponds to the energy minimum and separated by a distance a along the dislocation line. Then, in a high temperature limit, the oscillation mode entropy per one oscillator with a circular frequency ω can be expressed as

$$S = -k\ln\left[1-\exp\left(-\frac{\hbar\omega}{kT}\right)\right] \approx k\ln\frac{kT}{\hbar\omega}, \quad kT > \omega\hbar. \tag{6}$$

When a kink is formed, a new mode appears, namely, the oscillation one whose frequency ω_k corresponds to that of a kink oscillation around the equilibrium position. Since the total quantity of the oscillation modes is constant, one oscillation mode of the crystal or dislocation should vanish upon the appearance of the kink mode. Assume that the oscillator that vanishes has a frequency ω_p, with ω_p being the frequency of the oscillation of a dislocation in a Peierls valley. Then, at high temperatures, a change in the entropy can be written as

$$\Delta S_k = k\left(\ln\frac{kT}{\hbar\omega_k} - \ln\frac{kT}{\hbar\omega_p}\right) = k\ln\frac{\omega_p}{\omega_k} \tag{7}$$

In the temperature region $\hbar\omega_p \gg kT \gg \hbar\omega_k$, only kink oscillations will be excited classically, whereas a contribution to the entropy that arises from the oscillation of the height of the Peierls barrier is negligible. Accounting for this fact, we can express ΔS_k as

$$\Delta S_k = k\left(\ln\frac{kT}{\hbar\omega_k} - \ln\frac{kT}{\hbar\omega_p}\right) \tag{8}$$

At ordinary values of the oscillation frequencies, the term TS_k in Eq. (1) is insignificant in comparison with U_k. Thus, for this case,

$$F_k = W_k \tag{9}$$

is a good approximation.

The equilibrium concentration of kinks, c_k, is directly associated with the free energy of the kink formation, F_k, and, according to [10], is

$$c_k = \frac{1}{a^2}\exp\left(-\frac{2F_k}{kT}\right), \tag{10}$$

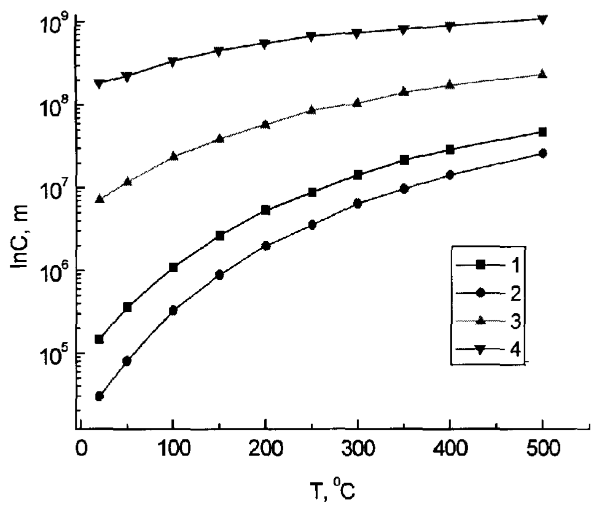

Fig. 3. Temperature dependence of $\ln c_k$ for ZnSe (*1*), NaCl (*2*), InSb (*3*), and Si (*4*) crystals

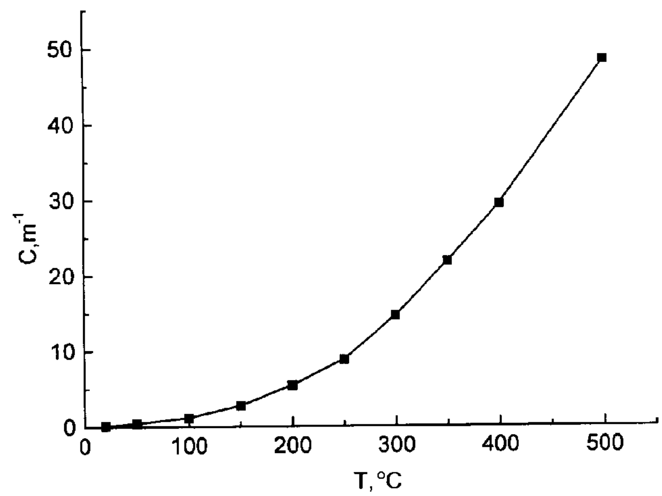

Fig. 4. Concentration of kinks as a function of temperature for NaCl crystals

where, accounting for (9) and (3),

$$F_k = W_f = \frac{\mu b^2 a}{4\pi(1-\nu)}\left[\ln\frac{a}{e\rho} - (1-\nu)\right]. \tag{11}$$

To determine the concentration of thermal jogs, the analysis analogous to that performed above should be carried out. On the dislocation which lies in the slip plane, a pair of jogs (a double jog) may be formed by means of the removal (or addition) of atoms from the dislocation and their subsequent approach to (or moving away from) a protruded segment on the crystal surface in such a way that the equilibrium chemical potential of the crystal remains conserved. With the equal probability, atoms can either turn into a vapor which is in equilibrium with the crystal, or enter the interstitial space when the concentration of interstitial atoms is equilibrium. For these processes, the total change in the free energy of a double jog is the free energy of the double jog formation, F_s. The energy of the double jog formation is far greater than that of the kink formation [10], but the interaction energy is nearly equal for both the cases. The same concerns also the entropy. Thus, the approximation

$$F_s = W_s, \tag{12}$$

is even better for the case under consideration than for the case of kinks. Here,

$$W_s = \frac{\mu b^2 a}{4\pi(1-\nu)}\left[\ln\frac{a}{e\rho}\right]. \tag{13}$$

When the whole dislocation line, except for thermal jogs, lies in the slip plane, the concentration of thermal jogs, c_s, is determined as

$$C_s = \frac{1}{a^2}\exp\left(-\frac{2F_s}{kT}\right). \tag{14}$$

The energies of the thermal kink formation calculated according to expression (11) for various kinds of crystals are presented in the Table. For these materials, the concentration of thermal kinks in the temperature range 20—500 °C was also calculated according to expression (10) (see Fig. 3). As follows from the figure, for the materials with a higher Peierls relief, the energy of the thermal kink formation is smaller and, thus, the concentration of kinks is higher.

For the crystals of sodium chloride, the energies of the formation of thermal kinks and jogs, calculated according to Eqs. (11) and (13), respectively, are $W_k = 0.23$ eV and $W_s = 0.66$ eV. Thus, the latter is almost thrice higher than the former. It is evident from expressions (10) and (14) that, for all the temperatures, the concentration of thermal kinks on the screw dislocations is by far exceeds that of jogs on the edge ones. At the same time, an intense growth of the kink concentration occurs upon the rise in temperature (see Fig. 4). Hence, the formation of kinks results in

Material	$(a, b)\times 10^{10}$, m	ν	$\mu \times 10^{-10}$, N/m^2	W_k, eV
ZnSe	5.65	0.4	0.38	0.28
NaCl	5.64	0.3	0.48	0.23
InSb	5.20	0.35	0.30	0.14
Si	3.00	0.26	1.00	0.07

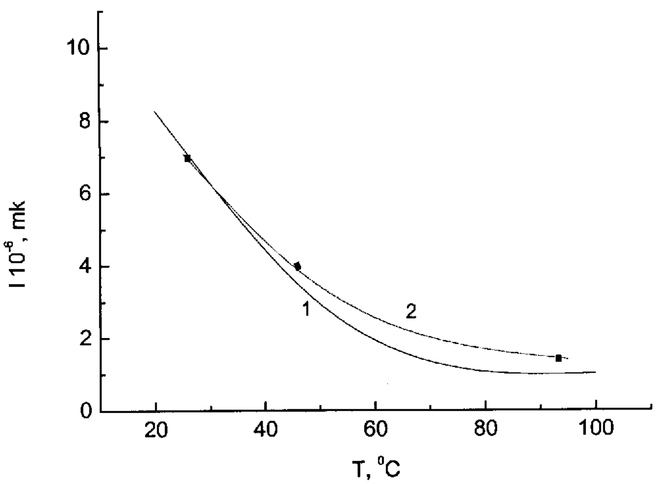

Fig. 5. Dependence of the length of the loose dislocation segment on temperature: *1* — theoretical curve, *2* — experimental data

an increase in the total length of the edge segments on those dislocations, which have a screw orientation near the surface and around which the impurity atmosphere may be formed. This, in turn, leads to an increase in the probability of the formation of pinning centers, and, as a result, a sharp decrease in the quantity of movable screw dislocations occurs. On the contrary, for the dislocations that have edge orientation near the crystal surface, the concentration of jogs grows slightly. In addition, an increase in c_s does not result in an increase of the total length of the edge segments of dislocations. Thus, for such dislocations, the probability of the formation of additional pinning centers grows exclusively owing to a rise in the diffusion coefficients of impurity atoms.

Assuming that the origin of the formation of the centers of strong pinning is the kinks on screw dislocations, we get that the distance between them should equal a length of a loose segment of the moving dislocation (l). In this case, as the Orowan's formula predicts,

$$\tau_c = \alpha\mu b/l, \qquad (15)$$

a movement of a dislocation segment with a length l, preliminary driven to a starting position, should occur at a stress τ_c, with α being approximately equal to 2. It is this quantity that can be determined experimentally from the curves of the distribution of dislocations over the unpinning stress presented in Fig. 1. The temperature dependence of the length of the loose dislocation segment calculated from Eq. (15) is shown in Fig. 5 (curve *2*). As is seen from the figure, the experimental data agree fairly well with the calculated ones.

As well as this, experimental results make it possible to calculate the actual energy of the formation of thermal kinks, and it is found to be 0.25 eV.

Conclusions

Basing on the results of both the experimental studies and theoretical calculations, it is shown that the ageing process gives rise to the formation of the centers of strong pinning of the dislocations on the impurity atoms in the regions where thermal kinks are formed. The energy of the formation of thermal kinks derived from the experimental data agrees well with the theoretically calculated value.

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ТЕМПЕРАТУРНІ ЗАЛЕЖНОСТІ ДЕФОРМАЦІЙНОГО СТАРІННЯ ГВИНТОВИХ І КРАЙОВИХ ДИСЛОКАЦІЙ В МОНОКРИСТАЛАХ NaCl

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Р е з ю м е

Вивчено температурні залежності деформаційного старіння гвинтових і крайових дислокацій. Встановлено, що температура сильно впливає на процес старіння гвинтових дислокацій та слабко — крайових. Показано, що потужні центри закріплення гвинтових дислокацій виникають в місцях утворення термічних перегинів. За експериментальними результатами визначено концентрацію термічних перегинів при температурах 20—100 °C та розраховано енергію їхнього утворення, значення якої добре узгоджується з розрахованим теоретично.