MECHANISM OF THE INFLUENCE OF ULTRASONIC AND ELECTRIC FIELDS ON THE VIBRATIONAL MOTION OF DISLOCATIONS IN THE ULTRASONIC VIBRATION OF ALKALI-HALIDE CRYSTALS

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The influence of electric and ultrasonic fields on the vibrational motion of disolocations in alkali-halide crystals was investigated by the method of current–voltage characteristics I(V) and the measurement of the amplitude dependence of the damping $Q^{-1}(\varepsilon_0)$ and the defect of the modulus $\Delta M/M(\varepsilon_0)$ in a composite piezoelectric oscillator. An abrupt decrease of I(t) is observed at amplitudes of the relative deformation $\varepsilon_0 = 10^{-6}$-10^{-5}. The internal friction at the same ε_0 reveals an amplitude dependence, while establishment of steady values is attained by passage through the maximum of $Q^{-1}(t)$. The electric field shifts the amplitude of the onset of the abrupt decrease of I(t) into the region of smaller ε_0. The displacement of the vibrating dislocation at an amplitude ε_0 corresponding to the onset of the singularity of I(t) is near the value of the radius of the Debye–Hückel cloud surrounding it. The characteristic times of the process correspond to the relaxation time of a free charge in an insulator.

The results for the influence of ultrasonic and electric fields on the behavior of dislocations in alkali-halide crystals in the kilohertz frequency range, obtained on the basis of an analysis of the current–voltage characteristics and the internal friction at room temperature, were given previously in [1, 2]. Specimens of solely zero orientations were studied. In the present paper, the investigations are augmented by a study of specimens of nonzero orientations, while the temperature interval is widened to 300°C. Analysis of the results made it possible to show the mechanism of the influence of the electric field on behavior of the dislocations in the alkali-halide crystals for small amplitudes ε_0 of the ultrasonic action, in the absence of translational dislocation motion.

EXPERIMENTAL PROCEDURE

Specimens of LiF, NaCl, KCl, and KBr with static yield points $3.5 \cdot 10^6$, $2 \cdot 10^6$, $7 \cdot 10^5$, and $9 \cdot 10^5$ $N \cdot m^{-2}$ and initial dislocation density N not exceeding $5 \cdot 10^8$ m^{-2} were investigated. The ultrasonic action on the specimen was effected by means of a composite piezoelectric oscillator in its two versions [3, 4]. The distribution of the elastic deformation along the length of the specimen has the form $\varepsilon = \varepsilon_0 \sin \frac{\pi n y}{L}$, where L is the specimen length, y is the distance measured from the joining point of the specimen and the quartz, n is the number of the harmonic. The frequency range of the investigations was 40-160 kHz. A false plug of fused quartz was placed between the quartz crystal and the specimen in the temperature investigations. The subsequent thermal expansion of the specimen was taken into account in the calculation of its length; the temperature gradients along the length did not exceed 10^2 $K \cdot m^{-1}$, and the frequencies of the quartz and the specimen differed by not more than 0.3 kHz. The orientation of the specimen is characterized by the angle Θ between the fourth-order axis and the direction of propagation of the ultrasonic wave. Specimens of zero and thirty-degree orientations were investigated. The $\Theta = 0°$ specimens were pricked out over the cleavage planes, and the specimens of NaCl, KCl, KBr with $\Theta = 30°$ were cut out by a fiber saw. The amplitudes of the cleavage stresses were calculated in accordance with the equation $\sigma_c^0 = m\varepsilon_0 M$, where M is Young's modulus, m is the Schmidt factor. For the specimens of zero orientation the same cleavage stresses σ_c^0 exist in the four planes of easy slip {110}

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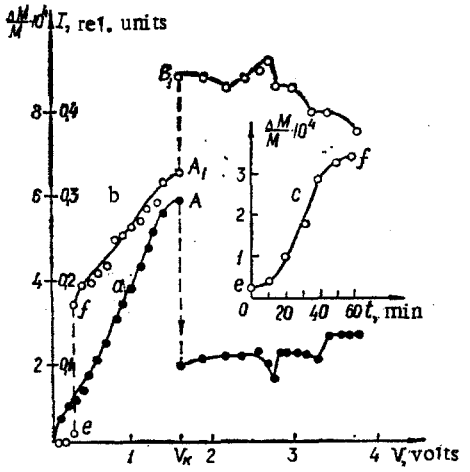

Fig. 1

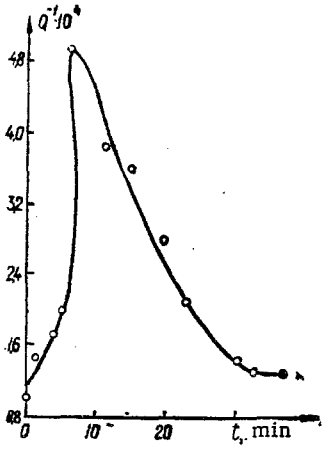

Fig. 2

Fig. 1. Current–voltage characteristic I(V) with abrupt decrease of I(t) (a). The change in the defect of the modulus $\Delta M/M(V)$ which corresponds to the curve I(V) (b). LiF, f = 120 kHz, third harmonic.

Fig. 2. Change in the damping $Q^{-1}(t)$ at the amplitude $\varepsilon_0 P$ which corresponds to the onset of the singularity of I(t), $\Theta = 0°$, f = 73 kHz, $\varepsilon_0 = 6.2 \cdot 10^{-6}$, KCl.

(m = 0.5). For the $\Theta = 30°$ specimens, σ_c^0 are present in all six planes {110}, but the Schmidt factor m is different for each pair of orthogonal planes [5]. By increasing the deformation in the specimen, we can investigate the action of ultrasound on the dislocation in planes with different m. The dependence of Young's modulus on the temperature was taken into account in the calculation of the cleavage stresses.

In the method of current–voltage characteristics, the dependence of the current I in the circuit of a two-component vibrator in the case of series resonance on the voltage V applied to the quartz is investigated. The quantity I is proportional to the amplitude of the relation deformation ε_0 in the specimen. The two-component vibrator system was also used to measure the internal friction at room temperature. The reciprocal of the Q factor, Q^{-1}, was taken as the measure of internal friction. A three-component vibrator is more convenient in temperature investigations and the study of effects which depend on time. The damping in this case is proportional to the ratio V_d/V_g, where V_d is the voltage applied to the quartz generator, V_g is the voltage taken from the quartz receiver. Since the elastic deformation in the specimen is proportional to V_g, the curve of the dependence $V_g(V_d)$ is similar to the curve I(V). The investigations are augmented by measurements of the defect of Young's modulus $\Delta M/M = 2f_0 - f/f_0$, where f_0 is the resonance frequency for the minimum amplitudes ε_0 used in the paper. An ultrasonic vibration was effected in the direction [001] for the specimens with $\Theta = 0°$, and at an angle of 30° to this direction for $\Theta = 30°$. An electric field was produced in the specimen by placing it in the field of an air-filled plane-parallel capacitor; the intensity vector $\boldsymbol{E}$ was directed along [100]. The damping and the defect of Young's modulus were investigated in a vacuum at the residual pressure 10^{-3} mm Hg.

The temperature dependence of the conductivity γ was investigated to determine the total concentration α of the bivalent impurity in the crystals (with the exception of LiF). For the temperature T_K at which the curve $\ln\gamma = f(1/T)$ changes slope, going over from the intrinsic conductivity region to the impurity conductivity region, $\alpha = \exp(S_S/2\kappa)\exp(-H_S/2\kappa T_K)$, S_S and H_S are the entropy and enthalpy of the production of a Schottky pair. The quantity H_S required for the calculation of α was determined from the slopes of the curve in these two regions [6]; the experimental data of other authors were used for S_S [7-9]. The concentration α thus calculated was $4.2 \cdot 10^{-6}$ mole fractions for NaCl, $8 \cdot 10^{-6}$ for KCl, and $2.2 \cdot 10^{-6}$ for KBr.

INFLUENCE OF ULTRASONIC FIELD

A linear dependence between the elastic deformation in the specimen and the voltage applied to the quartz is observed in the initial section of the curves I(V) and $V_g(V_d)$.

TABLE 1

Specimen	σ_c^p, N·m^{-2}		E, V·m^{-1}
	control specimen	test specimen	
LiF	$1 \cdot 10^6$	$8{,}2 \cdot 10^5$	$2 \cdot 10^6$
NaCl	$5{,}9 \cdot 10^5$	$5{,}6 \cdot 10^5$	$1{,}2 \cdot 10^6$
KBr	$5{,}8 \cdot 10^6$	$5{,}5 \cdot 10^5$	$8{,}3 \cdot 10^5$
KCl	$1{,}2 \cdot 10^5$	$8{,}8 \cdot 10^4$	$8{,}3 \cdot 10^5$

A section of microplasticity then follows; the transient effects associated with a change in the behavior of the dislocations appear in it. Figure 1a shows the linear section and the origin of the section of microplasticity of the curve I(V) and of the LiF specimen. The corresponding change in $\frac{\Delta M}{M}(V)$ is shown in Fig. 1b, from which it can be seen that the defect of the modulus $\frac{\Delta M}{M}$ reveals a time dependence even at small amplitudes ε_0. The increase in $\frac{\Delta M}{M}(t)$ in the section ef (Fig. 1c) may be due to the redistribution of the weak pinning centers along the dislocation; supplementary experiments are required to show the nature of these centers.

It can be seen from Figs. 1a and b that for the voltage on the quartz V_K a sharp decrease in I(t) is observed, which is accompanied by as sharp an increase in $\frac{\Delta M}{M}(t)$. The subsequent increase in V did not lead to a change in ε_0 and $\frac{\Delta M}{M}$ and the system sometimes went out of resonance. In a certain time, which depends on the type of crystal, the elastic properties of the specimen were again reestablished. Three singularities of I(t), which correspond to the processes in each pair of orthogonal planes of easy slip, were observed for the $\Theta = 30°$ specimens [10].

The distinguishing feature of the singularity of I(t) is its reproducibility: repeated measurements again reveal a region of abrupt decrease for the same $\varepsilon_0 P$, etc. The characteristic time of passing through the singularity is 30-50 min at room temperature. As the temperature was increased from room temperature to 300°C the stresses $\sigma_0 P$ of the onset of I(t) decreased by a factor of 5, while the time τ shortened to a few minutes. The internal friction at amplitudes near $\varepsilon_0 P$ reveals an amplitude dependence, and the stabilization of the steady value is attained by means of passage through the maximum. Figure 2 shows an example of such a maximum on the curve $Q^{-1}(t)$. The stabilization time of the steady value is near the time τ of passing through the singularity of I(t) in order of magnitude.

The energy applied to the quartz plate in the ultrasonic vibration of the specimen is expended on the production of the elastic field, the displacement energy of the dislocations, and the heat loss. Translational motion of the dislocations is not found after the singularity of I(t) has been passed, so that the decrease in ε_0 at the crest of the standing ultrasonic wave is due to the increase in the heat loss, i.e., the damping of the system.

INFLUENCE OF THE ELECTRIC FIELD

Two specimens with specular cleavages, a test and a control specimen, were used to investigate the influence of the electric field on the curves I(V) and $V_g(V_d)$; the control specimen was tested in the same ultrasonic regime, but without the electric field. The increase in the defect of the modulus $\frac{\Delta M}{M}(t)$ precedes the onset of the singularity of I(t) in the production of the electric field. The change in the product of the mean displacement $\bar{x}$ and the mobile dislocation density N for the NaCl specimen in the electric field $E = 1.2 \cdot 10^6$ V·m^{-1} ahead of the onset of the singularity of I(t), calculated in accordance with Baker's equation $\frac{\Delta M}{M} = \frac{N\bar{x}b}{2\varepsilon_0}$ [11], is shown in curve a of Fig. 3. The curve 2 corresponds to the measurement for the control specimen. The displacement of the vibrating dislocation segment when the field was switched on varied from 50 to 500 Å.

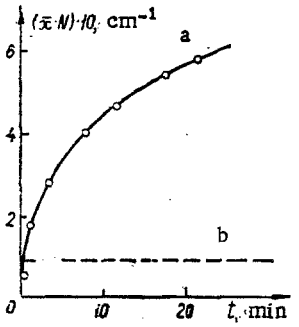

Fig. 3

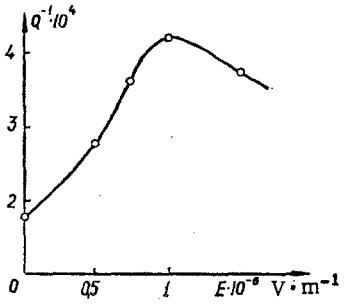

Fig. 4

Fig. 3. Increase (xN) which precedes the abrupt decrease of I(t) for the specimen in the electric field. NaCl, $\Theta = 0°$, f = 73 kHz, $\varepsilon_0 = 1.7 \cdot 10^{-5}$, $E = 1.2 \cdot 10^6$ V·m^{-1}.

Fig. 4. Dependence $Q^{-1}(E)$ for the amplitude ε_0 which corresponds to the origin of the section of microplasticity of the current–voltage characteristic I(V). NaCl, $\Theta = 0°$, $\varepsilon_0 = 1.5 \cdot 10^{-5}$, f = 160 kHz.

The cleavage stresses in the system {110} ⟨110⟩ which correspond to the singularity of I(t) for the test and control $\Theta = 0°$ specimens at a frequency of 73 kHz are compared in Table 1.

Figure 4 shows the dependence of the damping on the electric field strength E for the amplitudes ε_0 in the region of the singularity of I(t). When the electric field was switched off, the damping $Q^{-1}(t)$ slowly relaxed to its initial values.

DISCUSSION OF THE OBTAINED RESULTS

The dislocations in alkali-halide crystals have an electric charge [12, 13]. For crystals with an excess of bivalent cations at nearly room temperatures, the dislocations are negatively charged and are surrounded by a balancing Debye–Hückel cloud, whose radius is $\varkappa^{-1} = \frac{\varepsilon\varepsilon_0 \kappa T}{2e^2 n_\infty}$, where ε is the permittivity, n_∞ is the number of point defects in 1 m^3 far from the cloud. Table 2 shows the values of $\varkappa^{-2}$ calculated in accordance with this equation for the crystals investigated in this paper; the quantity n_∞ necessary for the calculation is determined on the basis of the values for the mole concentration α. The mean displacements $\bar{x}$ of the dislocation segments for the origin of the singularity of I(t), calculated in accordance with Baker's equation, are given in the same table.

The influence of the charge cloud on the vibrational motion of the dislocations is considered in [12-16]. Let β be the relaxation time of the cloud; it can be estimated from Einstein's relation for the diffusion coefficient $D = \frac{\bar{r}^2}{3}$ if we set $\bar{r}^2 = (\varkappa^{-1})^2$. At high temperatures for frequencies of the kilohertz range, $\omega\beta \ll 1$, i.e., the charge cloud is mobile and losses of the viscous type arise within its limit in the case of vibrations of the dislocation [14, 16]. At nearly room temperatures, $\omega\beta \gg 1$, i.e., the cloud does not manage to follow the vibrating dislocation. The restoring force F, which can be assumed proportional to the displacement for $\bar{x} \ll \varkappa^{-1}$, acts on the dislocation which has shifted with respect to the axis of the cloud, i.e., $F = -\varkappa_F x$, $\varkappa_F = \frac{\varkappa_0 q^2 l}{2\pi\varepsilon\varepsilon_0 \varkappa^{-2}}$, $\varkappa_0$ lies in the interval 1.8-4 [13]. It follows from the solution of the differential equation of the forced vibrations of a dislocation segment of length ℓ fixed at the ends, that for $\frac{1}{2}\sqrt{\frac{\varkappa_F}{C}}\bar{l} > 1$ the force exerted by the charge cloud plays a leading part in the limitation of the motion of dislocation. The linear tensile stress is decisive for $\frac{1}{2} = \sqrt{\frac{\varkappa_F}{C}}\bar{l} < 1$. Here $C \approx Gb^2$ is the coefficient of the restoring force that arises through the linear stress. The calculation performed for NaCl showed that the value of $\frac{1}{2}\sqrt{\frac{\varkappa_F}{C}}\bar{l}$ corresponding to the onset of the

TABLE 2

Crystal	Frequency f, kHz	Cloud radius $\varkappa^{-1}$, Å	Displacement $\bar{x}$, Å
LiF	120	—	500
NaCl	73	90	90
KBr	73	75	90
KCl	73	35	39

singularity of I(t) was 7.3; the linear charge density on the dislocation line q_1 for small ε_0, necessary for such an estimate, was taken from [17] and $\bar{\lambda}$ was determined from the data $\Delta M/M$ [18]. Therefore, at amplitudes of the relative deformation 10^{-6}-10^{-5} the decisive role in the limitation of the vibrational motion of the dislocation belongs to the charge cloud.

The most natural explanation of the observed abrupt decrease of I(t) is that for displacements $\bar{x} \approx \varkappa^{-1}$ part of the length of the dislocation lies outside the limits of the cloud, and this leads to an increase in the dislocation deformation and the damping of the system. As can be seen from Table 2, the values of $\bar{x}$ and $\varkappa^{-1}$ which correspond to the onset of the singularity of I(t) are, in fact, near in value. The electric field, acting directly on the dislocation charge, makes the vibrations of the dislocation asymmetric with respect to the cloud. The dislocation starts to lie outside the limits of the cloud at smaller amplitudes of the vibrations; therefore, the onset of the singularity of I(t) in the electric field shifts toward smaller ε_0. In time, the charge cloud assumes a symmetric shape round the vibrating dislocation, pinning it. This process is controlled by the motion of the charges of the cloud in the electric field of the charged dislocation. The time required for the stabilization of the equilibrium distribution of the charge in the insulator is $t = \varepsilon\varepsilon_0/\gamma$ [19]. The values of t calculated in accordance with this equation are near the values of τ for the time of passing through the singularity of I(t).

Thus, in alkali-halide crystals, at amplitudes of the ultrasonic vibration $\varepsilon_0 = 10^{-6}$-10^{-5} in the kilohertz region, the decisive role in the limitation of the vibrational motion of the edge dislocation belongs to the electrostatic force exerted by the charge cloud. For a displacement of the order of the dimensions of the cloud, part of the length of the dislocation lies outside its limit, and this leads to an increase in the damping $Q^{-1}(t)$. The electrostatic field changes the equilibrium position and makes it easier for the vibrating dislocation to lie outside the limits of the cloud.

LITERATURE CITED

1. É. P. Belozerova, N. A. Tyapunina, and A. A. Svetashov, in: Internal Friction in Metals, Semiconductors, Insulators, and Ferromagnets [in Russian], Nauka, Moscow (1978), pp. 152-157.
2. N. A. Tyapunina, A. A. Svetashov, and É. P. Belozerova, Vestn. Mosk. Univ. Ser. Fiz. Astron., 22, 68 (1981).
3. E. G. Shvidkovskii and A. A. Durgaryan, Nauchn. Dokl. Vyssh. Shk. Fiz.-Mat. Nauki, 1, 211 (1958).
4. J. Marx, Rev. Sci. Instrum., 22, 503 (1951).
5. É. P. Belozerova, V. V. Blagoveshchenskii, et al., Izv. Vyssh. Uchebn. Zaved. Fiz., No. 3, 52 (1984).
6. J. Hladik, Physics of Electrolytes, London (1972).
7. A. Huddart and R. W. Whitworth, Philos. Mag., 27, 107 (1973).
8. M. Suszýnska, Bull. Acad. Pol. Sci. Ser. Sci. Tekh., 2, 53 (1977).
9. S. Chandra and J. Rolfe, Can. J. Phys., 49, 2098 (1971).
10. É. P. Belozerova, A. A. Svetashov, and N. A. Tyapunina, Kristallografiya, 28, 346 (1983).
11. G. S. Baker, J. Appl. Phys., 33, 1730 (1962).
12. J. D. Eshelby, C. W. A. Newey, et al., Philos. Mag., 3, 75 (1958).
13. R. W. Whitworth, Adv. Phys., 24, 203 (1975).
14. L. M. Brown, Phys. Status Solidi, 1, 585 (1961).
15. W. H. Bobinson and H. K. Birnbaum, J. Appl. Phys., 37, 3754 (1966).
16. M. Tanibayashi, Philos. Mag., A, 44, 141 (1981).
17. A. R. Anderson and H. F. Pollard, J. Appl. Phys., 50 (8), 5262 (1979).
18. A. Granato and K. Luke, "Dislocation theory of absorption," in: Ultrasonic Methods of Investigation of Dislocations [Russian translation], IL, Moscow (1963), p. 27.

19. A. N. Gubkin, Physics of Insulators. Theory of Dielectric Polarization in Static and Alternating Electric Fields [in Russian], Vol. 1, Vysshaya Shkola, Moscow (1971).

STUDY OF THE ELECTRONIC STRUCTURE OF ALUMINUM COMPOUNDS WITH 3d-TRANSITION METALS

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Compounds of Al with 3d-transition metals with structures of the CsCl variety have a whole series of unique properties: the magnetic properties of FeAl, the high melting temperature of NiAl, properties related to the shape memory effect, increased hardness, etc.

Experimental and theoretical research into the electron properties (kinetic and optical) of compounds of aluminum with one of the transition elements permits one to suggest that the peculiarities in these compounds are caused by their electron structure. Theoretical investigation of the energy band structure of the FeAl, NiAl, and CoAl compounds was done in [1-4].

Calculation of the integrated characteristics of the electron structure, such as the density of states, the kinetic and optical coefficients, etc., requires knowledge of the electron energy spectrum at a large number of points of a Brillouin zone (BZ); therefore, it is most effective to use an interpolation model of the electron structure.

This work, which to some degree has a methodological character, based on a model Hamiltonian, calculates the energy spectrum, the density of states, the valence electron population numbers of different atomic orbitals, and the electron specific heat capacity. In addition, the kinetic stability of the FeAl, NiAl, and CoAl compounds with CsCl type structure is confirmed. It is shown that using the interpolation method for calculating the electron structure makes it possible to compute, relatively accurately in comparison with experimental data and calculations from first principles, the integrated characteristics of the electron structure and to predict the electrophysical properties of aluminides.

The equation for the eigenvalues of the band Hamiltonian has the form:

$$H\Psi_{\kappa n}(\boldsymbol{r}) = E_n(\boldsymbol{\kappa})\,\Psi_{\kappa n}(\boldsymbol{r}). \tag{1}$$

The model basis functions $\Psi_{\kappa n}(\boldsymbol{r})$ (n is the energy band index) are taken in the form of a sum of symmetrized linear combinations of orthogonal plane waves (OPW) $\Phi_{\kappa_j}(\boldsymbol{\kappa}, \boldsymbol{r})$ and linear combinations of Bloch functions of the 3d-electrons $\chi_\mu(\boldsymbol{\kappa}, \boldsymbol{r})$ (strong coupling approximation)

$$\Psi_{\kappa n}(\boldsymbol{r}) = \sum_{K_i} a_{nK_i}(\boldsymbol{\kappa})\,\Phi_{K_j}(\boldsymbol{\kappa}, \boldsymbol{r}) + \sum_{\mu} a_{n\mu}(\boldsymbol{\kappa})\,\chi_\mu(\boldsymbol{\kappa}, \boldsymbol{r}). \tag{2}$$

Here the summing is done over inverse lattice vectors with components (in units of $2\pi/a$, a is the lattice constant) (0, 0, 0), (1, 0, 0), (0, 1, 0), (1, 1, 0), (1, 0, 1), (0, 1, 1), (1, 1, 1) and over all population states with T_{2g} (μ = 1, 2, 3) and E_g (μ = 4, 5) symmetries of the orbitals in the irreducible 1/48 part of the BZ; $a_{nK_i}(\boldsymbol{\kappa})$, $a_{n\mu}(\boldsymbol{\kappa})$ are the linear combination coefficients.

The eight OPW describing the s-type band have the form

$$\Phi_{K_i}(\boldsymbol{\kappa}, \boldsymbol{r}) = C^{-\frac{1}{2}}\left(e^{i(\boldsymbol{\kappa}-K_i)\boldsymbol{r}} - \sum \langle \chi_\mu(\boldsymbol{\kappa}, \boldsymbol{r}) | e^{i(\boldsymbol{\kappa}-K_i)\boldsymbol{r}} \rangle \chi_\mu(\boldsymbol{\kappa}, \boldsymbol{r}),\right.$$

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