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Abstract

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ON THE RELATION BETWEEN THE ELECTRICAL PROPERTIES OF CRYSTALS AND THE PARAMETERS OF THE CRYSTAL LATTICE

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Works ([1–4]) have experimentally shown that there exists a relation between the electrical properties of crystals and the parameters of the crystal lattice. In particular, such a relation has been established between the electric strength, the tangent of the dielectric-loss angle, on the one hand, and the energy of the crystal lattice, on the other. In the present work an approximate calculation is carried out of the dependence of the electric strength of crystals on the parameters of the crystal lattice.

In the presence of a strong electric field, the mean energy of an electron, taking into account its interaction with the phonon gas, is equal to ([5])

$$\varepsilon \sim mv^2 \sim eEl\,\frac{v}{a} \sim eE\,\frac{l}{a}\sqrt{\frac{kT}{m}},$$

where m is the electron mass; k is Boltzmann' s constant; T is the absolute temperature; E is the electric-field strength; l is the electron mean free path; a is the velocity of propagation of phonons (in the present case the beginning of the acoustic branch of the vibrations is meant). Breakdown of the crystal will occur when the energy of the electrons is greater than or equal to the width of the forbidden band, i.e. the breakdown condition may be written as

$$eE_{\text{br}}\frac{l}{a}\sqrt{\frac{kT}{m}} \simeq u_0, \tag{1}$$

where u_0 is the width of the forbidden band in the energy spectrum of the crystal. The velocity of propagation of phonons ([6])

$$a = r_0\sqrt{\frac{\alpha}{2(M_1 + M_2)}},$$

Fig. 1

Figure 1: Fig. 1

where α is the coefficient of quasielastic coupling; M_1, M_2 are the masses of the particles forming the crystal; r_0 is the lattice constant. Substituting a into formula (1), we obtain:

$$E_{\text{br}} \simeq \frac{u_0}{el}\sqrt{\frac{m}{kT}}\, r_0 \sqrt{\frac{\alpha}{2(M_1+M_2)}};$$

but $l = Br_0$ ([5]), therefore

$$E_{\text{br}} \simeq \frac{u_0}{Be}\sqrt{\frac{m}{kT}}\sqrt{\frac{\alpha}{2(M_1+M_2)}}. \qquad (2)$$

To estimate the magnitude of E_{br}, let us calculate E_{br} from formula (2) for NaCl; the value of α, according to the data of T. A. Kontorova ([7]), is equal to $3.45 \cdot 10^4$; B may be taken equal to 10. Then $E_{\text{br, NaCl}} \simeq 1.92 \cdot 10^6$ V/cm. The calculated value is in sufficiently good agreement with the experimental value.

The quasi-elastic coupling coefficient is equal to ([7])

$$\alpha = \frac{mnU}{r_0^2}, \qquad (3)$$

where U is the crystal-lattice energy per ion pair; $m = 1$; n, according to various authors, varies for alkali-halide crystals within different limits. Substituting (3) into (2) and replacing all constants by their values, we obtain

Fig. 1

$$E_{\text{br}} \simeq 30.85\, \frac{n^{1/2}U^{1/2}u_0}{r_0\sqrt{2(M_1+M_2)}}. \qquad (4)$$

The plot of the dependence of E_{br} on

$$u_{\text{br}} = \frac{n^{1/2}U^{1/2}u_0}{r_0\sqrt{2(M_1+M_2)}}$$

should be a straight line. As is seen from Fig. 1, Hippel' s values of E_{br} lie approximately on a straight line. By formula (2) or (4) one can theoretically calculate the breakdown voltages for alkali-halide crystals.

Table 1 gives the calculated and experimental values of E_{br}. The values of u_0 are taken from work ([8]). As is seen, the calculated values of E_{br} for various alkali-halide crystals are in good agreement with the experimental data ([1]).

Table 1

Crystal	$E_{\mathrm{br}} \cdot 10^{-6}$ in V/cm, exp.	$E_{\mathrm{br}} \cdot 10^{-6}$ in V/cm, theor.
NaCl	1.5	1.92
NaBr	1	1.15
KCl	1	1.54
KBr	0.7	1.02
KJ	0.6	0.65
RbCl	0.7	1.00
RbBr	0.6	0.8
RbJ	0.5	0.55
NaJ	0.8	0.65

An important electrical characteristic of a crystal is also the value of the electric-field strength at which the electrical conductivity begins to deviate from Ohm' s law. Experimental investigations show that the field E_r at which deviation from Ohm' s law begins is different for different crystals ([9]). In this case, too, one can establish a dependence of E_r on the parameters of the crystal lattice.

As is known ([10]), the spherical part of the electron distribution function in the presence of an electric field has the form

$$n_0 = A \exp\left[-\frac{1}{kT}\int \frac{b d\varepsilon}{b + \frac{2}{3}\tau(eEv)^2}\right], \qquad (5)$$

where $b = \Delta\bar{\varepsilon}^2/2t$ ($\Delta\bar{\varepsilon}^2$ is the mean value of the square of the energy transferred in collisions; t is the time of energy transfer); ε is the mean electron energy; τ is the mean free time.

For a semiconductor or dielectric $\Delta\bar{\varepsilon}^2 = \frac{2}{3}\varepsilon m a^2$.

Substituting b into (5), we have

$$n_0 = A \exp\left[-\frac{1}{kT}\int \frac{\varepsilon\, d\varepsilon}{\varepsilon + \frac{2\tau^2}{ma^2}(eEv)^2}\right]. \qquad (6)$$

If, in the denominator of the expression under the integral, the second term may be neglected, then the dependence of the electrical conductivity on the field strength obeys Ohm' s law; conversely, if the first term may be neglected—

then for the electrical conductivity a deviation from Ohm' s law is obtained[^10]. Consequently, the magnitude of the critical field (i.e., the field at which the deviation from Ohm' s law begins) can be estimated from the relation

$$\varepsilon \simeq \frac{2\tau^2}{ma^2}(eE_r v)^2.$$

Substituting $\tau = l/v$, ε, a, and taking into account that $l = Br_0$, we obtain

$$E_r \simeq \frac{\sqrt{kTm}}{2Be}\sqrt{\frac{\alpha}{2(M_1+M_2)}} = \frac{\sqrt{kTm}}{2Be}\,\frac{n^{1/2}U^{1/2}}{r_0\sqrt{2(M_1+M_2)}}. \tag{7}$$

Thus, in agreement with the experimental data, the electrical strength of crystals and the magnitude of the critical field at which a deviation from Ohm' s law occurs depend on the energy of the crystal lattice, on the lattice constant, and on the masses of the particles composing the crystal. The functional dependence of these quantities is determined by formulas (4) and (7) of the present work.

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References

1. A. V. Hippel, *Zs. f. Phys.*, **88**, 358 (1934).
2. A. A. Vorob' ev, E. K. Zadovskaya, *DAN*, **81**, No. 3 (1951).
3. A. A. Vorob' ev, *ZhTF*, **26**, 2, 330 (1956).
4. A. A. Vorob' ev, K. A. Vodop' yanov, M. A. Krivov, *DAN*, **106**, No. 6 (1954).
5. L. Z. Gurevich, *Fundamentals of Physical Kinetics*, 1940, p. 178.
6. K. F. Herzfeld, *Theory of the Solid State*, 1936.
7. G. A. Kontorova, *ZhTF*, **26**, 9, 2021 (1956).
8. A. A. Vorob' ev, *DAN*, **108**, No. 1 (1956).
9. P. Tomka, *Magyar. fiz. folyóirat*, **2**, No. 3, 173 (1954).

10. L. Z. Gurevich, *Fundamentals of Physical Kinetics*, 1940, p. 231.

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