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CONNECTION BETWEEN SHOCK POLARIZATION OF IONIC CRYSTALS AND THE LATTICE CHARACTERISTICS

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In order to clarify the role of the ion mass in shock polarization of ionic crystals, we investigated the polarization of the single crystals Li^7H and Li^6D in shock waves. The results of the experiments show that the ion masses do not influence the polarization current. Results are presented of an investigation of the shock polarization of RbI and KI single crystals, and it is concluded on the basis of an analysis of expanded experimental material on 10 ionic compounds that the polarization on the shock wave front (P_0) is determined by the dimension of the cation. The obtained data confirm the previously established[2] correlation between P_0 and the low-frequency dielectric constant of ionic crystals under normal conditions.

WE have previously obtained[1,2] experimental data showing that the polarization of alkali-halide crystals in shock waves (SW) is connected with the main lattice of these compounds. It has been noted, in particular, that a correlation exists (up to a value $\sigma \sim 1.3$, where σ is the compression behind the SW front) between the polarization on the SW front (P_0) and the relative dimensions of the ions, the low-frequency dielectric constant (ϵ_1), and the activation energy of the displacement of the cation vacancy (E_+).

Inasmuch as alkali-halide crystals are typical representatives of the class of ionic compounds, it is natural to assume that the observed connection is typical also of other compounds of this class. However, the question of the role of such a fundamental lattice characteristic as the ion mass in the phenomenon under consideration remains open.

It is simplest to ascertain whether the ion masses influence the value of P_0 in experiments analogous to those of[1], on compounds that differ only in the isotopic composition of the elements contained in them. We present the results of such experiments on Li^7H and Li^6D crystals. In addition, we present the results of an investigation of the shock polarizations of RbI and KI crystals, and analyze, on the basis of expanded experimental material (using also data on CsI[3] and MgO[4]), the regularities observed in[2].

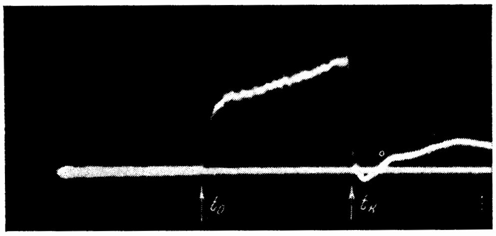

FIG. 1. I(t) oscillogram of experiment with Li^6D crystal.

Values of j_0 and j_k in shock loading of Li^7H and Li^6D crystals.

Crystal	Number of experiment	j_0, mA/cm²	$\bar{j}_0$, mA/cm²	j_K, mA/cm²	$\bar{j}_K$ mA/cm²
Li^7H	1	740	640 ± 100	1290	1010 ± 180
	2	540		730	
Li^6D	3	420	490 ± 40	750	930 ± 120
	4	530		1000	
	5	520		1040	

EXPERIMENT

The arrangement of the explosion experiment was analogous to that described earlier[1]. A plane shock wave propagated in the [100] direction. We registered in the experiments the polarization current as a function of the time I(t)[1]. Samples of Li^7H, Li^6D, RbI, and KI were plates of thickness l_0, cut parallel to the (100) plane.

1. Li^7H and Li^6D. The shock wave amplitude was 100 kbar, $l_0 = 0.3$ cm. The crystals used had low transparency, a fact connected either with the state of the surfaces (in view of the hygroscopic nature of Li^7H and Li^6D), or with the presence of a noticeable number of color centers. The parameter $(r_- - r_+)/r_-$ (where r_- and r_+ are the radii of the anion and the cation), characterizing the relative dimensions of the ions, has the same value for the lithium hydride and deuteride, whereas the masses of the anions in these compounds differ by a factor of two, and the masses of the cations by 17%. The reduced masses M ($M = m_-m_+/(m_- + m_+)$, where m_- and m_+ are the masses of the anion and the cation) of lithium hydride and deuteride are respectively 0.875 and 1.50 at. un. In all the experiments, the plots of I(t) had the same form. A typical oscillogram is shown in Fig. 1. The results of the experiments are listed in the table, where j_0 is the density of the current I at the instant t_0 when the shock wave enters the sample[1], and j_k is the current density at the instant t_k when the shock wave leaves the sample.

2. RbI and KI. The polarization of ionic RbI crystals

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[1] In all cases, j_0 was determined from the oscillograms by the procedure of [1].

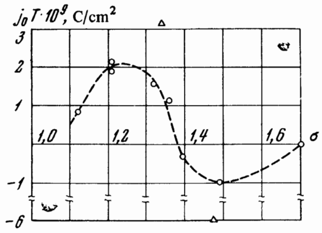

FIG. 2. Plot of j_0T against the compression σ behind the shock wave front in loading of RbI (○) and KI (△).

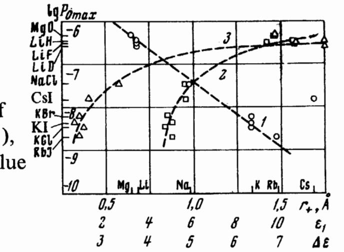

FIG. 3. Curves illustrating the connection between P_{0max} and the characteristics of the main lattice of the investigated crystals: r_+ (curve 1), ϵ_1 (curve 2) and $\Delta\epsilon$(curve 3). The value of P_{0max} is expressed in C/cm².

was investigated in the pressure range 6–160 kbar, and that of KI at 42 and 79 kbar. The dynamic adiabats of RbI and KI were taken from a compendium[5] kindly supplied to the authors by A. N. Dremin. The value of l_0 varied from 0.18 to 0.21 cm. The experimental data are shown in Fig. 2 in coordinates j_0T and σ, where $T = l_0/D$ is the time of travel of the shock wave through the sample (D—shock wave velocity).

DISCUSSION

1. According to Allison[6]

$$P_0 = \alpha \frac{\varepsilon_2}{\varepsilon_1} j_0, \tag{1}$$

where $\alpha = \sigma T$ and ϵ_2 is the dielectric constant of the substance behind the shock wave front. In all the experiments with the Li hydride and deuteride, we had ω = const. If we assume that $(\epsilon_2/\epsilon_1)_{\mathrm{Li^7H}} = (\epsilon_2/\epsilon_1)_{\mathrm{Li^6D}}$, which is very likely in view of the similarity of the physical properties of the investigated compounds, then it follows from the table that the values of P_0 in Li^7H and Li^6D are equal, accurate to the experimental scatter.

The relatively large scatter of the value of j_0 in the case of Li^7H is not unexpected, for in the heretofore investigated ionic crystals (for example NiCl[1]), this scatter reached ± 50%.

It follows from the foregoing that the possible change of P_0 as a result of the change of the masses of the ions on going from Li^6D to Li^7H is by not more than a factor of two, whereas the interval of variation of P_0 in the investigated ionic crystals amounts to three orders of magnitude (see Fig. 3). We can therefore conclude that P_0, at least, depends little on the ion masses. Inasmuch as in the final analysis the polarization is determined only by two fundamental lattice constants—the masses and the dimensions of the ions—the performed experiments actually confirm the hypothesis[2] that up to $\sigma \sim 1.3$ a decisive role in shock polarization of ionic crystals is played by the dimensions of the ions.

2. The experimental material obtained in the present investigation on four ionic compounds allows us to verify and refine the regularities observed earlier[2] for a smaller group of crystals.

An analysis of the experimental data on the 10 ionic crystals investigated to date (Li^6D, Li^7H, LiF, MgO, NaCl, CsI, KBr, KCl, KI, and RbI) shows that, other conditions being equal (constant σ and constant orientation of the crystals relative to the direction of propagation of the shock wave), P_0 is connected in the following manner with the lattice characteristics under normal conditions: a) for compounds with the lattice of the NaCl type, for a given cation, the value of P_0 remains constant when the anion is replaced, accurate to within the experimental scatter; b) in the same compound, P_0 decreases with increasing cation radius; c) regardless of the type of lattice, P_0 increases with increasing ϵ_1 and $\Delta\epsilon = \epsilon_1 - \epsilon_\infty$, where ϵ_∞ is the high-frequency dielectric constant.

It should be noted that the new experimental data do not confirm the correlation between P_0 and $(r_- - r_+)/r_-$, which was reported in[2].

On the basis of the same data we can conclude that P_0 is a function of the structure of the crystal, and that for compounds with a lattice of one type the value of P_0 is determined only by the dimension of the cation2).

The foregoing conclusions are illustrated by the plots of Fig. 3, which show the logarithms of the maximum positive values of $P_0 = P_{0max}$ ($\sigma \sim 1.3$), calculated from formula (1) (under the assumption that $\epsilon_2 = \epsilon_1$), as functions of r_+ (curve 1), ϵ_1 (curve 2), and $\Delta\epsilon$ (curve 3) for all the investigated compounds. It is interesting that the lower part of curve 1 corresponds to crystals (KCl, KBr, KI, and RbI) which experience a polymorphic transformation in the region of σ up to 1.3. On the other hand, in the CsI crystal, which has already under normal conditions the type CsCl lattice (into which the lattice of the aforementioned crystals becomes transformed under pressure), the value of p_{0max} is approximately 50 times larger than that expected on curve 1 for CsI. This circumstance indicates that the polarization of the aforementioned four crystals occurs in the initial lattice, of the NaCl type, and not in the modified one.

In conclusion we note that there are no published data on the value of E_+ for the majority of compounds indicated in Fig. 3, so that at the present time it is impossible to establish whether a correlation exists between P_0 and E_+ for the expanded group of compounds.

Although in light of the experimental data on the 10 ionic crystals the notions developed in[2] concerning the mechanism of the shock polarization (polarization of the main lattice with relaxation times much greater than the relaxation times of the ionic polarization) remain apparently in force, nonetheless, the dynamics of the processes leading to polarization, and their connection with the dimensions of the cations and the polarizability of the lattice (Δϵ), are still unclear.

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[1] A. G. Ivanov, E. Z. Novitskiĭ, V. N. Mineev, Yu. V.

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2) Strictly speaking, this and other conclusions of the present paper can be extended only to compounds of chemical purity (with individual impurities having a concentration on the order of 10^{-4} – 10^{-5} wt. %), since all the experiments performed to date on shock polarization of ionic crystals were performed exclusively on chemically pure compounds.

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