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71.15.Mb**SOUND VIBRATIONS IN IONIC CRYSTAL TAKING
ELECTRIC FIELD CORRELATIONS INTO ACCOUNT**

Small vibrations in a solid insulator in the presence of a self-consistent electric field with the first strength moment at the equilibrium equal to zero and the second one different from zero have been considered. A new variable, the second moment of electric field strength, was introduced into the Euler equation, and a temporal equation for this variable was derived on the basis of Maxwell equations in the hydrodynamic approximation. A wave equation was obtained, and its solutions – two transverse and one longitudinal sound vibration branches – are found. The transverse sound velocity is calculated; the results obtained correspond to those calculated using the shear modulus to an accuracy of about 10%.

Keywords: sound vibrations, electric field correlation, Euler equation.

Consider low-frequency long-wave sound vibrations in an ionic crystal. Suppose that ions interact with one another only by means of a self-consistent electrostatic field [1]. This approach generalizes the consideration of sound vibrations in metals [2], where a self-consistent electromagnetic field was used only to describe the interaction between oppositely charged subsystems. For simplicity, let the system be uniform and isotropic. Its positive and negative components will be described with the use of the common local mass density ρ , pressure P , and mass velocity \mathbf{v} . Besides the indicated purely hydrodynamic quantities, we need to describe a microscopic electric field in the crystal, which is responsible for both the attraction of ions at large distances and their repulsion at small ones. This field is a random variable, with the first moment of the electric field strength \mathbf{E} equal to zero (we do not consider piezoelectrics), but the second moment is different from zero after its averaging over a physically small volume. The standard Euler equation includes the Maxwell stress tensor [3], which is quadratic in the electric field strength and, in our approximation, is completely determined by the tensor $\langle E_l E_m \rangle$. For the latter, we will derive a temporal equation in the hydrodynamic approximation. It is known [4] that, in the case of a perfect crystal free of defects like vacancies or excess interstitial atoms (we consider only this case), the velocity of medium points coincides with the time derivative of their displacement, $\mathbf{v} = \partial \mathbf{u} / \partial t$, where u_α is the shear

field (the deformation vector [4]) that characterizes the motion of a point in this medium. Therefore, we can describe the dynamics of the crystal in terms of the mass velocity.

Let us write down the standard equations of classic hydrodynamics for an insulator, neglecting all dissipation effects, such as viscosity and heat conductivity [3]. These are the continuity equation

$$\partial_t \rho + \operatorname{div} \rho \mathbf{v} = 0 \quad (1)$$

and the Euler equation

$$\partial_t (\rho v_i) + \partial_k \pi_{ik} = 0, \quad (2)$$

in which we introduced the notation $\partial / \partial x_k = \partial_k$ for the derivative and

$$\pi_{ik} = \rho v_i v_k + P \delta_{ik} - (\langle E_i E_k \rangle - \langle E^2 \rangle \delta_{ik} / 2) \varepsilon / (4\pi) \quad (3)$$

for the tensor of momentum flow. The dielectric permittivity ε is taken to be constant. One can see that Eq. (3) contains the Maxwell stress tensor, which is completely determined by the second moment $\langle E_i E_k \rangle$. The temporal equation for the indicated moment can be obtained from the Maxwell equation for the electric field as a random variable,

$$\partial_\varepsilon \mathbf{E} / \partial t = c \operatorname{rot} \mathbf{B} - 4\pi \sigma \mathbf{v}, \quad (4)$$

where σ is the electric charge density. For this purpose, we multiply Eq. (4) by E_k taken at the same

Transverse sound velocities for some alkali halides

Crystal	ρ , g/cm ³	$G \times 10^{10}$, dyne/cm ²	$u_s^G \times 10^5$, cm/s	$W \times 10^{-11}$, erg	$u_s^\perp \times 10^5$, cm/s	u_s^\perp / u_s^G
LiF	2.601	51.2	4.44	1.68	5.10	1.15
NaF	2.805	31.4	3.35	1.49	3.77	1.13
NaCl	2.165	15.2	2.65	1.27	2.95	1.11
NaBr	3.200	11.8	1.92	1.21	2.17	1.13
KCl	1.990	12.7	2.53	1.15	2.49	0.99
KBr	2.750	10.2	1.93	1.10	1.93	1.00
KI	3.130	7.0	1.50	1.04	1.59	1.06
RbCl	2.799	8.9	1.78	1.11	1.92	1.08
RbBr	3.351	7.5	1.50	1.06	1.60	1.07
RbI	3.554	6.1	1.31	1.01	1.38	1.05

space-time point and symmetrize the product with respect to tensor indices. The equation for the second moment of the magnetic induction was obtained analogously in work [5] in the magnetohydrodynamic approximation. We should take into account that the equilibrium field \mathbf{E} exists in a fixed coordinate system. Therefore, according to the Galilean transformation [3], $\mathbf{B}' = \mathbf{B} + [\mathbf{v}, \mathbf{E}]\varepsilon/c$,

$$\begin{aligned} \partial \varepsilon E_i E_k / \partial t &= c \operatorname{rot}_i (\mathbf{B} + [\mathbf{v}, \mathbf{E}]\varepsilon/c) E_k + \\ &+ c \operatorname{rot}_k (\mathbf{B} + [\mathbf{v}, \mathbf{E}]\varepsilon/c) E_i - 4\pi\sigma (v_i E_k + v_k E_i). \end{aligned} \quad (5)$$

The thermal fluctuations of the field are also neglected. After averaging over a small volume, the last term turns out nonlinear, and it can be omitted. For a substance that is not magnetoactive, the internal magnetic field is small in comparison with the electric one; therefore, the correlations between the electric and magnetic fields can be neglected. In view of the isotropic character of the problem, we obtain

$$\langle E_l E_m \rangle_0 = \langle E^2 \rangle_0 \delta_{lm} / 3 = \text{const.} \quad (6)$$

Therefore, from Eq. (5) and with the use of Eq. (6), we obtain the linearized equation

$$\partial \langle E_i E_k \rangle / \partial t = (\partial_k v_i + \partial_i v_k - 2\partial_l v_l \delta_{ik}) \langle E^2 \rangle_0 / 3. \quad (7)$$

The tensor of momentum flow (2) includes the entropy deviation. However, sound is an adiabatic process. Therefore, after the linearization, we obtain

$$\partial_i v_i + \partial_k \{ \delta_{ik} v_s^2 \rho - (\langle E_i E_k \rangle - \langle E_l E_l \rangle \delta_{ik} / 2) \varepsilon / 4\pi \} / \rho_0 = 0. \quad (8)$$

Here, $v_s^2 = (\partial P / \partial \rho)_s$, and ρ_0 is the equilibrium value of mass density. Using Eqs. (1) and (7), we can differentiate Eq. (8) with respect to the time,

$$\partial_t^2 v_i - v_s^2 \partial_i \partial_k v_k - \partial_k (\partial_i v_k + \partial_k v_i) \langle E^2 \rangle_0 \varepsilon / (12\pi\rho_0) = 0. \quad (9)$$

Hence, we obtained the wave equation (9) for sound vibrations in an isotropic solid. It is convenient to change to the Fourier components according to the rule

$$\mathbf{v}(\mathbf{x}, t) = \int d^3k d\omega \mathbf{v}(\mathbf{k}, \omega) e^{i\mathbf{k}\mathbf{x} - i\omega t} / (2\pi)^4. \quad (10)$$

Substituting Eq. (10) into Eq. (9), we find the dispersion equations for two transverse, $\omega^2 = \langle E^2 \rangle_0 \varepsilon / (12\pi\rho_0) k^2$, and one longitudinal, $\omega^2 = (v_s^2 + \langle E^2 \rangle_0 \varepsilon / (6\pi\rho_0)) k^2$, branches of sound vibrations. Therefore, we can determine the velocities for the transverse,

$$u_s^\perp = \sqrt{\langle E^2 \rangle_0 \varepsilon / (12\pi\rho_0)}, \quad (11)$$

and longitudinal,

$$u_s^\parallel = \sqrt{v_s^2 + \langle E^2 \rangle_0 \varepsilon / (6\pi\rho_0)}, \quad (12)$$

sound waves. One can see from Eq. (12) that, in the case $\langle E^2 \rangle_0 = 0$, we obtain the sound velocity in a liquid [6]. As is known from elasticity theory, the transverse sound velocity in a solid can be expressed in terms of the shear modulus G [4],

$$u_s^G = \sqrt{G / \rho_0}. \quad (13)$$

Now, it is easy to see from expression (11) that the introduced equilibrium field correlation can also be expressed in terms of the shear modulus,

$$G = \langle E^2 \rangle_0 \varepsilon / (12\pi). \quad (14)$$

This provides elastic properties in the system. It is known [7] that the cohesion energy W in ionic crystals is almost completely electrostatic by nature. This means that its density can be used to estimate the introduced correlation of the electric field,

$$W n_0 \approx \langle E^2 \rangle_0 \varepsilon / (8\pi). \quad (15)$$

Here, n_0 is the concentration of ionic pairs, because the cohesion energy in an ionic crystal is measured just per ionic pair. Assumption (15) allows us to estimate the transverse sound velocity (Eq. (11)),

$$u_s^\perp = \sqrt{2W/(3M)}, \quad (16)$$

where $M = M_+ + M_-$ is the mass of an ionic pair. A comparison of the numerical values for the transverse sound velocity in a number of alkali halides calculated according to formulas (13) and (16) demonstrates a good agreement for them (see Table). The values of density ρ and shear modulus G were taken from work [8], and those of cohesion energy from work [7, Table 20.5]. All the data were measured at the temperature $T = 298$ K.

To summarize, proceeding from the hydrodynamic model for the description of small vibrations in an ionic crystal and making allowance for a self-consistent electric field with the first moment equal to zero and the second one different from zero, two transverse and one longitudinal branches of sound vibrations are calculated. The values obtained for the

transverse sound vibrations correspond to those obtained in the framework of elasticity theory to an accuracy of about 10%.

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ЗВУКОВІ КОЛИВАННЯ В ІОННОМУ КРИСТАЛІ ПРИ ВРАХУВАННІ КОРЕЛЯЦІЙ ЕЛЕКТРИЧНОГО ПОЛЯ

Резюме

Розглянуто малі коливання в твердому діелектрику в самоузгодженому електричному полі, яке має в рівновазі перший нулю перший момент і відмінний від нуля другий момент напруженості. У рівнянні Ейлера запроваджено нову змінну – другий момент напруженості електричного поля, для якого отримано часове рівняння на основі рівнянь Максвелла в гідродинамічному наближенні. Отримано хвильове рівняння та знайдено дві поперечні та поздовжню звукові гілки коливань. Обчислено значення швидкості поперечного звуку, які відповідають з точністю порядку 10 відсотків знайденим за модулем зсуву значенням.