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Coulomb interaction effect on the shock wave process in ionic crystals at nanosecond impact pulse

© B.A. Zimin¹, Yu.V. Sudenkov^{2,†}, S.A. Chertishcheva²

¹ Baltic State Technical University "VOENMEKH" named after Marshal D.F. Ustinov, St. Petersburg, Russia

² St. Petersburg State University, St. Petersburg, Russia

[†] E-mail: y.sudenkov@yandex.ru

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Acoustic vibrations of ionic crystal exposed to a short impact pulse are addressed. The study evaluates the contribution of the Coulomb bond energy of ionic crystals to the dependence of moduli of elasticity on stress field induced by RMS electromagnetic field in the absence of the field at the initial time point. Dynamic vibration equations are written using the Maxwell stress tensor defined by the second electromagnetic stress field moment. It is shown that non-equilibrium Poisson's ratio in ionic crystals describes qualitatively the experimental results.

Keywords: impact loading, electrostatic interaction, Maxwell tensor, relaxation processes, Poisson's ratio.

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1. Introduction

The great majority of the existing models of impact disturbance propagation in solid bodies are currently based on the analysis of the steady-state shock wave process [1,2]. At the same time the most interesting and informative field of impact studies includes a non-steady shock wave process near the loading surface. However, there is extremely small body of information about strongly non-equilibrium and non-steady processes near the impact loading surface that define the evolution of initial disturbance profiles to those typical of the steady-state process. This is due to a number of restrictions inherent in traditional experimental methods of investigating the shock wave process and to a limited nature of existing theoretical capabilities of describing non-steady strongly non-equilibrium processes [3–5].

Therefore, it is important to develop picosecond and nanosecond impact loading techniques and to study the evolution of shock wave process variables in materials exposed to such short impact disturbances. The features of evolution of impact disturbance conditions during steady-state wave propagation and formation were noted in theoretical and experimental studies [6–9].

Findings of the experimental study of solid body response to nanosecond pressure pulses are discussed in [8,9]. Focus was made on the stress relaxation processes near the impact surface. In particular, a liquid-like immediate response of alkali-halide crystal to short impact pulses was noted.

Impact loads were excited by a laser pulse through an optical glass to a thin (3–5 μm) layer of a radiation-absorbing material being in acoustic contact with the test samples.

Impact load variables were controlled in a series of longitudinal stress measurements by a piezoceramic transducer placed on the rear side of samples with different thicknesses. For a series of lateral stress measurements, a polyvinylidenefluoride film (25 μm) piezoelectric transducer was placed in the center of impact disturbance area at different distances from the loading plane of a sample consisting of two bonded together parallelepipeds of the test material.

Experimentally obtained normalized dependences of longitudinal and lateral stress pulse component amplitude variations on the sample thicknesses $\sigma_l(h)$, $\sigma_t(h)$ in ionic NaCl crystals are shown in Figure 1 [8].

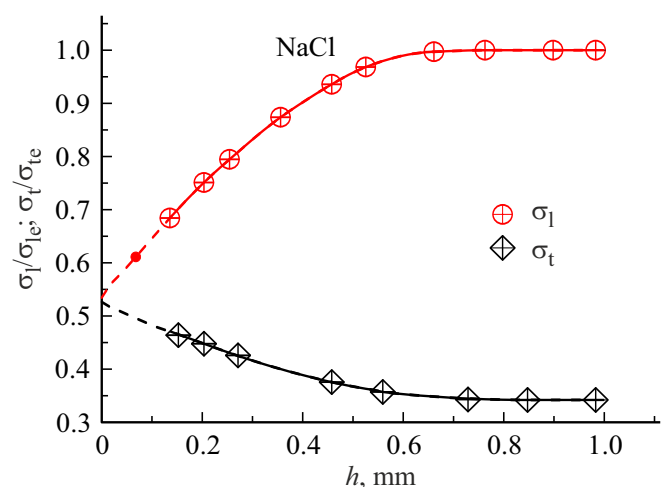


Figure 1. Normalized dependence of the amplitude of longitudinal stresses $\sigma_l(h)$ and lateral stresses $\sigma_t(h)$ on the sample thickness h .

2. Theoretical analysis of the findings of experimental study of ionic crystal response to nanosecond pressure pulses

The Coulomb energy plays the key role in the ion interaction in ionic crystals. The total electric charge of each lattice cell is equal to zero. During long-wavelength acoustic vibrations, ions contained in the lattice cell are displaced uniformly and the electrical neutrality of the lattice cell is not disturbed, only elastic forces are involved in the vibrations. Acoustic vibrations in ionic crystals are virtually identical to those in conventional dielectric materials. However, optical modes related to the relative motion of electrically charged ions differ from each other due to a peculiar nature of interatomic forces in ionic crystals. It is generally assumed that these crystals consist of slightly distorted localized ions interacting through the electrostatic field.

Let's consider the acoustic vibrations in ionic crystals assuming that such system is homogeneous, isotropic and is described by density, pressure P and particle mass velocity $\bar{V}$. In deriving the equations of ionic crystal motion, electric field components will be treated as independent dynamic variables. The Maxwell stress tensor is added to the equations of state of such materials.

As a result of ionic displacement from an equilibrium position, a dipole moment is generated in the crystal. The dipole moment induces a Coulomb field consisting of a macroscopic field and Lorenz field [10]. Variation of the thermodynamic properties of dielectric materials is defined by an electric field that penetrates a body and, unlike metals, affects considerably the thermodynamic potentials [10]. Since the deformability and polarizability of ions are defined by the electronic subsystem and cannot be included into the lattice vibration theory based on the expansion of the lattice potential in ionic displacements, then additional analysis of vibrational processes is implied to consider the electromagnetic field effect in such materials during rapid dynamic disturbances.

The Euler equations are the initial system of equations for investigating continuum motion [11]:

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho \bar{V}) = 0, \quad (1)$$

$$\frac{\partial(\rho V_i)}{\partial t} + \partial_k \sigma_{ik} = 0, \quad (2)$$

where

$$\partial_k = \frac{\partial}{\partial X_k}.$$

Dielectric properties of a body vary not only with density variation, but also in strain, because strain disturbs the body isotropy and dielectric anisotropy appears. Analysis of such situation is simplified, if only the change of volume is considered [10].

Continuum electrodynamics generally considers macroscopic variables by averaging the corresponding microscopic

variables. Field E_i is a random variable, whose average is equal to zero $\langle E_i \rangle = 0$, therefore the Euler equations of motion shall include the Maxwell stress tensor that is quadratic with respect to E_i and is defined by the tensor $\langle E_i E_k \rangle$ [10].

Then the analysis of dielectrics in an electric field allows us to write an equation for the stress tensor as [10]:

$$\sigma_{ik} = P \delta_{ik} - (\langle E_i E_k \rangle - \langle E_0^2 \rangle \delta_{ik} / 2) \frac{\varepsilon}{4\pi}. \quad (3)$$

where P is the pressure, $\langle E_i E_k \rangle - \langle E_0^2 \rangle \delta_{ik} / 2$ is the Maxwell stress tensor, ε is the permittivity, $E_0^2 = E_1^2 + E_2^2 + E_3^2$.

We write the Maxwell equation for E_i [10]:

$$\frac{\partial E_i}{\partial t} = c \text{rot}_i \bar{B}' - 4\pi \sigma V_i, \quad (4)$$

where σ is the density of electric charges, c is the speed of light, $\bar{B}'$ is the magnetic field induction vector, μ is the permeability. Taking into account that $\varepsilon = 1/(\mu c^2)$, we obtain for $(1 - \mu\varepsilon)/c \approx 1/c$.

Relation of the induction B and magnetic field strength H , $B = \mu H$ is valid in fixed bodies. For a moving medium at low velocities $V \ll c \bar{B}'$, it is written as [10]

$$\bar{B}' = \bar{B} + [\bar{V}, \bar{E}] \frac{1 - \mu\varepsilon}{c}. \quad (5)$$

To find $E_i E_k$, we multiply (4) by E_k and symmetrize the product by indices i, k (1, 2, 3):

$$\begin{aligned} \frac{\partial}{\partial t}(E_i E_k) &= c \text{rot}_i \left(\bar{B} + [\bar{V}, \bar{E}] \frac{1}{c} \right) E_k \\ &+ c \text{rot}_k \left(\bar{B} + [\bar{V}, \bar{E}] \frac{1}{c} \right) E_i - 4\pi \sigma (V_i E_k + V_k E_i). \end{aligned} \quad (6)$$

The ionic crystals, in which a magnetic field is almost non-existent — $\bar{B} \ll [\bar{V}, \bar{E}](1)/c$. Nonlinear terms $(V_i E_k + V_k E_i)$ in (6) may be neglected because the velocity gradients $\nabla \times [\bar{V}, \bar{E}]$ in sort impact are much higher than $(\bar{V}, \bar{E}) \sim E^2 \approx 0$.

For an isotropic medium, the rms value of $\langle E_i E_k \rangle$ is equal to [12]

$$\langle E_i E_k \rangle = \langle E_0^2 \rangle \frac{\delta_{ik}}{3}. \quad (7)$$

Considering all assumptions and expression (7), we obtain a system of differential equations for linearized

equations (6):

$$\left\{ \begin{array}{l} \frac{\partial}{\partial t}(E_1^2) = -2(\partial_2 V_2 + \partial_3 V_3) \frac{\langle E_0^2 \rangle}{3}, \\ \frac{\partial}{\partial t}(E_2^2) = -2(\partial_1 V_1 + \partial_3 V_3) \frac{\langle E_0^2 \rangle}{3}, \\ \frac{\partial}{\partial t}(E_3^2) = -2(\partial_1 V_1 + \partial_2 V_2) \frac{\langle E_0^2 \rangle}{3}, \\ \frac{\partial}{\partial t}(E_1 E_2) = -2(\partial_1 V_2 + \partial_2 V_1) \frac{\langle E_0^2 \rangle}{3}, \\ \frac{\partial}{\partial t}(E_1 E_3) = -2(\partial_1 V_3 + \partial_3 V_1) \frac{\langle E_0^2 \rangle}{3}, \\ \frac{\partial}{\partial t}(E_2 E_3) = -2(\partial_2 V_3 + \partial_3 V_2) \frac{\langle E_0^2 \rangle}{3}, \\ \frac{\partial}{\partial t}(E_i E_k) = \frac{\partial}{\partial t}(E_k E_i). \end{array} \right. \quad (8)$$

Equation (2) taking into account (3) is written as

$$\partial_t V_i + \partial_k \left[\delta_{ik} \rho C^2 - (\langle E_i E_k \rangle - \langle E_0^2 \rangle \delta_{ik} / 2) \frac{\varepsilon}{4\pi} \right] \frac{1}{\rho_0} = 0, \quad (9)$$

where

$$C^2 = \frac{\partial P}{\partial \rho} \Big|_{\rho_0},$$

C is the speed of sound, ρ_0 is the equilibrium density. After time differentiation of equation (9) taking into account equation (8), we obtain the system of equations

$$\left\{ \begin{array}{l} \partial_t^2 V_1 - C^2 \partial_1 (\partial_1 V_1 + \partial_2 V_2 + \partial_3 V_3) - [\Delta^2 V_1 + \partial_1 (\partial_1 V_1 + \partial_2 V_2 + \partial_3 V_3)] \frac{\langle E_0^2 \rangle}{2\pi\rho_0} = 0, \\ \partial_t^2 V_2 - C^2 \partial_2 (\partial_1 V_1 + \partial_2 V_2 + \partial_3 V_3) - [\Delta^2 V_2 + \partial_2 (\partial_1 V_1 + \partial_2 V_2 + \partial_3 V_3)] \frac{\langle E_0^2 \rangle}{2\pi\rho_0} = 0, \\ \partial_t^2 V_3 - C^2 \partial_3 (\partial_1 V_1 + \partial_2 V_2 + \partial_3 V_3) - [\Delta^2 V_3 + \partial_3 (\partial_1 V_1 + \partial_2 V_2 + \partial_3 V_3)] \frac{\langle E_0^2 \rangle}{2\pi\rho_0} = 0. \end{array} \right. \quad (10)$$

We seek a solution to (10) as

$$\bar{V}(\bar{x}, t) = \tilde{V}(k, \omega) e^{i\bar{k}\bar{x} - i\omega t}, \quad (11)$$

Substituting (11) in (10), we derive dispersion relations

$$\omega^2 = \frac{\langle E_0^2 \rangle \varepsilon}{12\pi\rho_0} k^2, \quad (12)$$

$$\omega^2 = \left(C^2 + \frac{\langle E_0^2 \rangle \varepsilon}{6\pi\rho_0} \right) k^2. \quad (13)$$

Relations (12) and (13) are dispersion relations for transverse and longitudinal modes demonstrating substantial

difference in frequencies and corresponding propagation velocities. Velocities of transverse C_t and longitudinal C_l waves are equal.

$$C_t = \sqrt{\frac{\langle E_0^2 \rangle \varepsilon}{12\pi\rho}}, \quad C_l = \sqrt{C^2 + \frac{\langle E_0^2 \rangle \varepsilon}{6\pi\rho}}. \quad (14)$$

These differences probably define the behavior of longitudinal and transverse stress components (Figure 1) demonstrating the relaxation response of NaCl crystals to a short impact disturbance with duration in the order of $\tau \approx 10^{-9} - 10^{-8}$ s and loading rates of $\partial\sigma/\partial t \approx 10^{11} - 10^{10}$ MPa/s. Wave process relaxation behavior in various materials and ionic crystals exposed to short impact pulses was studied in [8,9].

3. Relaxation behavior of Poisson's modulus in ionic crystals in nanosecond pulse loading

In deriving the equations of ionic crystal motion, the electric field components were assumed as independent dynamic variables, and the Maxwell stress tensor is added to the equation of state of such materials. As a result of ionic displacement from an equilibrium position, a dipole moment is generated in the crystal. The dipole moment induces a Coulomb field consisting of a macroscopic field and Lorenz field [10].

During long-wavelength acoustic vibrations, ions contained in the lattice cell are displaced uniformly and the electrical neutrality of the lattice cell is not disturbed. But the optical modes related to the relative motion of electrically charged ions might introduce differences in the electrical neutrality of the lattice cell. Delayed relative motion of positive and negative ion sublattices with much different sizes and molecular weights of ions may cause considerable failure of electrical neutrality of the cells.

Energy of ionic crystals in this case may be written as [10]:

$$G = G_{el} + \langle E^2 \rangle \frac{\varepsilon}{4\pi}, \quad (15)$$

where G_{el} is the elastic component of energy, $\langle E^2 \rangle \frac{\varepsilon}{4\pi}$ is the electric field energy.

The equation of energy balance will be written as

$$\frac{\partial}{\partial t} \left(G_{el} + \langle E^2 \rangle \frac{\varepsilon}{4\pi} \right) + \frac{\partial}{\partial x} \left(G_{el} + \langle E^2 \rangle \frac{\varepsilon}{4\pi}, V_{gr} \right) = 0, \quad (16)$$

where V_{gr} is the group velocity.

Non-equilibrium response behavior of ionic dielectrics will be analyzed using the simplest kinetic equation with a relaxation term [13], relaxation time τ and variable ξ defining the degree of relaxation process development [3]:

$$\frac{d\xi}{dt} = -\frac{\xi - \xi_0}{\tau}, \quad (17)$$

where ξ_0 corresponds to the equilibrium state of medium.

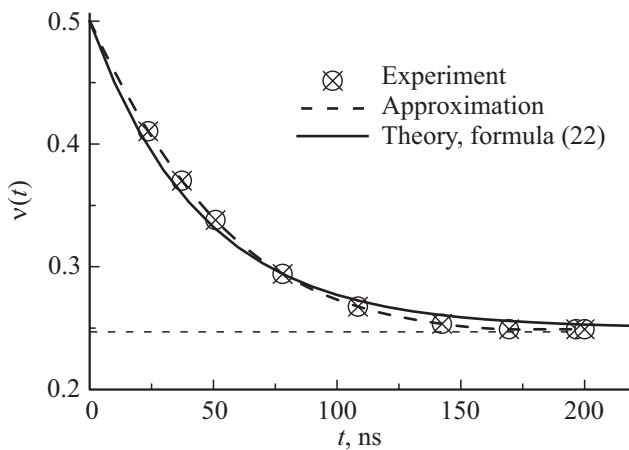


Figure 2. Dependence of Poisson's ratio of NaCl on time in impact loading with 10^{-9} – 10^{-8} s pulses (dashed line) and calculation according to (22) (solid line).

A variable describing the weak interaction of elastic and electric fields is chosen [11]:

$$\xi = \langle E^2 \rangle \frac{\varepsilon}{4\pi} - G_{\text{el}}. \quad (18)$$

Here, G_{el} , $\langle E^2 \rangle \frac{\varepsilon}{4\pi}$ are the elastic and Coulomb interaction energies induced by impact loading, $\xi_0 = \langle E_0^2 \rangle \frac{\varepsilon}{4\pi}$ is the Coulomb interaction in the equilibrium state of medium.

Taking into account equation of balance (16) and smallness of τ ($\partial x \cong \tau V_{\text{gr}}$), kinetic equation (17) is written as

$$\frac{\partial}{\partial t} \left(\langle E^2 \rangle \frac{\varepsilon}{4\pi} \right) + \frac{\langle E^2 \rangle \frac{\varepsilon}{4\pi}}{\tau} = \frac{1}{2} \frac{\langle E_0^2 \rangle \frac{\varepsilon}{4\pi}}{\tau}. \quad (19)$$

Then a solution to equation (19), taking into account that at the initial time $\langle E^2 \rangle \frac{\varepsilon}{4\pi} = 0$, is given by

$$\langle E^2 \rangle \frac{\varepsilon}{4\pi} = \left[\frac{1}{2} \langle E_0^2 \rangle \frac{\varepsilon}{4\pi} - \frac{1}{2} \langle E_0^2 \rangle \frac{\varepsilon}{4\pi} \exp\left(-\frac{t}{\tau}\right) \right]. \quad (20)$$

Using the known relation for Poisson's ratio [14]

$$\nu = \frac{1}{2} \frac{C_l^2 - 2C_t^2}{C_l^2 - C_t^2} \quad (21)$$

and substituting the current value of $\langle E^2 \rangle$ from (20) to (14), we obtain for Poisson's ratio

$$\nu = \frac{1}{2} \frac{12\pi\rho C^2}{12\pi\rho C^2 + \frac{1}{2} \langle E_0^2 \rangle \frac{\varepsilon}{4\pi} [1 - \exp(-\frac{t}{\tau})]}. \quad (22)$$

Analyzing the relation for Poisson's ratio (22), it turns out that the Coulomb interaction energy variation at the initial time ($t = 0$) $\langle E^2 \rangle \frac{\varepsilon}{4\pi} = 0$ and Poisson's ratio is equal to $\nu = 0.5$.

At the equilibrium process stage at $t \gg \tau$, the Coulomb interaction energy is equal to the equilibrium energy

$$\langle E^2 \rangle \frac{\varepsilon}{4\pi} = \frac{1}{2} \langle E_0^2 \rangle \frac{\varepsilon}{4\pi},$$

and therefore $\nu < 0.5$. When the Coulomb and elastic energies in the equilibrium state are equal, Poisson's ratio will correspond to the tabulated value $\nu \approx 0.25$.

Figure 2 shows the dependences of Poisson's ratio plotted according to the data of [8] and calculated using relation (22).

Note that for the rigorous substantiation of the non-equilibrium behavior of Poisson's ratio, the full theory of kinetic equations for interacting systems shall be used [11]. Nevertheless, the assumptions made in our model allow us to derive a time dependence of Poisson's ratio that correlates quantitatively with the time dependence of Poisson's ratio plotted using the experimental data of [8] in impact loading of NaCl samples with 10^{-9} – 10^{-8} s pulse (see Figure 2).

4. Conclusion

Non-equilibrium moduli, variation of which is caused by the electromagnetic field effect on vibrational processes in rapid mechanical disturbances, shall be used for correct description of mechanical phenomena in ionic crystals.

In case of quite weak interaction between these fields, energy exchange between them is hampered, therefore a tendency to the equilibrium state takes place step-by-step. Equilibrium within each of the subsystems is set initially and only then the whole system tends to the equilibrium state. I.e. ionic crystals might be treated as a medium where wave propagation disturbs the equilibrium between the internal thermodynamic system variables.

Thus, expression of Poisson's ratio ν through the longitudinal and transverse speeds of sound makes it possible to describe the relaxation behavior at short impact loading times $\tau \approx 10^{-9}$ – 10^{-8} s.

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Conflict of interest

The authors declare no conflict of interest.

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