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MECHANISM OF SPACE CHARGE GENERATION IN SHOCK COMPRESSION OF IONIC CRYSTALS

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During shock loading of solids (dielectrics, semiconductors, metals) electromagnetic phenomena such as electromagnetic radiation and emission, development of a current between the plates of a shortcircuited capacitor upon their compression, etc. occur [1-3]. In a phenomenological description of such processes the shock front is considered as a discontinuity on which polarization, dielectric permittivity, and conductivity of the material are given, and the mechanism of charge liberation in the shock front is not concretized [1]. The present study will employ a different approach, based on study of the kinetics of point defects and dislocations in a shock front and will calculate the dependence of the change in potential (or polarization) over front width on the amplitude of shock compression, explaining a number of experimentally observed dependences. The materials which have been most studied at present are ionic crystals having an NaCl-type structure, in which the charge carriers are positive ion vacancies under normal circumstances. Electrification of crystals upon quasistatic loading (the Stepanov effect) is related to displacement of charged dislocations. In shock compression experiments the velocity and charge of the dislocations have different values, so that the role of dislocations in charge formation within the shock front is not known [1]. Attempts at explaining the effect in terms of diffusion of Na^+ vacancies through the shock front do not produce quantitative agreement with experiment [1]. The present study will examine both diffusion and over-barrier mechanisms of point defect and dislocation displacement with consideration of their multiplication in the shock front.

In the shock front multiplication of Frenkel defects occurs ($\sim 10^{17}$ cm^{-3} per percent plastic deformation), so that interstitial ions also take on an important role. Lattice compression in the shock front leads to distortion of the equilibrium atomic configuration in the vicinity of a defect, as a result of which the latter may be displaced. Given a thermofluctuation mechanism, the probability that a detect of the k-th type will move from one equilibrium position to another is given by the expression

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$$\nu_k^{\pm} = \nu_{0k} \exp\left(-u_k^{\pm}/kT\right), \tag{1}$$

where ν_k^+ is the transition frequency; the indices + and − denote displacement along and opposite the direction of wave propagation [4]; T is the absolute temperature; ν_{0k} = 10^{12}-10^{14} sec^{-1}; u_k^+ is the activation energy characterizing the corresponding potential barrier, dependent on the coordinates x, t of the given defect. If a point defect is captured by a moving dislocation, its velocity will be equal to the velocity of the dislocation c_d, and the transition frequency $\nu = c_d/a$. In this case charge transport in the shock front is accomplished by dislocations, and the sign of the dislocation charge is determined by the difference in binding energies of defects of various types to dislocations [5]. Initially we will consider charge transport by point defects. We denote the quantity of particles per unit volume in the sections (x − a/2) and (x + a/2) (where a is the lattice constant) by n_1 and n_2. Then the particle flux density through the section x has the form $j_k = (\nu_{k1}^+ n_{k1} - \nu_{k2}^- n_{k2})a$. Expanding this expression in the parameter a and considering the transport of defects together with matter under the action of the electric field, we obtain

$$j_k = an_k\left[\nu_k^+ - \nu_k^- - \frac{a}{2}\frac{\partial}{\partial x}(\nu_k^+ + \nu_k^-)\right] - \frac{a^2}{2}(\nu_k^+ + \nu_k^-)\frac{\partial n_k}{\partial x} + n_k v + \frac{\sigma_k E}{q_k}. \tag{2}$$

Here v is the mass velocity of matter in the shock front; q_k is the charge of a given type of particle; $\sigma_k = a^2 q_k^2 n_k(\nu_k^+ + \nu_k^-)/2kT$ is the ionic conductivity; $\nu_k^{\pm}$ are functions solely of temperature and stress, affecting the height of the potential barrier, in as much as the dependence on E, the external electric field intensity and the field created by the charged defects is considered in Eq. (2) in the linear approximation by the last term.

We write the continuity equation and Maxwell's equation as

$$\frac{\partial n_k}{\partial t} + \frac{\partial j_k}{\partial x} = f_k - \mu_{km} n_k n_m, \quad f_k = M_k\left|\frac{d\gamma}{dt}\right|, \tag{3}$$

$$\varepsilon_0 \frac{\partial \varepsilon E}{\partial x} = \sum_k q_k (n_k - n_{k0}),$$

where f_k is a function of the source of defects formed in the shock wave; M_k is the multiplication coefficient; the coefficient $d\gamma/dt$ is proportional to the probability of recombination of vacancies and interstitial ions, with it following from the law of charge conservation that $M_k = M_m$ and $\mu_{km} = \mu_{mk}$; ε is the dielectric permittivity; n_{k0} is the initial defect density. The coefficient μ_{km} is proportional to the particle scattering section $\sim 4a^2$ and the particle velocity $\sim \nu a$, i.e., $\nu_{km} \sim \nu a^3$. Evaluations for $a = 3\cdot 10^{-10}$ m and $n = 10^{18}$ cm^{-3} indicate that the recombination term is small in comparison to the first term in Eq. (3) at frequencies up to 10^{14} sec^{-1}, so it will not be considered further. The ratio of the last term of Eq. (2) to the first terms $\sim qE\lambda/kT$ where λ is the characteristic scale of the shock front. At a field intensity of $E \sim 10^8$ V/m (the dielectric breakdown intensity) this ratio is ~0.4, i.e., the last term can also be neglected.

With these assumptions the particle behavior is determined by independent equations. Substituting Eq. (2) in Eq. (3), for the particle density we obtain a Fokker–Planck type equation with source (subscript k is omitted)

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x}\left[\left\{v + a\left(\nu^+ - \nu^- - \frac{a}{2}\frac{\partial}{\partial x}[\nu^+ + \nu^-]\right)\right\}n - \frac{a^2}{2}(\nu^+ + \nu^-)\frac{\partial n}{\partial x}\right] = M\left|\frac{d\gamma}{dt}\right|. \tag{4}$$

Under the action of the external stresses the directions along and opposite the x axis become nonequivalent. This causes ν^+ and ν^- calculated at the same point to differ. However analysis shows that consideration of this effect does not qualitatively change the result. Therefore for the future we will assume that $\nu^+(x) = \nu^-(x) = \nu(x)$. The term in brackets is caused by motion of defects in the shock wave force field. At ν = const we obtain a diffusion equation from Eq. (4). If in the first approximation in a we consider the difference between ν^+ and ν^- in the form $\nu^- - \nu^+ \sim a\partial\nu/\partial x$, then the general character

of the solutions presented below does not change, the basic expressions coinciding to the accuracy of a numerical factor.

In the case of charge transport by dislocations n represents the number of dislocations per unit area. Correspondingly, Eq. (2) gives the dislocation flux per unit length. The charge of the dislocations is independent of the load applied [5], while the rate at which they multiply is proportional to $d\gamma/dt$, just as for point defects. In the final outcome, we again arrive at Eq. (4) with different parameters: $\nu = c_d/a$, $M = M_d \sim 10^{16}$ m^{-2} [6] is the dislocation multiplication coefficient [6].

We will analyze a steady-state shock front in which all parameters depend on a single parameter $\xi = (x - Dt)\lambda$, where D = const is the shock wave velocity. Transforming the variables, we integrate Eq. (4) over ξ. Neglecting v in the final expression in comparison to D, we have

$$h - m = \alpha d\mu m/d\xi, \; m = n/n_0, \; \mu = \nu/\nu_1, \qquad (5)$$
$$\alpha = a^2\nu_1/(D\lambda), \; h = 1 + M\gamma(\xi)/n_0.$$

Here the condition $\mu = m = 1$ as $\xi \to +\infty$ is used, and it is also considered that all derivatives vanish at infinity.

Integration of Eq. (5) gives

$$m(\xi) = \frac{1}{\alpha\mu(\xi)} \int_{-\infty}^{\xi} h(\xi') \exp\left[\frac{1}{\alpha}\int_{\xi}^{\xi'} \frac{d\xi''}{\mu(\xi'')}\right] d\xi'. \qquad (6)$$

For weak shock waves it is more convenient to use the asymptotic expansion of the solution in the small parameter α. For example, at $\nu_1 = 10^5$ sec^{-1}, $a = 3\cdot10^{-10}$ m, D = 2.5 km/sec, $\lambda = 10^{-4}$ m we find that $\alpha = 3\cdot10^{-14}$. Equation (5) is a singularly perturbed equation as described in [7]. Nevertheless there is no boundary series in the asymptotic expansion of its solution, since the zeroth approximation satisfies the initial conditions. Thus, integrating the exact solution of Eq. (6) by parts k times, we write the expressions

$$m = h - \alpha\frac{d}{d\xi}\mu h + \alpha^2\frac{d}{d\xi}\mu\frac{d}{d\xi}\mu h - \ldots + \frac{(-1)^k\alpha^k}{\mu}\left(\mu\frac{d}{d\xi}\right)^k \mu h + \frac{(-1)^k\alpha}{\mu} I,$$
$$I = \int_{-\infty}^{\xi} \exp\left[\frac{1}{\alpha}\int_{\xi}^{\xi'}\frac{d\xi''}{\mu(\xi'')}\right]\frac{1}{\mu(\xi')}\left(\mu(\xi')\frac{d}{d\xi'}\right)^{k+1}\mu(\xi')h(\xi')\,d\xi',$$

whence in the first approximation

$$m = h - \alpha\frac{d}{d\xi}\mu h. \qquad (7)$$

In weak shock waves ($p \ll K$, where p is the pressure and K is the modulus of volume compression), when effects of lattice oscillation anharmonics are insignificant, in Eq. (1) we can take $u = u_0 - \beta\gamma$, where $\gamma = p/K$. Then, using Eq. (7), we obtain the charge density distribution ρ over the width of the shock front for a thermofluctuation mechanism of point defect or dislocation displacement. Neglecting defect multiplication at this stage and considering that they are generated in pairs (electrical neutrality condition) we find

$$\rho = -\frac{qa\beta n_0}{D\lambda kT} v(\gamma)\frac{d\gamma}{d\xi}, \; E_x = -\frac{qan_0}{\varepsilon\varepsilon_0 D}[v(\gamma) - v(0)], \qquad (8)$$
$$v(\gamma) = a\nu_0 \exp[-(u_0 - \beta\gamma)/(kT)]$$

(where $v(\gamma)$ is the defect velocity). For dislocations q indicates the linear charge density of the dislocation. In the case of point defects Eq. (8) must be summed over all types of defects.

For above-barrier displacement of charges in Eq. (7) we take μ = const. Considering multiplication of defects and dislocations, in place of Eq. (8) we have

$$\rho = -\frac{qav_0M}{D\lambda}\frac{d\gamma}{d\xi}, \; E_x = -\frac{qav_0M}{\varepsilon\varepsilon_0 D}[\gamma(\xi) - \gamma_0] + E_{0x} \qquad (9)$$

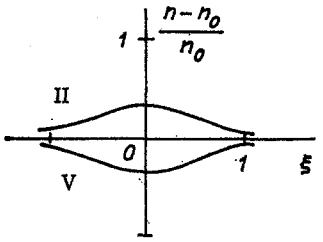

Fig. 1

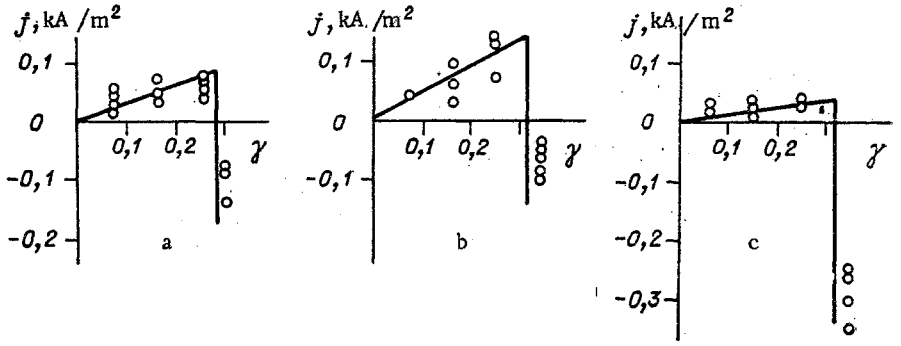

Fig. 2

where $v_0 = a\nu_0$ is the limiting defect velocity (for dislocations v_0 is of the order of the transverse wave velocity). The constant E_0 can be determined from Eq. (8) at $\gamma = \gamma_0 = u_0/\beta$, γ_0 being the critical deformation at which the potential barrier vanishes. For dislocations, generally speaking, the linear charge density q is different for the dynamic stage, Eq. (8) and for the thermofluctuation displacement mechanism, Eq. (9).

If we approximate the shock front by an expression of the form $\gamma = (\gamma_*/2)(1 - \text{th}\ \xi)$ (where γ_* is the shock compression amplitude), then it follows from Eqs. (8), (9) that $\rho \sim \text{ch}^{-2}\xi$. Consequently, the charge is essentially concentrated within the shock front width, and its distribution is that of a soliton (asymmetric in the case of Eq. (8)).

We will evaluate the parameters describing point defects. Since the radius of Cl^- ions is greater than that of Na^+ ions, we will limit our study to the latter, using the index i for interstitial ions and v for Na^+ vacancies. We will consider an infinite lattice containing an isolated interstitial ion. Let the lattice be compressed in the direction [1, 0, 0]. Using the ion interaction energy in the form [8]

$$u_{ij} = \chi \exp(-r_{ij}/b) \pm q^2/r_{ij}.$$

Here r_{ij} is the distance between i-th and j-th ions; χ and b are empirical parameters (for NaCl $b = 0.321 \cdot 10^{-10}$ m, $\chi = 1.09 \cdot 10^3$ eV). If we do not consider lattice distortions near the defect then for u_i we can take the difference between the potential energies of an interstitial ion positioned at the center of a cell and shifted in the direction of compression by half the width of the cell face. For such a displacement the Coulomb potential of the interstitial ion does not change, and consideration of repulsion of nearest neighbors (eight and four respectively) gives

$$u_i = 4\chi[\exp(-a/b\sqrt{2}) - 2\exp(-\sqrt{a^2 + s^2}/2b)], \tag{10}$$

where s and a are the lattice parameters along and across the compression direction. For a lattice with Na^+ vacancy the potential maximum is reached upon displacement of the nearest Na^+ ion half the distance separating it form the vacancy. With analogous assumptions we find

$$u_v = 2\chi[\exp(-\sqrt{a^2 + s^2}/2b) + 4\exp(-\sqrt{5a^2 + s^2}/2b) - \exp(-s/b) - 2\exp(-a/b)] + V, \tag{11}$$

$$V = \frac{q^2}{4\pi\varepsilon_0}\left[\sum_{i,j,k}^{+\infty\prime}(-1)^{i+j+k}\left\{\frac{1}{\sqrt{s^2(i-1/2)^2 + a^2[k^2 + (j-1/2)^2]}}\right.\right.$$

TABLE 1

Direction	$M_d \cdot 10^{-16}$, m^{-2}	$M_T \cdot 10^{-24}$, m^{-3}	$E_* \cdot 10^{-5}$, V/m
[1, 0, 0]	1,9	2,0	2,7
[1, 1, 0]	2,8	3,0	4,7
[1, 1, 1]	0,8	0,8	1,1

$$\left. - \frac{1}{\sqrt{s^2 i^2 + a^2 (j^2 + k^2)}} \right\} - \frac{1}{\sqrt{s^2 + a^2}} \Bigg]. \qquad (11)$$

(the point i = j = k = 0 is excluded from the summation).

The relationship between volume and pressure in the shock wave is defined by the adiabatic equation of state up to $p \sim K$ [9], whence we obtain the relationship between s and γ for uniaxial compression

$$s = a(\gamma\Gamma + 1)^{-1/\Gamma}, \qquad (12)$$

where Γ is the adiabatic index. Equations (10)-(12) define the functions $u_k(\gamma)$, while in the range $a\gamma/b \ll 1$ these relations becomes linear. A corresponding calculation for an interstitial Na^+ ion gives $u_{i0} = 4.5$ eV, $\beta_i = 11$ eV. The value of u_{i0} is apparently elevated, since it exceeds the Frenkel defect formation energy ($\sim$3.5 eV). To evaluate u_V it is simpler to consider uniform compression, so that the lattice sum in Eq. (11) becomes independent of s and can be eliminated, if in the linear expansion we use the experimental value $u_{V0} = 0.86$ eV. In this case $\beta_V = -5.7$ eV (an experimental value of $\beta_V = -1.5$ eV has been found [10]).

Charge density Eq. (8) proves to be positive for both a vacancy and an interstitial ion. This means that the shock front contains an excess quantity of interstitial ions and insufficient number of Na^+ vacancies (V) (Fig. 1). The potential barrier for vacancies increases, and their role decreases, with increase in pressure. For an interstitial Na^+ ion the threshold value $\gamma_0 \approx 0.4$. However, consideration of motion of the nearest neighbors of the interstitial ion away from each other and anharmonism of lattice oscillations may decrease γ_0.

For dislocations the threshold value of γ_0 is determined by stresses of the order of magnitude of the yield point Y (for NaCl $Y \sim 0.05$ GPa, i.e., $\gamma_0 \sim 2 \cdot 10^{-3}$), which is significantly less than γ_0 for an interstitial Na^+ ion. Therefore in a weak shock wave charge transport is apparently caused by defects related to dislocations.

For comparison with the experiment of [1] involving shock compression of a shortcircuited capacitor we will use an expression for the increase in potential in the shock wave which follows from Eq. (9). Neglecting γ_0, $E_0(\xi < 0)$, we have

$$\Delta\varphi = \frac{E_*\lambda}{2} [\xi - \ln(2 \operatorname{ch} \xi)], \quad E_* = \frac{qav_0 M\gamma_*}{\varepsilon\varepsilon_0 D}. \qquad (13)$$

Over the time required for establishment of the electrical signal in the measurement circuit $\tau \approx 10^{-9}$ sec a potential difference $\Delta\phi \approx E_* D\tau$ is formed, proportional to the amplitude of the current density j_* recorded at the output. Equation (13) is supported by the experimentally observed linear dependence $j_*(\gamma_*)$. This effect can be explained by the fact that with increase in the degree of compression of the material the number of dislocations and point defects increases proportionately.

Figure 2 shows calculated functions for NaCl which are compared to experimental results of [1] for various crystallographic axes (a, [1, 0, 0]; b, [1, 1, 0]; c, [1, 1, 1]). The following parameter values were used: $q = 1.7 \cdot 10^{-11}$ C/m [5], $\nu_0 = 5 \cdot 10^{12}$ sec^{-1}, D = 3 km/sec, $\varepsilon = 6$. The data were reconciled by selection of the parameter M. For a dislocation charge transport mechanism the multiplication coefficient M_d presented in Table 1 is in good agreement with the results of [6]. For motion of point defects the coefficient M_p also agrees with experimental values of M_p [10]. Nevertheless, preference must be given to dislocations, for which, as has already been indicated above, γ_0 is 1-2 orders of magnitude smaller.

Considering that the experimental values of M_d and M_p are in the ratio $M_d q_d/e \sim M_p$ (where s is the elementary charge), it can be proposed that all defects of a given type are transported by dislocations, which determines the charge of the latter. Measurement of threshold j_* and γ_0 values would aid in refinement of the theoretical parameter values.

The analysis performed above is invalid for pressures close to the value K ($\gamma \approx 0.3$-0.4), at which a change in electrical signal polarity is observed. This effect may be related to the interstitial ion achieving the threshold γ_0 value at which their displacement velocity is comparable to or even higher than the dislocation velocity. The change in the charge transport mechanism in the shock front (for $u_0 >> kT$ for point defects) will be quite abrupt. We note that electrical breakdown of the crystal cannot be excluded as an explanation for such an abrupt change in sign.

Table 1 presents maximum E_* values for the cusp points of Fig. 2. They are two orders of magnitude smaller than the critical field $E_c \approx 1.3 \cdot 10^8$ V/m for NaCl. However it should be considered that increase in defect concentration in the shock wave and significant lattice deformation ($\gamma_0 \approx 0.3$) may lead to formation of additional local levels in the forbidden zone, i.e., to a reduction in E_c.

Thus, by studying the kinetics of defects and locations in the shock front, a number of experimental principles can be explained. The role of multiplication of charged defects and dislocations has been clarified, permitting description of the experimentally observed linear increase in current density over a certain pressure range as a function of degree of pressure, as well as calculation of the initial voltage step in the measurement circuit. Estimates of threshold deformations in NaCl have shown that at $\gamma \lesssim 0.4$ the charge distributed in the shock front is produced by motion of dislocations. With increase in pressure the potential barrier for interstitial ions decreases, and at $\gamma \gtrsim 0.4$ they also become current carriers. Calculation of electric fields in the shock front shows that at such deformations breakdown phenomena are possible. On the basis of the expressions obtained for the known shock-wave geometry it is possible to calculate the dipole moment and radiation of the shock-compressed region as a function of pressure amplitude.

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