Local optical oscillations near point and extended defects in ionic crystals

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It is shown that the vector-like field of the relative displacements of the ions in the unit cell during optical oscillations of an ionic crystal leads to a nonexponential (power-law) decrease of the amplitude of the local optical oscillations at large distances from point and linear defects. In the case of a planar defect the amplitude decreases exponentially over a macroscopic distance equal to the wavelength. The dispersion laws of oscillations localized near linear and planar defects are obtained.

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The theory of local oscillations in a crystal have been quite fully developed and expounded in detail in many reviews and monographs (see, e.g., Refs. 1–4). Principal attention was paid in the study of defects to the spectrum of the local oscillations; there was little interest in the coordinate dependence of the local-oscillation amplitude. It turns out, however, that in ionic crystals, where the mechanical oscillations of the atoms are inevitably connected with electric fields, the question of the coordinate dependence is not trivial and is worthy of a detailed examination.

We consider in this paper optical local oscillations near various types of defects in an ionic crystal and discuss the nonexponential dependence of the local-oscillation amplitude near point and linear defects.

It is customarily assumed that the amplitude of a local oscillation of a crystal with a point or linear defect (the discrete local-oscillation frequencies lies outside the continuous frequency spectrum of an ideal crystal) decreases exponentially with the distance from the defect.[1-4] A similar decrease takes place in the wave function of an electron localized near a short-range attraction center in a crystal. The electron wave function, however, is a scalar quantity, so that the character of the decrease of the function itself is the same as that of its gradient. The crystal oscillations are described by a vector function, therefore the character of the decrease of the displacement itself and of its divergence or curl can be different. When it comes to optical oscillations of an ionic crystal, they are inevitably connected with quasistatic electric oscillations that manifest themselves differently when the oscillations are longitudinal and transverse. As a result the decrease of the local-oscillation amplitude may turn out to follow a power law. This was already pointed out in an investigation[5] of impurity absorption of infrared in ionic crystals.

We discuss here both the physical and the formal causes of the nonexponential amplitude decrease of local optical oscillations in an ionic crystal such as NaCl.

1. POINT DEFECT

The coordinate dependence of the relative atom displacements ξ that describe the local optical oscillations near a symmetric point defect is given by the expression[1,2]

$$\xi_i(\mathbf{r}) = a^3 U G_{ij}^{\omega}(\mathbf{r}) \xi_j(0), \tag{1}$$

where G_{ij}^{ω} is the Green's tensor of the stationary oscillations of an ideal crystal, U is the intensity of the perturbation introduced by the defect (in the case of an isotropic defect $U = \omega^2(\Delta\mu/\mu)$, where $\Delta\mu = \mu - \mu_g$ is the defect of the reduced mass of the atom pair in the unit cell of the crystal), and a^3 is the atomic volume.

It is known (see, e.g., Ref. 2) that in a crystal of the NaCl type the internal electric field splits the long-wave edge ($\mathbf{k} = 0$) of the optical branch into a longitudinal oscillations (with limiting frequency ω_l) and two degenerate transverse oscillations (with limiting frequency ω_0). The frequencies ω_l and ω_0 are connected by the relation $\omega_l^2 = \omega_2^0 + 4\pi e^2/\mu a^3$. The difference between the frequencies ω_l and ω_0 is the main effect of the action of the quasistatic electric field on the dynamics of the mechanical oscillations of the ionic crystal. It is this which is the main cause of the power-law decrease of the Green's function at large $|\mathbf{r}|$.

In a number of crystals, for example NaCl, KI, KBr, and KCl the frequency ω_l is the maximum frequency of the long-wave longitudinal optical mode. In a coordinate system connected with the principal crystallographic axes of the crystal the dispersion of the longitudinal oscillations at small values of the wave vector $\mathbf{k}$ can be expressed in the form[6,7]

$$\omega^2(\mathbf{k}) = \omega_l^2[1 - m(ak)^2 - na^2(k_x^4 + k_y^4 + k_z^4)/k^2]. \tag{2}$$

The values of m and n for different crystals are given in Ref. 6, where it is indicated that $|n| > |m|$ for a number of crystals.

Consider a defect whose local oscillations have a frequency ω close to the edge of the longitudinal optical mode: $\omega > \omega_l$ and $\omega - \omega_l \ll \omega_l - \omega_0$ (this can take place, for example, at $\Delta\mu = 0$). The Green's tensor of the considered crystal is then determined in the long-wave approximation mainly by its "longitudinal" part

$$G_{ij}^{\omega}(\mathbf{r}) = \frac{1}{(2\pi)^3} \int \frac{n_i n_j e^{i\mathbf{k}\mathbf{r}} \, d^3k}{\omega_l^2 - \omega^2 - \beta^2(\mathbf{n}) k^2}, \tag{3}$$

where $\mathbf{n}$ is a unit vector in the $\mathbf{k}$ direction, and the function

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$\beta^2(\mathbf{n})$ reflects the angular dependence of the dispersion law (2)

$$\beta^2(\mathbf{n}) = \omega_l^2 \{ma^2 + na^2(n_1^4 + n_2^4 + n_3^4)\}. \tag{4}$$

This includes the projections (n_1, n_2, n_3) of the unit vector $\mathbf{n}$ on the crystallographic axes of the cubic crystal.

For a more lucid illustration of the calculation of the main contribution to the integral in (3), we consider first a spherical dispersion law, when $\beta^2(\mathbf{n}) = \beta^2 = $ const, and then take into account deviations from sphericity.

We direct the z axis along the vector $\mathbf{r}$ and consider the asymptotic behavior, as $r \to \infty$, of the element $i = j = z$ of the tensor (3)

$$G_{zz}^\omega(\mathbf{r}) = -\frac{1}{(2\pi)^2} \int_0^\infty \frac{dk\, k^2}{\Omega^2 + \beta^2 k^2} \int_0^\pi \cos^2\theta\, e^{ikr\cos\theta} \sin\theta\, d\theta$$

$$= \frac{1}{2\pi} \frac{1}{\Omega^2} \left[\left(\frac{\Omega^2}{2\beta^2} \frac{1}{r} + \frac{\Omega}{\beta} \frac{1}{r^2} + \frac{1}{r^3} \right) e^{-\Omega r/\beta} - \frac{1}{r^3} \right], \tag{5}$$

where $\Omega^2 = \omega^2 - \omega_l^2$. It can be seen that (5) contains components of two types. The first, traditionally discussed, contains as a factor the exponential $\exp(-\Omega r/\beta)$ and decreases over distances on the order of several lattice constants; it is "generated" by elastic forces. The main contribution to the pre-exponential factor of this component is made at large distances by the term inversely proportional to the first power of the distance. The second component, proportional to $1/r^3$, is unexpected from the viewpoint of defect-containing crystals with nonelectrostatic interaction, and reflects in fact the long-range interaction in ionic crystals. At distances $r > \beta/\Omega$ the components of the first type can be left out, and we are left only with the last term of (5), proportional to $1/r^3$. Analysis of the remaining elements of the Green's tensor of the optical oscillations leads to the conclusion that its asymptotic form describes a dipole field

$$G_{ij}^\omega(\mathbf{r}) = \frac{1}{4\pi} \frac{1}{\omega^2 - \omega_l^2} \frac{r^2 \delta_{ij} - 3x_i x_j}{r^5}. \tag{6}$$

The asymptotic form (6) thus causes the relative displacements (1) to have a coordinate dependence described by a power-law decrease. Expression (6) was in fact obtained in Ref. 5.

We call attention to the fact that the exponentially decreasing terms in (5) depend on the parameter β, i.e., are determined by the character of the dispersion of the crystal longitudinal oscillations. The last term, which has a power-law decrease and remains at distances $r \gg \beta/\Omega$ does not contain the parameter β, i.e., does not depend at all on the dispersion of the longitudinal oscillations. Therefore expression (6) can be obtained from (3) by putting $\beta = 0$ and by using, after integration with respect to $\cos\theta$, the formula

$$\int_0^\infty e^{ikr} k^{\nu-1}\, dk = \lim_{\delta \to +0} \int_0^\infty e^{ikr - \delta k} k^{\nu-1}\, dk = \frac{\Gamma(\nu)}{r^\nu} e^{i\nu\pi/2}.$$

Let us discuss the causes of the unusual (power-law) decrease of the amplitude of the local oscillation. The displacement of interest to us is in the long-wave approximation in fact the "longitudinal" solution of the following system of equations:

$$(\omega^2 - \omega_0^2)\boldsymbol{\xi} - \beta^2 \Delta\boldsymbol{\xi} + e\mu^{-1}\mathbf{E} = a^3 U \boldsymbol{\xi}(0)\delta(\mathbf{r}),$$
$$\mathrm{div}\, \mathbf{D} = 0, \quad \mathbf{D} = \mathbf{E} + (4\pi e/a^3)\boldsymbol{\xi}, \quad \mathrm{rot}\, \mathbf{E} = 0. \tag{7}$$

The formal cause of the power law decrease of the asymptotic form of the Green's tensor is the absence of a gap in the spectrum of the differential operator, whose eigenvalue problem is equivalent to the system (7). Indeed, assuming that curl $\boldsymbol{\xi} = 0$, we can put $\boldsymbol{\xi} = \nabla\psi$ and easily verify that the system (7) is equivalent to a single equation for the scalar function ψ, namely

$$\hat{L}\psi \equiv (\Omega^2 - \beta^2 \Delta)\Delta\psi = a^3 U \boldsymbol{\xi}(0)\, \mathrm{grad}\, \delta(\mathbf{r}). \tag{8}$$

At all the allowed values of ω^2 the spectrum of the operator $\hat{L}$ is gapless (it begins with zero), so that it is not at all surprising that the eigensolutions of (8) decrease nonexponentially with distance. Clearly, the decrease of the eigensolutions of (8) with distance is determined by the coordinate dependence of the Green's tensor of the operator $\hat{L}$. In the usual situation one studies the Green's function of the operator $\Omega^2 - \beta^2\Delta$, which decreases exponentially with distance like $r^{-1} \exp(-\Omega r/\beta)$. This coordinate dependence sets the coordinate dependence of the function $\Delta\psi = \mathrm{div}\, \boldsymbol{\xi}$. The coordinate dependence of $\boldsymbol{\xi}$ at large distances, however, follows then a power law, since the function $\Delta\psi$ determines in fact the distribution function of a field of electrostatic type:

$$\mathrm{div}\, \boldsymbol{\xi} = \Delta\psi, \quad \mathrm{rot}\, \boldsymbol{\xi} = 0.$$

Thus, in an ionic crystal the relative displacements at large distances from a defect should have a power-law decrease. The polarization field of the crystal, $\mathbf{P} = (e/a^3)\boldsymbol{\xi}$, behaves similarly: the density $\rho = \mathrm{div}\, \mathbf{P}$ of the bound charge decreases exponentially while the polarization vector has a power-law decrease. The same can be said concerning the electric field $\mathbf{E}$. It follows from the latter that the dynamic interaction between the considered defects in an ionic crystal has a power-law dependence on the distance between the defects, and this determines the specific concentration effects.[5]

We proceed now to investigate the influence of the nonsphericity of the dispersion (2) on the coordinate dependence of the Green's tensor. We transform (3) into

$$G_{ij}^\omega(\mathbf{r}) = -\frac{1}{(2\pi)^3} \frac{\partial^2}{\partial x_i\, \partial x_j} J(\mathbf{r}),$$
$$J(\mathbf{r}) = \int \frac{dk\, do\, e^{i\mathbf{k}\mathbf{r}}}{\Omega^2 + \beta^2(\mathbf{n})k^2}, \tag{9}$$

where do is a solid-angle element in the direction of the unit vector $\mathbf{n}$.

To calculate the integral $J(\mathbf{r})$ we write $\mathbf{k}\cdot\mathbf{r} = kr\cos\theta$ and introduce an angle φ in a plane perpendicular the vector $\mathbf{r}$. We can then write

$$J = \int_0^{2\pi} d\varphi \int_1^{-1} du \int_0^\infty \frac{dk\, e^{ikru}}{\Omega^2 + \beta^2(u,\varphi)k^2}, \tag{10}$$

where $u = \cos\theta$, and the function $\beta^2(u,\varphi)$ contains the angular dependence of the dispersion (2) in a new coordinate

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frame. We use the fact that the function $\tilde{\beta}^2(u,\varphi)$ is symmetric because the initial dispersion law is invariant to the replacement of $\mathbf{k}$ by $-\mathbf{k}$. After performing the last integration in (10) we then obtain

$$J=-\frac{\pi}{2\Omega}\int_0^{2\pi}d\varphi$$
$$\times\int_0^1 du\left[\frac{\exp[-\Omega ru/\beta(u,\varphi)]}{\beta(u,\varphi)}+\frac{\exp[-\Omega ru/\beta(-u,\varphi)]}{\beta(-u,\varphi)}\right].$$
$$(11)$$

To find the behavior of the Green's tensor at large distances, we find the asymptotic form of the integral J as $r\to\infty$. The internal integral in (11) can be calculated by the Laplace method. The main contribution to the asymptotic value is given by integration near $u=0$, so that we can write

$$\int_0^1 du\,\frac{\exp[-\Omega ru/\beta(u,\varphi)]}{\beta(u,\varphi)}\approx\int_0^\infty\frac{du}{\beta(0,\varphi)}$$
$$\times\exp[-\Omega ru/\beta(0,\varphi)]=\frac{1}{\Omega r}.$$
$$(12)$$

Substituting (12) in (11) we obtain the final result

$$J=-2\pi^2/\Omega^2 r. \qquad (13)$$

The asymptotic form of the Green's tensor is consequently

$$G_{ij}^{\circ}(\mathbf{r})=-\frac{1}{4\pi\Omega^2}\frac{\partial^2}{\partial x_i\,\partial x_j}\frac{1}{r}, \qquad (14)$$

and coincides with (6) in the case of spherical dispersion.

We arrive thus at the very important conclusion that the anisotropy of the dispersion law (2) does not influence the asymptotic form of the Green's tensor, a form characterized by a power-law decrease at large distances. Peculiarities of the dispersion law, however, can manifest themselves in the behavior of the Green's tensor at short distances from the defect, i.e., when the frequency of the local oscillation are determined.[1-4]

2. LINEAR DEFECT

In the case of a linear defect, when the perturbation is concentrated, say, on the z axis, the solution of Eq. (8) must be sought in the form

$$\psi=\varphi(x,y)\exp(ik_z z).$$

The operator $\hat{L}$ in (8) is then replaced by a two-dimensional one

$$\hat{L}_2\equiv(\Omega^2+\beta^2k^2-\Delta_2)(k_z^2-\Delta_2);\quad\Delta_2=\partial^2/\partial x^2+\partial^2/\partial y^2, \quad(15)$$

in which we assume $\beta^2=$ const. At a fixed value of k_z, the operator $\hat{L}_2$ has an eigenvalue spectrum with a gap (the spectrum begins with k_z). Consequently, at sufficiently large distances the amplitudes of the optical oscillations (if they appear) decrease exponentially (at $k_z\neq0$). For example, in the case $\rho\gg1/k_z$ we have

$$\xi_i(\rho,k_z)=-\frac{a^2|U|k_z^{3/2}}{(8\pi)^{1/2}(\omega^2-\omega_l^2)\rho^{1/2}}\frac{x_ix_j\xi_j^{\,0}}{\rho^2}$$
$$\times\exp[-k_z\rho+i(k_z z-\omega t)],$$
$$(16)$$
$$\xi_z=0,\quad\rho^2=x^2+y^2,\quad i=1,2.$$

At distances $\beta/\Omega\ll\rho\ll1/k_z$, however, a power law decrease of the amplitude sets in, and the displacement field is the field of the linear dipole in the two-dimensional problem. There exist thus intermediate distances $(\beta/\Omega\ll\rho\ll1/k_z)$ at which $\xi_i(\rho,z)$ takes the form

$$\xi_i(\rho,z)=\frac{a^2|U|}{2\pi(\omega^2-\omega_l^2)}\frac{\rho^2\delta_{ij}-2x_ix_j}{\rho^4}\,\xi_j(0)\,e^{i(k_zz-\omega t)}, \quad(17)$$
$$\xi_z=0.$$

It must be emphasized that Eqs. (17) are valid at $\rho\ll\beta/\Omega\sim a$, and therefore cannot yield a dispersion equation that determines the frequencies of the local oscillations. It is obtained from the asymptotic solution as $\rho\to0$, and takes the form $(k_0\sim a^{-1})$

$$\omega^2=\omega_l^2+(\beta k_0)^2\exp\left\{-\frac{8\pi\beta^2}{a^2|U|}\right\}-(\beta k_z)^2\left|\ln\frac{k_z^2}{k_0^2}\right|. \quad(18)$$

The local oscillations described by Eqs. (15)–(18) appear only at $U<0$ and their dependence on the perturbation U is that typical of linear defects.[1,2]

3. PLANAR DEFECT

We consider now the oscillations near a planar defect, such as a stacking fault. Let the plane of the defect coincide with the plane $z=0$. Such a defect is described in the initial equation by a one-dimensional δ function

$$\ddot{\xi}+\omega_0^2\xi+\beta^2\Delta\xi=\frac{e\mathbf{E}}{\mu}+a\delta(z)\sum U(n_x-n_x',n_v-n_v')$$
$$\times\xi(n_x',n_v',0). \quad(19)$$

Assuming as before that $\omega-\omega_l\ll\omega_l-\omega_0$, we can confine ourselves only to the "longitudinal" part of the Green's tensor and obtain

$$\xi_i(z,\varkappa)=\frac{aU(\varkappa)}{2\pi}\int\frac{dk_zk_ik_j\xi_j^{\,0}e^{ik_zz}}{k^2(\omega_l^2-\omega^2-\beta^2k^2)}. \quad(20)$$

Here $\varkappa$ is the projection of the wave vector $\mathbf{k}$ on the (x,y) plane, i.e., $k^2=\varkappa^2+k_z^2$, and

$$U(\varkappa)=\frac{1}{a^2}\int dx\,dy\,U(x,y)e^{-i\varkappa\mathbf{r}},$$
$$\xi_i^{\,0}\equiv\xi_i(0,\varkappa)=\frac{1}{a^2}\int dx\,dy\,\xi_i(x,y,0)e^{-i\varkappa\mathbf{r}}.$$

Putting $z=0$ in (20) we obtain the dispersion equation for the local oscillations. It breaks up into two independent dispersion-law modes $\omega^2=\omega_{1,2}^2(\varkappa)$ whose frequencies are given by the relations

$$1+\frac{aU(\varkappa)}{2(\omega_l^2-\omega_i^2)}\left(\frac{\alpha_l}{\beta}-\varkappa\right)=0, \quad(21)$$

$$1+\frac{aU(\varkappa)\varkappa^2}{2(\omega_2^2-\omega_l^2)}\left(\frac{1}{\varkappa}-\frac{\beta}{\alpha_2}\right)=0, \quad(22)$$

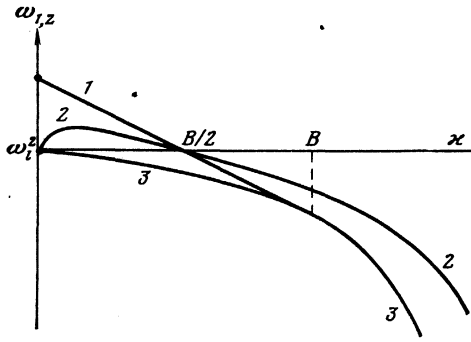A. M. Kosevich and V. A. Pogrebnyak   1092

FIG. 1. 1 and 2) plots of dispersion laws of local oscillations $\omega_{1,2}^2$, 3) plot of dispersion law $\omega^2 = \omega_l^2 - (\beta\varkappa)^2$.

where $\alpha_{1,2}^2 = \omega_{1,2}^2 - \omega_l^2 + \beta^2 \varkappa^2$ and $\alpha_{1,2}^2 > 0$.

Solving (21) and (22) for $\omega_{1,2}^2$ we easily obtain the explicit form of the dispersion laws for the first mode (Fig. 1)

$$\omega_1^2(\varkappa) - \omega_l^2 = (aU/2\beta)^2 - a|U|\varkappa, \quad \varkappa \leqslant B \equiv a|U|/2\beta^2 \quad (23)$$

and for the second mode

$$\omega_2^2(\varkappa) - \omega_l^2 = -\beta^2\varkappa^2$$
$$+ \tfrac{1}{2}\{a|U|\varkappa + (\beta\varkappa)^2 - [2a|U|\beta^2\varkappa^3 + (\beta\varkappa)^4]^{1/2}\}. \quad (24)$$

Both dispersion laws correspond to local oscillations $(\omega_{1,2}^2 > \omega_l^2)$ and their eigenfrequencies are separated from the continuous spectrum by some gap. For oscillations of the first type the gap remains finite and equal to $\omega_1^2(0) - \omega_l^2 = (aU(0)/2\beta)^2$, as $\varkappa \to 0$, while for the second the gap is proportional to $\varkappa$. The frequency spectrum of the first mode at the point $\varkappa = B$ (see Fig. 1) merges with the frequency spectrum of the bulk oscillations. At $\varkappa > B$ there are no oscillations of the first type. The oscillation frequencies of the second type are separated at $\varkappa \gg B$ from the edge of the bulk-oscillation frequencies by a gap

$$\omega_2^2(\varkappa) - \omega_l^2 + \beta^2\varkappa^2 = (aU(\varkappa)/2\beta)^2.$$

A characteristic feature of both spectra is the nonanalytic dependence of the frequency on the wave vector $\varkappa$. This nonanalyticity is due to separation, in the initial equations of motion, of the macroscopic electric field,[8] whose Fourier component is an nonanalytic function of $\mathbf{k}$ as $k \to 0$, namely $\mathbf{E}(\mathbf{k}) \sim \mathbf{k}(\mathbf{k}\cdot\xi^0)/k^2$ [see Eq. (20)]. A detailed discussion of this question can be found, e.g., in Refs. 7–10.

The linear dependence of $\omega_{1,2}$ on $\varkappa$ at small $\varkappa$, i.e, at $\varkappa \ll a|U|/2\beta^2$, is a manifestation of the dimensionality of the effect (in this case, its two-dimensionality) and does not depend on the dispersion law of the ideal crystal. We note that a similar (linear) dependence of the frequency on the wave vector appears in surface oscillations of optically active crystals.[11,12]

We see that the $\omega_1^2(\varkappa)$ and $\omega_2^2(\varkappa)$ curves intersect at the point $\varkappa = B/2$. The intersection of the dispersion curves is due to simplified model of the perturbation. It can be seen from (19) that the perturbation matrix is chosen in diagonal form, and by the same token the interaction between the different displacement components is excluded. The situa-

tion here is similar to that in a layered crystal.[13] When account is taken of the simplest off-diagonal elements of the perturbation matrix $(U_{xz} = U_{yz} = -U_{zx} = -U_{zy} \equiv U_1)$ we obtain in place of (21) and (22) the dispersion equation

$$\left[1 + \frac{aU}{2(\omega^2 - \omega_l^2)}\left(\frac{\alpha}{\beta} - \varkappa\right)\right]\left[1 + \frac{aU\varkappa^2}{2(\omega^2 - \omega_l^2)}\left(\frac{1}{\varkappa} - \frac{\beta}{\alpha}\right)\right]$$
$$= -U_1^2 \left[\frac{a(k_x + k_y)}{2(\omega^2 - \omega_l^2)}\left(1 - \frac{\beta\varkappa}{\alpha}\right)\right]^2 \frac{\alpha}{\beta\varkappa}.$$

As expected, the interaction $\propto U_1$ leads to "pushing apart" of the modes at the intersection point and has little effect on the dispersion law (21)–(22) far from this point.

We investigate now the coordinate dependence of the amplitude of the local oscillations. The first type of oscillations corresponds to the following displacement components:

$$\xi_x = \pm i\xi_z^0 A\varkappa(e^{-\varkappa|z|} - e^{-\alpha_1|z|/\beta})e^{i(\varkappa\mathbf{r} - \omega_1 t)},$$
$$\xi_z = -\xi_z^0 A\varkappa\left(e^{-\varkappa|z|} - \frac{\alpha_1}{\beta\varkappa}e^{-\alpha_1|z|/\beta}\right)e^{i(\varkappa\mathbf{r} - \omega_1 t)}, \quad (25)$$

where

$$\xi_x = \frac{\xi\varkappa}{\varkappa}, \quad A = \frac{a|U|}{2(\omega_1^2 - \omega_l^2)} = \frac{2\beta^2}{a|U|}.$$

In Eq. (25) for ξ_x the plus sign is for the half-space $z > 0$ and the minus sign for $z < 0$. At $z = 0$ only the z-component of the displacement is left, and $\xi_x(0) = \xi_y(0) = 0$.

It follows from (25) that a wave localized near the surface defect is a superposition of two oscillations. One is characterized by the standard decrease of the amplitude with increasing $|z|$, which is determined by the local-oscillation frequency, away from the edge of the continuous spectrum: $\xi_{(1)} \propto \exp(-\alpha|z|/\beta)$. The second oscillation is due to the onset of a macroscopic electric field; the amplitude of this oscillation decreases over a distance determined only by the wavelength. At distances $z \gg \beta/\alpha_1$ with $\varkappa \ll \alpha_1/\beta$, only the second wave remains:

$$\xi_x = \pm i\xi_z^0 A\varkappa \exp\{-\varkappa|z| + i(\varkappa\mathbf{r} - \omega_1 t)\},$$
$$\xi_z = -\xi_z^0 A\varkappa \exp\{-\varkappa|z| + i(\varkappa\mathbf{r} - \omega_1 t)\}. \quad (26)$$

At a fixed point of space, the wave (26) has circular polarization, and in the upper and lower half-spaces the polarization vectors rotate in opposite directions.

Notice should be taken of the formal similarity of the wave described by (26) to a Rayleigh surface wave.

Homogeneous oscillations $(\varkappa = 0)$ of the first type are concentrated near the defect

$$\xi_z = \xi_z^0 A(\alpha_1/\beta)e^{-\alpha_1|z|/\beta}, \quad \xi_x = 0. \quad (27)$$

It can be assumed that this is the eigenoscillation of the defect (the remainder of the lattice remains at rest). Since the condition $U < 0$ corresponds to an increased "rigidity" of the defect region in the crystal, the frequency of local oscillations of this type will exceed ω_l. This explains the presence of activation energy of the oscillations of the first type.

We proceed now to the second type of oscillations with dispersion law $\omega_2(\varkappa)$. This wave has the following displace-

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ment components:

$$\xi_\varkappa = \xi_\varkappa{}^0 \left(e^{-\varkappa|z|} - \frac{\varkappa\beta}{\alpha_2} e^{-\alpha_2|z|/\beta} \right) e^{i(\varkappa\mathbf{r} - \omega_2 t)},$$

$$\xi_z = \pm i\xi_\varkappa{}^0 \left(e^{-\varkappa|z|} - e^{-\alpha_2|z|/\beta} \right) e^{i(\varkappa\mathbf{r} - \omega_2 t)}, \tag{28}$$

where $\xi_\varkappa{}^0 = \xi^0 \varkappa/\varkappa$. An essential feature of this wave is that its amplitude, unlike practically all surface waves (acoustic and electrosonic), it does not contain the wave number $\varkappa$ as a factor. The reason is that the oscillations considered are of the optical type (they do not vanish as $\varkappa \to 0$).

At $z = 0$ the x and y components of the displacements differ from zero, and $\xi_z(0) = 0$. Far from the defect plane, at $z \gg \beta/\alpha_2$ and $\varkappa \ll \alpha_2/\beta$ the wave is described [in analogy with (25) and (26)] by the following equations:

$$\xi_\varkappa = \xi_\varkappa{}^0 \exp\{-\varkappa|z| + i(\varkappa\mathbf{r} - \omega_2 t)\},$$

$$\xi_z = \pm i\xi_\varkappa{}^0 \exp\{-\varkappa|z| + i(\varkappa\mathbf{r} - \omega_2 t)\}. \tag{29}$$

Just as before, the plus sign is taken for $z > 0$ and the minus sign for $z < 0$. The polarization vector in the wave (29) rotates in a direction opposite that of the wave of the first type. As $\varkappa \to 0$ the oscillations of the second type are transformed into bulk oscillations, so that the gap in their spectrum vanishes as $\varkappa \to 0$.

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