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MICROSCOPIC AND MACROSCOPIC SURFACE DYNAMICS OF HIGHLY ANISOTROPIC CRYSTALS

E.S. SYRKIN

Institute for Low Temperature Physics and Engineering,
Academy of Sciences of the Ukrainian SSR,
Kharkov 310164, USSR

Highly anisotropic crystals, owing to the unusual character of bonding forces, are of interest in terms of both fundamental research in solid state physics and their technological application. They are a good model of quasi- low-dimensional structures, where transitions are now actively studied. Besides, such a quasi-two-dimensional structure in laminar crystals (LC) (or quasi-one-dimensional in chain crystals) causes high anisotropy of spectra of various excitations (phonon, magnon, electron, etc.) of the system and essentially influences its dynamical, thermodynamical and kinetic characteristics. In an elastic medium, essential differences between the transverse velocities of found results in strong elastic anisotropy show up in particular near phase transitions associated with softening of acoustic phonons. High anisotropy is often the case in magnetically ordered materials and recently has been observed in superconductors with a high superconducting transition temperature. We are reporting a study of the influence of strong anisotropy of elastic properties and the interatomic interaction on vibrational states localized near the surface. The study was performed both in terms of elasticity theory and with consideration for the lattice discreteness.

Let us first consider propagation of Rayleigh surface waves (SW) in a laminar crystal of the hexagonal system where the interactions of atoms in the basal plane XY and along the sixth order axis (the Z axis) are substantially distinct. The equations of motion in classical elasticity theory are as follows:

$$\rho \ddot{u}_i = c_{iklm} \nabla_k \nabla_l u_m \tag{1}$$

where c_{iklm} is the elastic modulus tensor and ρ is the density of the medium. Introduce the notation: $c_{xxzz}/c_{xxxx}=\delta$, $c_{zzzz}/c_{xxxx}=\xi$, $c_{xzxz}/c_{xxxx}=j$. For a laminar crystal,

$$\delta \sim \xi \sim \gamma \ll 1 \tag{2}$$

Let the crystal fill the half-space $Z>0$ and the x axis be in the direction of the wave vector $\vec{k}$ of the surface wave. The solution of (1) with the boundary conditions

$$(\nabla_x u_z + \nabla_z u_x)|_{z=0} = 0\,, \quad (\delta \nabla_x u_x + \xi \nabla_z u_z)|_{z=0} = 0 \tag{3}$$

and with taking account of (2) leads to the following results:

$$\omega_s^2(k) = \omega_{\min}^2(k)(1-\gamma^2/\xi) \tag{4}$$

$$\vec{u}(x,z) = u_0\{\vec{u}_1 \exp(-kz\gamma^{3/2}/\xi) + i\sqrt{\gamma}\vec{u}_2 \exp(-kz\gamma^{-1/2})\}\, e^{ikx} \tag{5}$$

$$\vec{u}_1 = \begin{pmatrix} -i(\delta+\gamma)\gamma^{3/2}/\xi \\ 1 \end{pmatrix}, \quad \vec{u}_2 = \begin{pmatrix} 1 \\ i(\delta+\gamma)\sqrt{\gamma/\xi} \end{pmatrix}$$

Here $\omega_{\min}^2(k) = \gamma k^2 c_{xxxx}/\rho$ is the lower boundary of the continuous spectrum of the layered crystal, $\omega_s(k)$ is the SW frequency, and u_0 is a normalizing factor. Therefore, the above obtained SW contains two components, as does the customary Rayleigh wave, which damp exponentially in the bulk of the crystal. However, in an isotropic medium both the components are elliptically polarized and have comparable amplitudes, and penetrate into the medium to a depth of the order of the wavelength. For a laminar medium, one of the components (the first term in (5)) becomes main, its polarization is almost linear (normal to the surface), and the depth of penetration into the medium considerably exceeds the wavelength. The second component has a small amplitude and penetrates into the medium to a depth which is small as compared to the wavelength. The above results obtained without taking account of spatial dispersion, are valid only for exceedingly long waves. Thus, (4) is only applicable if $a^2k^2 \ll \gamma^2/\xi \ll 1$. In this connection, it is of interest to investigate the vibrational spectrum of a semi-infinite LC not only in the long-wave region, but also for a two-dimensional wave vector varying to the boundary of the planar Brillouin zone.

Let us consider a simple LC model, described by a minimum number of parameters, namely the model of a body-centered tetragonal crystal with central interactions between nearest neighbours in the same layer and in neighbouring layers. For atoms within the same layer, the force constant matrix in this model is

$$\Phi_{ik}(a,0,0) = -\alpha\delta_{i1}\,\delta_{k1} \tag{6}$$

while for atoms of neighbouring layers it is

$$\Phi_{ik}\left(\frac{a}{2},\frac{a}{2},\frac{\varepsilon a}{2}\right) = -\gamma\alpha \begin{pmatrix} 1 & 1 & \varepsilon \\ 1 & 1 & \varepsilon \\ \varepsilon & \varepsilon & \varepsilon^2 \end{pmatrix} \tag{7}$$

where a is the interatomic distance in the basal plane, the parameter ε characterizes the lattice "stretching" along the Z-axis, α is the force constant for atoms of the same layer, and $\gamma\alpha$ is the force constant for atoms of neighbouring layers (for an LC, $\gamma \ll 1$). Taking into account the two-dimensional periodicity in the XY plane, the equations of motion of intralayer atoms become as follows

$$\omega^2 u_x(n) = (2+8\gamma-2\cos k)\,u_x(n) - 4\gamma\cos\frac{k}{2}\,[u_x(n+1)+u_x(n-1)]$$
$$-4i\varepsilon\gamma\sin\left(\frac{k}{2}\right)[u_z(n+1)-u_z(n-1)]$$
$$\omega^2 u_y(n) = 8\gamma u_y(n) - 4\gamma\cos\frac{k}{2}\,[u_y(n+1)+u_y(n-1)] \tag{8}$$
$$\omega^2 u_z(n) = 8\gamma\varepsilon^2 u_z(n) - 4\gamma\varepsilon^2\cos\frac{k}{2}\,[u_z(n+1)+u_z(n-1)]$$
$$-4i\varepsilon\gamma\sin\frac{k}{2}\,[u_x(n+1)-u_x(n-1)]$$

($n \geqslant 1$ is the serial number of a layer). The equation of motion of surface layer atoms ($n=0$) are

$$\omega^2 u_x(0) = (2+4\gamma-2\cos k)\,u_x(0) - 4\gamma\cos\frac{k}{2}\,u_x(1) - 4i\varepsilon\gamma\sin\frac{k}{2}\,u_z(1)$$
$$\omega^2 u_y(0) = 4\gamma u_y(0) - 4\gamma\cos\frac{k}{2}\,u_y(1) \tag{9}$$
$$\omega^2 u_z(0) = 4\gamma\varepsilon^2 u_z(0) - 4\gamma\varepsilon^2\cos\frac{k}{2}\,u_z(1) - 4i\varepsilon\gamma\sin\frac{k}{2}\,u_x(1)$$

In the direction under consideration waves of two types can propagate independently: shear waves polarized along the Y-axis, and waves polarized in the XZ-plane. The shear SW are described by the relations

$$\omega_s^2 = 4\gamma\sin^2\frac{k}{2}, \quad u(n) = u(0)\left(\cos\frac{k}{2}\right)^n \tag{10}$$

For $k\to 0$, these waves are non-Rayleigh SW deeply penetrating into the medium. Cosider now waves polarized in the XZ-plane. The solution of Eqs. (8) and (9) is the sum of the two components, decaying with distance from the surface as $\tilde{u}_j q_j$ ($j=1,2$) where q_j ($|q_j|<1$) is the solution of the equation

$$\left(q+\frac{1}{q}\right)^2 - 2\cos\frac{k}{2}\left(q+\frac{1}{q}\right)\left[2+\frac{1}{2\gamma}\sin^2\frac{k}{2}-\frac{\omega^2}{8\gamma\varepsilon}\left(\varepsilon+\frac{1}{\varepsilon}\right)\right]$$
$$-4\sin^2\frac{k}{2}+4\left(\varepsilon-\frac{\omega^2}{8\gamma\varepsilon}\right)\left(\frac{1}{\varepsilon}+\frac{1}{2\gamma\varepsilon}\sin^2\frac{k}{2}-\frac{\omega^2}{8\gamma\varepsilon}\right)=0 \tag{11}$$

Equation (9) leads to the relation

$$\left(\frac{\omega^2}{8\gamma\varepsilon}\right)^2 + \frac{\omega^2}{16\gamma}\,\frac{(1-q_1q_2)^2}{q_1q_2} - \frac{\varepsilon^2(1+q_1^2q_2^2+q_1^2+q_2^2)}{4q_1q_2} - \varepsilon^2\cos^2\frac{k}{2} \tag{12}$$
$$+\varepsilon^2\cos\frac{k}{2}\,\frac{(q_1+q_2)(1+q_1q_2)}{2q_1q_2}=0$$

For $k^2 \ll \gamma$ there exists one SW of the present polarization in the LC, namely:

$$\vec{u}(x,z)=u_0\left[\begin{pmatrix}-2i\varepsilon\gamma^{3/2}\\ 1\end{pmatrix}\exp\left(-\frac{\sqrt{\gamma}kz}{\varepsilon a}\right)+i\varepsilon\sqrt{\gamma}\begin{pmatrix}1\\ 2i\sqrt{\gamma/\varepsilon}\end{pmatrix}\exp\left(\frac{-kz}{\varepsilon\sqrt{\gamma}a}\right)\right]e^{ikx/a}$$

$$\omega_s^2=\gamma k^2\varepsilon^2(1-\gamma) \tag{13}$$

These results are similar to (4) and (5), which were obtained in terms of elasticity theory. SW for larger wave vector values, up to the Brillouin zone boundary, may be found in [1].

The high elastic anisotropy essentially affects also the properties of Love waves propagating in a system consisting of a highly anisotropic crystal layer and an isotropic substrate. In particular, as the parameters are varied, there can arise in this system SW with a dispersion law unusual for acoustics. It can be shown [2] that the lowest-frequency mode of the system of LC-isotropic substrate has a frequency range in which the SW dispersion law is as follows:

$$\omega^2=k\frac{\rho_0}{\rho H}S_0^2 \tag{14}$$

(H is the layer thickness and S_0 the transverse sound velocity in the substrate), which is similar to the two-dimensional plasmon law.

REFERENCES

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[2] Yu.A. Kosevich and E.S. Syrkin, *Acustic. Zh.* (USSR) **34** (1988), 113.