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Contribution of optical phonons to sound velocity in piezoelectric semiconductors

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The influence of optical phonons on the sound velocity is investigated in piezoelectric semiconductors. In a large-wave-number region near the electron Fermi wave number, the contribution of optical phonons to the sound velocity is appreciable in connection with the wave-number dependence of the dielectric function of electrons.

The amplified acoustic phonons in piezoelectric semiconductors have been studied in the high-frequency range for which the wave number q satisfies the condition

$$ql \gg 1 ,$$

where l is the electron mean free path. In the high-frequency range, it must be significant to investigate the terms which have been neglected in the low-frequency range on account of small effects. Miranda and ter Haar[1,2] have predicted that the phonon amplification may be enhanced by plasmons in the high-frequency region. Their prediction has been supported by Kagoshima and Ishiguro[3] experimentally.

In polar semiconductors, the optical-phonon frequency is the same order as that of the electron plasma frequency, which is given by

$$\omega_p = (4\pi n_0 e^2/m\epsilon)^{1/2} ,$$

where n_0 is the average carrier density, and ϵ is the dielectric constant. In these materials, conduction electrons interact with acoustic waves through the piezoelectric coupling and with longitudinal-optical phonons through the polar coupling. In this report, we investigate the explicit contribution of optical phonons to acoustic waves by making use of a renormalization procedure.[4,5] In the low-frequency region, the polarization field induced by optical phonons is almost screened by conduction electrons and therefore does not give rise to the modification of acoustic waves. But, in the high-frequency region, we may expect that the polarization field induced by optical phonons gives a contribution to the modification of acoustic waves, as a screening effect decreases.

We suppose the longitudinal acoustic waves propagating parallel to the c axis in CdS and also suppose the special configuration where the stress components are zero except for the diagonal component concerned with the c axis, corresponding to the experimental configuration.[6] We take the c axis of a crystal as the z axis. In this configuration, the piezoelectric polarization induced by acoustic waves can be expressed by making use of the effective piezoelectric constant,[6]

$$e_{33}^{*} = e_{33} - 2e_{31}c_{13}/(c_{11}+c_{12}) ,$$

where e_{ij} and c_{ij} are the piezoelectric and elastic constants, respectively. As the electron-phonon interaction in piezeoelectric semiconductors, the piezoelectric coupling gives a main contribution and the deformation-potential coupling can be neglected in comparison with that. This is valid up to a frequency value of $10^{13}\ \mathrm{s}^{-1}$ in CdS.[7]

We develop our calculation after the method of Born and Huang.[8] We introduce the longitudinal vector field $\mathbf{w}$ which is defined by

$$\mathbf{w} = (\mathbf{u}_+ - \mathbf{u}_-)(M/\Omega_0)^{1/2} .$$

Here, $\mathbf{u}_+$ and $\mathbf{u}_-$ are the longitudinal lattice displacements of cations and anions in a unit cell, respectively, M is the reduced mass, and Ω_0 is the volume of a unit cell. The longitudinal vector field $\mathbf{w}$ obeys the equation of motion

$$\frac{\partial^2 \mathbf{w}}{\partial t^2} = -b_{11}\mathbf{w} + b_{12}\mathbf{E} , \tag{1}$$

where

$$b_{11} = \omega_T^2, \quad b_{12}^2 = \frac{\epsilon_\infty}{4\pi}(\omega_L^2 - \omega_T^2) .$$

Here, ω_L and ω_T are the frequencies of longitudinal and transverse optical phonons, respectively, $\mathbf{E}$ is the longitudinal electric field, and ϵ_∞ is the high-frequency dielectric constant. The equation of motion of the longitudinal lattice displacement $\mathbf{u}$ is written by

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \kappa \frac{\partial^2 \mathbf{u}}{\partial z^2} - e_{33}^{*} \frac{\partial \mathbf{E}}{\partial z} , \tag{2}$$

with

$$\kappa = c_{33} - 2c_{13}^2/(c_{11}+c_{12}) .$$

κ is the effective elastic constant and ρ is the mass density. The polarization $\mathbf{P}$ is related to $\mathbf{w}$, $\mathbf{u}$, and $\mathbf{E}$ through the equation

$$\mathbf{P} = b_{12}\mathbf{w} + e_{33}^{*}\frac{\partial \mathbf{u}}{\partial z} + b_{22}\mathbf{E} , \tag{3}$$

where

$$b_{22} = (\epsilon_\infty - 1)/4\pi .$$

Next we have to include the contribution from free-carrier density fluctuation to the self-consistent field $\mathbf{E}$. The electric displacement $\mathbf{D}$ defined by

$$\mathbf{D}=\mathbf{E}+4\pi\mathbf{P} \tag{4}$$

is related to the deviation of carrier density $n_1(\mathbf{r},t)$ from its average value n_0 through the following Poisson's equation:

$$\nabla\cdot\mathbf{D}=4\pi n_1(\mathbf{r},t) . \tag{5}$$

We note that we are dealing with jellium, a uniform positively charged medium against which the electrons move. The time dependence of $n_1(\mathbf{r},t)$ obeys the continuity equation. Thus we have

$$\frac{\partial}{\partial t}n_1(\mathbf{r},t)+\nabla\cdot\mathbf{j}(\mathbf{r},t)=0 . \tag{6}$$

The current density $\mathbf{j}(\mathbf{r},t)$ will be linearly related to the electric field $\mathbf{E}$ by the constitutive equation

$$\mathbf{j}(\mathbf{r},t)=\int d\mathbf{r}'\int_{-\infty}^{t} dt'\sigma(\mathbf{r}-\mathbf{r}',t-t')\mathbf{E}(\mathbf{r}',t') . \tag{7}$$

Taking the Fourier transforms of Eqs. (1)–(7), we have the following dispersion equation for the coupled modes:

$$\epsilon(\mathbf{q},\omega)(\omega^2-\omega_T^2)\left[\omega^2-\frac{\kappa}{\rho}q^2\right]-\frac{4\pi e_{33}^{*2}}{\epsilon_\infty\rho}q^2(\omega^2-\omega_T^2) -(\omega_L^2-\omega_T^2)\left[\omega^2-\frac{\kappa}{\rho}q^2\right]=0 . \tag{8}$$

$\epsilon(\mathbf{q},\omega)$ is the dielectric function of electrons and is set as

$$\epsilon(\mathbf{q},\omega)=1+i4\pi\sigma(\mathbf{q},\omega)/\epsilon_\infty\omega , \tag{9}$$

which is the standard relation between dielectric function and conductivity. Equation (8) yields the dispersion relation of acoustic waves as follows:

$$\omega^2=q^2\left[\kappa+\frac{4\pi e_{33}^{*2}}{\epsilon_\infty\epsilon(\mathbf{q},\omega)}\omega_T^2/[\omega_T^2+(\omega_L^2-\omega_T^2)/\epsilon(\mathbf{q},\omega)]\right]\Big/\rho \tag{10}$$

We see that the polarization field which causes the difference $(\omega_L^2-\omega_T^2)$ is screened by the presence of conduction electrons. When the electron–optical-phonon interaction is not taken into account, we have the following dispersion relation of acoustic waves:

$$\omega^2=q^2[\kappa+4\pi e_{33}^{*2}/\epsilon_\infty\epsilon(\mathbf{q},\omega)]/\rho . \tag{11}$$

From Eqs. (10) and (11), the contribution of optical phonons to the sound velocity is given by

$$\left|\frac{\Delta S}{S_0}\right|=\frac{2\pi e_{33}^{*2}}{S_0^2\epsilon_\infty\rho\epsilon(\mathbf{q},\omega)} \times\{1-\omega_T^2/[\omega_T^2+(\omega_L^2-\omega_T^2)/\epsilon(\mathbf{q},\omega)]\} . \tag{12}$$

with

$$S_0=[(\kappa+4\pi e_{33}^{*2}/\epsilon_\infty)/\rho]^{1/2} .$$

For the numerical computation, we use the expression obtained by Lindhard[9] as the value of $\epsilon(\mathbf{q},\omega)$. Figure 1 shows $\Delta S/S_0$ and $\epsilon(\mathbf{q},\omega)$ as a function of wave number q. The computation is carried out for CdS. The numerical values of parameters used are as follows:

$$e_{33}^*=1.822\times10^5 \text{ esu (Ref. 10)} ,$$

$$\kappa=5.884\times10^{11} \text{ dyn/cm}^2 \text{ (Ref. 10)} ,$$

$$\omega_L=295 \text{ cm}^{-1},\quad \omega_T=261 \text{ cm}^{-1} ,$$

$$\rho=4.819 \text{ g/cm}^3,\quad \epsilon_\infty=9.53,\quad m=0.205m_e ,$$

and the number density of electrons $n_0=10^{16}$ cm^{-3} which leads to a Fermi velocity $v_F=3.76\times10^6$ cm/s.

For a small q range, the polarization field induced by optical phonons is almost screened by electrons and does not contribute to the modification of a sound velocity. Hence in the long-wavelength limit, Eq. (10) reduces to Eq. (11). However, for a large q range, but smaller than the Fermi wave vector k_F, the contribution of optical phonons to the sound velocity is appreciable but not so large, as shown in Fig. 1. In the region of consideration, the dielectric function of electrons may be expressed as

$$\epsilon(\mathbf{q},\omega)=1+q_{\mathrm{TF}}^2/q^2 , \tag{13}$$

where q_{TF} is the Thomas-Fermi screening wave vector. The wave-number dependence of the dielectric function shown in Fig. 1 can be understood by Eq. (13). The change in the renormalized sound velocity can be interpreted by the behavior of $\epsilon(\mathbf{q},\omega)$. When the carrier density n_0 increases, the ratio $\Delta S/S_0$ decreases on account of increase of a screening effect.

We have derived the dispersion relation Eq. (8) based upon the method of Born and Huang from the macroscopic viewpoint. This method is an intuitively clear way to understand the physical properties of the system. However, we note here that the dispersion equation can be also derived by the quantum-mechanical method to be outlined below. The full Hamiltonian of the system is written by

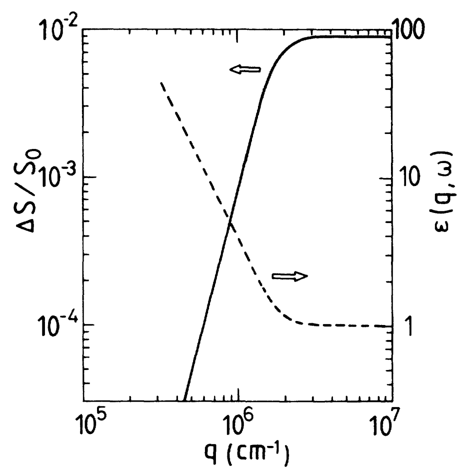

FIG. 1. The ratio of the change in the renormalized sound velocity due to optical phonons, $\Delta S/S_0$, is shown as a function of wave number q for a carrier density $n_0=10^{16}$ cm^{-3}. The dielectric function of electrons $\epsilon(\mathbf{q},\omega)$ is also plotted (dashed line).

$$H = H_0 + H_C + H_1 ,$$

$$H_0 = \sum_{\mathbf{k}} E_k a_k^\dagger a_k + \tfrac{1}{2}\sum_{\mathbf{k}} (P_k^* P_k + \omega_L^2 Q_k^* Q_k) + \tfrac{1}{2}\sum_{\mathbf{k}} \left[p_k^* p_k + \frac{k^2}{\rho}(\kappa + 4\pi e_{33}^{*2}/\epsilon_\infty) q_k^* q_k \right] , \tag{14}$$

$$H_C = \tfrac{1}{2} \sum_{\mathbf{kk'q}} \frac{4\pi e^2}{\epsilon_\infty q^2} a_{k+q}^\dagger a_{k'-q}^\dagger a_{k'} a_k ,$$

$$H_1 = \sum_{\mathbf{k}} v_1(k) Q_k n_{-k} + \sum_{\mathbf{k}} v_2(k) q_k n_{-k} + \sum_{\mathbf{k}} v_3(k) Q_{-k} q_k ,$$

where

$$v_1(k) = \frac{ie}{k} \left[\frac{4\pi}{\epsilon_\infty} (\omega_L^2 - \omega_T^2) \right]^{1/2} ,$$

$$v_2(k) = -4\pi e e_{33}^{*2}/\epsilon_\infty \sqrt{\rho} ,$$

$$v_3(k) = i e_{33}^{*2} k \left[\frac{4\pi}{\epsilon_\infty \rho} (\omega_L^2 - \omega_T^2) \right]^{1/2} .$$

Here, $a_k^\dagger$ and a_k are the creation and annihilation operators of electrons, respectively, P_k and Q_k are the normal coordinates of longitudinal-optical phonons, and p_k and q_k are those of acoustic phonons. H_0 is the zeroth-order Hamiltonian of the three-components system. H_C is the Coulomb interaction between electrons. The terms in H_1 represent the optical-phonon–electron, acoustic-phonon–electron, and acoustic-phonon–optical-phonon interactions, respectively. n_k is the Fourier component of the electron-density operator,

$$n_k = \sum_{\mathbf{p}} a_p^\dagger a_{p+k} .$$

By calculating the equations of motion of n_k, Q_k, and q_k in the random-phase approximation, we have

$$\epsilon(\mathbf{k},\omega) n_k + [\epsilon(\mathbf{k},\omega) - 1][v_1(k) Q_k + v_2(k) q_k] 4\pi e^2/(\epsilon_\infty k^2) = 0 , \tag{15}$$

$$(\omega^2 - \omega_L^2) Q_k - v_1(-k) n_k - v_3(k) q_k = 0 , \tag{16}$$

$$\left[\omega^2 - \frac{k^2}{\rho}(\kappa + 4\pi e_{33}^{*2}/\epsilon_\infty \rho) \right] q_k - v_2(-k) n_k - v_3(-k) Q_k = 0 . \tag{17}$$

Here, $\epsilon(\mathbf{k},\omega)$ is the electron dielectric function which is defined by

$$\epsilon(\mathbf{k},\omega) = 1 + \frac{4\pi e^2}{\epsilon_\infty k^2} \sum_{\mathbf{p}} \frac{f_{p+q} - f_p}{\hbar\omega - E(p+q) + E(p)} , \tag{18}$$

where f_p is the Fermi-Dirac distribution function. Explicit values of $\epsilon(\mathbf{k},\omega)$ were obtained by Lindhard as stated above.[9] Solving Eqs. (15)–(17), we have the same dispersion equation of the coupled modes as that of Eq. (8).

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