phys. stat. sol. (b) 140, 421 (1987)

Subject classification: 77.55; 68.30; 71.38

Changchun Institute of Physics, Chinese Academy of Sciences[1])

Electron–Phonon Interaction in Dielectric Interface Systems[2])

By

PAN JIN-SHENG

The integral and differential equations for the polarization eigenmodes of the dielectric interface systems are given by making use of the macroscopic electric field caused by the bulk and interface polarization charges. It is shown that the polarization eigenmodes should be normalized according to the ortho-normalized relation interpreted in the text. It is also shown that the interaction of the charged particles with SO phonons can be described by Fröhlich-like coupling constant α^{so} characterizing the interface system.

Представляется интегральное и дифференциальное уравнение, которые принадлежат поляризованной собственной моде в слойной системе диэлектрика, с помошью макроскопического электрического поля вызванными поляризованными зарядами в диэлектрике и границе раздела. Доказали то, что поляризованная собственная мода дожна нормирована в соотвествии с ортонормированныи отношением, изложеным в тексте. Также доказали, что взаймодействие между заряженными частицами и SO фонона можно описывать подобным Fröhlich постоянному связи α^{so}, которая характеризует двухслойная система.

1. Introduction

The electron–phonon interaction in a dielectric layer was firstly considered by Lucas et al. [1], followed by the works of Wang and Mahan [2], Evans and Mills [3]. However, these authors did not consider the influence of the electronic polarizability. In view of this situation, Licari and Evrard [4] pointed out the importance of the electronic polarizability and took it into account. The electron–phonon interaction in a bilayer system without considering the electronic polarizability was studied by Lenac and Sunjic [5]. Recently, Wendler [6] deduced the equation of motion for the polarization eigenmodes of the dielectric bilayer system from the microscopic dynamical equation, and calculated the strength of the interaction between the electron and the phonon for a certain wave vector $\boldsymbol{q}_{||}$ of the phonon. All the works of the above authors are important for gaining insight into the behavior of the electron–phonon interaction near the surface or interface of the dielectric layer.

In Section 2 of this paper, we will deduce the integral and differential equations of the polarization vector by making use of the electrostatic potential caused by the bulk and interface polarization charges. It is also proved that the polarization eigenvectors should be normalized to $(L_3^0 q_{||})^{-1}$, where L_3^0 is unit length of the system in x_3-direction. In the Section 3, we use the orthonormalized relation obtained in Section 2 and the Hamiltonian density from the equation of motion (1) to deduce the operator represen-

[1]) Changchun, Jilin, People's Republic of China.

[2]) This subject was supported by the Science fund of the Chinese Academy of Sciences.

tation of the Hamiltonian and the electron–phonon interaction energy. It is found that the commutation relation between the creation and annihilation operators of the phonon is also changed. In Section 4 the electron–phonon interaction is considered. The interaction of the charged particles with SO phonons can be described by a Fröhlich-like coupling constant α^{SO}.

2. The Polarization Eigenmodes of the Dielectric Bilayer

We assume two different polar materials which are diatomic ionic crystals or polar semiconductors consisting of one pair of positive and negative ions per Wigner-Seitz cell to be in contact at $x_3 = 0$ (Fig. 1). Making use of the long-wave approximation, the equation of motion for the relative displacement of the ions in the layer n ($n = 1$ or 2) is given by [7]

$$\mu_n \boldsymbol{u}(\boldsymbol{x}, t) = -\mu_n \omega_{on}^2 \boldsymbol{u}(\boldsymbol{x}, t) + e_n \boldsymbol{E}^{loc}(\boldsymbol{x}, t) , \tag{1}$$

where $\boldsymbol{u}(\boldsymbol{x}, t) = \boldsymbol{u}^+(\boldsymbol{x}, t) - \boldsymbol{u}^-(\boldsymbol{x}, t)$ is the relative displacement of the positive and negative ions, $\mu_n = m_n^+ m_n^- / (m_n^+ + m_n^-)$ their reduced mass, $\omega_{on}^2 = f_n/\mu_n$ the characteristic frequency associated force constant f_n, $\boldsymbol{E}^{loc}(\boldsymbol{x}, t)$ the local electric field. The displacement of the ions will result in polarization: one is the ionic polarization caused by the relative separation of the positive and negative ions, the other is the electric polarization caused by the local field acting on the electron shell of the ions. Thus, we have

$$\boldsymbol{p}(\boldsymbol{x}, t) = n_n e_n \boldsymbol{u}(\boldsymbol{x}, t) + n_n \alpha_n \boldsymbol{E}^{loc}(\boldsymbol{x}, t) , \tag{2}$$

where n_n is the number of Wigner-Seitz cells per unit volume; α_n the electronic polarizability per cell in the layer n. Assuming the media to be nonmagnetic and uncharged, the macroscopic electric potential $\varphi(\boldsymbol{x}, t)$ at $\boldsymbol{x}$ produced by the surface and bulk polarization charges at $\boldsymbol{x}'$, is

$$\varphi(\boldsymbol{x}, t) = \frac{1}{4\pi\varepsilon_0} \left\{ \sum_k \int \mathrm{d}S_k \frac{1}{|\boldsymbol{x} - \boldsymbol{x}_k'|} \boldsymbol{N}_k \cdot \boldsymbol{p}(\boldsymbol{x}_k', t) - \int \mathrm{d}\boldsymbol{x}' \frac{1}{|\boldsymbol{x} - \boldsymbol{x}'|} \nabla_{\boldsymbol{x}} \cdot \boldsymbol{p}(\boldsymbol{x}', t) \right\} , \tag{3}$$

where the first term comes from the contribution of the surface polarization charges of the k-th interface, $\boldsymbol{N}_k$ is the unit vector along the normal direction of the interface k; the second term comes from the bulk polarization charges. Using

$$\boldsymbol{E}(\boldsymbol{x}, t) = -\nabla_{\boldsymbol{x}} \varphi(\boldsymbol{x}, t) , \tag{4}$$

and the Lorentz relation between the local field $\boldsymbol{E}^{loc}$ and the macroscopical electric field $\boldsymbol{E}$

$$\boldsymbol{E}^{loc} = \boldsymbol{E} + \frac{1}{3\varepsilon_0} \boldsymbol{p} , \tag{5}$$

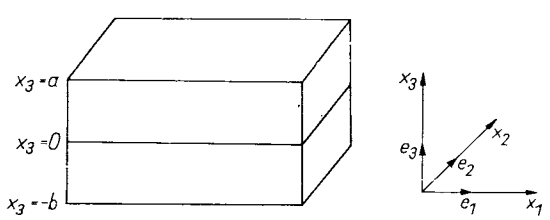

Fig. 1. The geometry of the interface system

from (2) and (3) we have

$$\left(1-\frac{1}{3\varepsilon_0}n_n\alpha_n\right)[\ddot{p}_{n,\alpha}(\boldsymbol{x},t)-\omega_{on}^2 p_{n,\alpha}(\boldsymbol{x},t)]-\frac{n_n e_n^2}{3\varepsilon_0\mu_n}p_{n,\alpha}(\boldsymbol{x},t)$$
$$=\sum_1^2{}_{n'}\frac{1}{\varepsilon_0}n_{n'}\alpha_{n'}\left\{\int_{n'}\mathrm{d}\boldsymbol{x}'\,\Gamma_\alpha(\boldsymbol{x}'-\boldsymbol{x}')\,\nabla_{\boldsymbol{x}'}\cdot\ddot{\boldsymbol{p}}_{n'}(\boldsymbol{x}',t)-\right.$$
$$\left.-\sum_k\int_{n'}\mathrm{d}S_k\,\Gamma_\alpha(\boldsymbol{x}-\boldsymbol{x}_k)\,\boldsymbol{N}_k\cdot\ddot{\boldsymbol{p}}_{n'}(\boldsymbol{x}_k,t)\right\}+\sum_1^2{}_{n'}\frac{1}{\varepsilon_0}\left(n_{n'}\alpha_{n'}\omega_{on'}^2+\frac{n_{n'}e_{n'}^2}{\mu_{n'}}\right)\times$$
$$\times\left\{\int_{n'}\mathrm{d}\boldsymbol{x}'\,\Gamma_\alpha(\boldsymbol{x}-\boldsymbol{x}')\,\nabla_{\boldsymbol{x}'}\cdot\boldsymbol{p}_{n'}(\boldsymbol{x}',t)-\right.$$
$$\left.-\sum_k\int_{n'}\mathrm{d}S_k\,\Gamma_\alpha(\boldsymbol{x}-\boldsymbol{x}_k)\,\boldsymbol{N}_k\cdot\boldsymbol{p}_{n'}(\boldsymbol{x}_k,t)\right\},\tag{6}$$

where n and n' take 1 or 2, and

$$\Gamma_\alpha(\boldsymbol{x}-\boldsymbol{x}')=\frac{1}{4\pi}\frac{\partial}{\partial x_\alpha}\frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|}.\tag{7}$$

Assuming the polarization to have a harmonic time dependence

$$\boldsymbol{p}(\boldsymbol{x},t)=\boldsymbol{p}(\boldsymbol{x})\,\mathrm{e}^{i\omega t},$$

(6) becomes

$$-\frac{(\lambda_n-\lambda_{on})\,[1-(1/3\varepsilon_0)\,n_n\alpha_n]+(1/3\varepsilon_0)}{1-n_n\alpha_n(\lambda_n-\lambda_{on})}\,p_n(\bar{x})$$
$$=\frac{1}{\varepsilon_0}\sum_1^2{}_{n'}\frac{\bar{\theta}_n^{1/2}}{\bar{\theta}_{n'}^{1/2}}\left\{\int_{n'}\mathrm{d}\boldsymbol{x}'\,\Gamma_\alpha(\boldsymbol{x}-\boldsymbol{x}')\,\nabla_{\boldsymbol{x}'}\cdot\boldsymbol{p}_{n'}(\boldsymbol{x}')-\right.$$
$$\left.-\sum_k\int_{n'}\mathrm{d}S_k\,\Gamma_\alpha(\boldsymbol{x}-\boldsymbol{x}_k)\,\boldsymbol{N}_k\cdot\boldsymbol{p}_{n'}(\boldsymbol{x}_k)\right\},\tag{8}$$

where we have used the following abbreviations:

$$\lambda_{on}=\frac{\omega_{on}^2}{\varepsilon_0\omega_{pn}^2},\qquad\lambda_n=\frac{\omega^2}{\varepsilon_0\omega_{pn}^2},\qquad\omega_{pn}^2=\frac{n_n e_n^2}{\varepsilon_0\mu_n},\tag{9a}$$

$$\theta_n^{1/2}=[1-n_n\alpha_n(\lambda_n-\lambda_{on})]^{-1},\qquad\bar{\theta}_n^{1/2}=\frac{\theta_r^{1/2}}{\omega_{pn}^2}.\tag{9b}$$

Here ω_{pn} is the ion plasma frequency. We assume $\boldsymbol{q}_{||}$ to be the two-dimensional wave vector parallel to the interface, and $\boldsymbol{x}_{||}$ the two-dimensional position vector in the same plane. Because of the translational invariance for continuous displacements in $\boldsymbol{q}_{||}$ direction, we can introduce the two-dimensional Fourier transforms for $\boldsymbol{p}(\boldsymbol{x})$ and $1/|\boldsymbol{x}-\boldsymbol{x}'|$,

$$\boldsymbol{p}(\boldsymbol{x})=\frac{1}{4\pi^2}\int\mathrm{d}\boldsymbol{q}_{||}\,\mathrm{e}^{i\boldsymbol{q}_{||}\cdot\boldsymbol{x}_{||}}\,\boldsymbol{p}(\boldsymbol{q}_{||},x_3),\tag{10a}$$

$$\frac{1}{4\pi\,|\boldsymbol{x}-\boldsymbol{x}'|}=\frac{1}{8\pi^2}\int\mathrm{d}\boldsymbol{q}_{||}\,\mathrm{e}^{i\boldsymbol{q}_{||}\cdot(\boldsymbol{x}_{||}-\boldsymbol{x}'_{||})}\frac{1}{q_{||}}\,\mathrm{e}^{-q_{||}|x_3-x'_3|}.\tag{10b}$$

Making use of the above transforms, the integral equation (8) can be rewritten as

$$\chi^{-1}(\omega)\,[\boldsymbol{e}_1 p_{n,1}(\boldsymbol{q}_{||}, x) + \boldsymbol{e}_2 p_{n,2}(\boldsymbol{q}_{||}, x_3) + \boldsymbol{e}_3 p_{n,3}(\boldsymbol{q}_{||}, x)] =$$

$$= \frac{1}{2}\sum_1^2 {}_{n'} \frac{\bar{\theta}_n^{1/2}}{\bar{\theta}_{n'}^{1/2}} \left\{ \int_{n'} \mathrm{d}x_3' \,[\boldsymbol{e}_1 i q_1 + \boldsymbol{e}_2 i q_2 - \boldsymbol{e}_3 q_{||} \operatorname{sgn}(x_3 - x_3')] \frac{\mathrm{e}^{-q_{||}|x_3 - x_3'|}}{q_{||}} \times \right.$$

$$\left. \times \left(\boldsymbol{e}_1 i q_1 + \boldsymbol{e}_2 i q_2 + \boldsymbol{e}_3 \frac{\partial}{\partial x_3'} \right) \cdot \boldsymbol{p}_{n'}(\boldsymbol{q}_{||}, x_3) \right\} -$$

$$- \frac{1}{2}\sum_1^2 {}_{n'} \frac{\bar{\theta}_n^{1/2}}{\bar{\theta}_{n'}^{1/2}} \left\{ \sum_k [\boldsymbol{e}_1 i q_1 + \boldsymbol{e}_2 i q_2 - \boldsymbol{e}_3 q_{||} \operatorname{sgn}(x_3 - x_{k,3})] \times \right.$$

$$\left. \times \frac{\mathrm{e}^{-q_{||}|x_3 - x_{k,3}|}}{q_{||}} p_{n',3}(\boldsymbol{q}_{||}, x_{k,3}) \right\} \tag{11}$$

where $\boldsymbol{e}_1$, $\boldsymbol{e}_2$, $\boldsymbol{e}_3$ are Cartesian unit vectors directed along the x_1, x_2, x_3-axis, respectively, and

$$\frac{\chi_n^{-1}(\omega)}{\varepsilon_0} = -\frac{(\lambda_n - \lambda_{on})\,[1 - (1/3\varepsilon_0)\, n_n \alpha_n] + (1/3\varepsilon_0)}{1 - n_n \alpha_n (\lambda_n - \lambda_{on})}. \tag{12}$$

Here $\chi_n(\omega)$ is, in fact, the isotropic susceptibility. This relation is easily obtained by making use of (1), (2), and (5) with the linear relation between the polarization $\boldsymbol{p}$ and the macroscopic electric field $\boldsymbol{E}$,

$$\boldsymbol{p}(\boldsymbol{q}_{||}, x_3) = \varepsilon_0 \chi_n(\omega)\, \boldsymbol{E}(\boldsymbol{q}_{||}, x_3)\,. \tag{13}$$

Because there is the relation $\chi_n(\omega) = \epsilon_n(\omega) - 1$ between $\chi_n(\omega)$ and the dielectric function $\epsilon_n(\omega)$, from (12) one can obtain the dielectric function for the layer n,

$$\epsilon_n(\omega) = \varepsilon_{\infty n} \frac{\omega_{\mathrm{L}n}^2 - \omega^2}{\omega_{\mathrm{T}n}^2 - \omega^2}, \tag{14a}$$

with

$$\varepsilon_{\infty n} = 1 + \frac{1}{\varepsilon_0} \frac{n_n \alpha_n}{1 - (1/3\varepsilon_0)\, n_n \alpha_n}, \tag{14b}$$

$$\omega_{\mathrm{L}n}^2 = \omega_{on}^2 + \frac{(2/3\varepsilon_0)\, \omega_{\mathrm{p}n}^2}{1 + (2/3\varepsilon_0)\, n_n \alpha_n}, \qquad \omega_{\mathrm{T}n}^2 = \omega_{on}^2 \frac{(1/3\varepsilon_0)\, \omega_{\mathrm{p}n}^2}{1 - (1/3\varepsilon_0)\, n_n \alpha_n}. \tag{14c}$$

$\varepsilon_{\infty n}$ is the optical dielectric constant, $\omega_{\mathrm{L}n}$ and $\omega_{\mathrm{T}n}$ are, respectively, the longitudinal and the transverse optical (LO and TO) phonon frequencies. If the coordinates are transformed from the old system ($\boldsymbol{e}_1$, $\boldsymbol{e}_2$, $\boldsymbol{e}_3$) to the new one ($\boldsymbol{e}_{||}$, $\boldsymbol{e}_{\mathrm{s}}$, $\boldsymbol{e}_3$) according to

$$\begin{pmatrix} \boldsymbol{e}_{||} \\ \boldsymbol{e}_{\mathrm{s}} \end{pmatrix} = \frac{1}{q_{||}} \begin{pmatrix} q_1 & q_2 \\ -q_2 & q_1 \end{pmatrix} \begin{pmatrix} \boldsymbol{e}_1 \\ \boldsymbol{e}_2 \end{pmatrix},$$

the polarization denoted by (11) can be separated into an s-polarized part $p = (0, p_{\mathrm{s}}, 0)$

and a p-polarized one $p_{||} = (p_{||}, 0, p_3)$ which are, respectively,

$$\chi_n^{-1}(\omega)\, p_{n,s}(\boldsymbol{q}, x_3) = 0\,, \tag{15a}$$

$$\chi_n^{-1}(\omega)\, p_{n,||}(q, x_3) = \frac{i}{2} \sum_1^2 n' \left\{ \int \mathrm{d}x_3' \, \mathrm{e}^{-q_{||}|x_3 - x_3'|} \left(\boldsymbol{e}_{||} i q_{||} + \boldsymbol{e}_3 \frac{\partial}{\partial x_3'} \right) \cdot \boldsymbol{p}_{n'}(\boldsymbol{q}_{||}, x_3') - \right.$$
$$\left. - \sum_k \mathrm{e}^{-q_{||}|x_3 - x_{k,3}|}\, p_{n',3}(\boldsymbol{q}_{||}, x_{k,3}) \right\} \frac{\bar{\theta}_n^{1/2}}{\bar{\theta}_{n'}^{1/2}}\,, \tag{15b}$$

$$\chi_n^{-1}(\omega)\, p_{n,3}(q, x_3) = -\frac{1}{2} \sum_1^2 n' \left\{ \int \mathrm{d}x_3' \, \mathrm{e}^{-q_{||}|x_3 - x_3'|} \operatorname{sgn}(x_3 - x_3') \times \right.$$
$$\times \left(\boldsymbol{e}_{||} i q_{||} + \boldsymbol{e}_3 \frac{\partial}{\partial x_3'} \right) \cdot \boldsymbol{p}_{n'}(\boldsymbol{q}_{||}, x_3') +$$
$$\left. + \sum_k \mathrm{e}^{-q_{||}|x_3 - x_{k,3}|} \operatorname{sgn}(x_3 - x_{k,3})\, p_{n',3}(\boldsymbol{q}_{||}, x_{k,3}) \right\} \frac{\bar{\theta}_n^{1/2}}{\bar{\theta}_{n'}^{1/2}}\,. \tag{15c}$$

Thus, the analytical relations for the s-polarized and p-polarized parts are completely decoupled. The usual way for solving this system of equations is, as done by Wendler [6], to transform it into a differential equation. Differentiating (15b) and (15c) with respect to x_3 gives

$$\chi_n^{-1}(\omega) \frac{\mathrm{d}}{\mathrm{d}x_3}\, p_{n,||}(\boldsymbol{q}_{||}, x_3) = i q_{||} \chi_n^{-1}(\omega)\, p_{n,3}(\boldsymbol{q}_{||}, x_3)\,,$$

$$\chi_n^{-1}(\omega) \frac{\mathrm{d}}{\mathrm{d}x_3}\, p_{n,3}(\boldsymbol{q}_{||}, x_3) = -i q_{||} [\chi_n^{-1}(\omega) + 1]\, p_{n,||}(\boldsymbol{q}_{||}, x_3) - \frac{\mathrm{d}}{\mathrm{d}x_3} p_{n,3}(\boldsymbol{q}_{||}, x_3)\,. \tag{16a}$$

Because of $\chi_n^{-1}(\omega) + 1 = \chi_n^{-1}(\omega)\, \epsilon_n(\omega)$, the second equation obtained above can be changed to

$$\chi_n^{-1}(\omega)\, \epsilon_n(\omega) \frac{\mathrm{d}}{\mathrm{d}x_3}\, p_{n,3}(\boldsymbol{q}_{||}, x_3) = -i q_{||} \chi_n^{-1}(\omega)\, \epsilon_n(\omega)\, p_{n,||}(\boldsymbol{q}_{||}, x_3)\,. \tag{16b}$$

From the above three equations (15a), (16a), and (16b) one can determine the polarization eigenmodes for various concrete conditions.

Now, the problem is how the polarization eigenvectors are normalized. If the orthonormalized expression is taken in the form

$$\sum_\alpha \sum_n \int_n \mathrm{d}x_3 \, \frac{\theta_n^{1/2}(\omega_j)\, \theta_n^{1/2}(\omega_i)}{\omega_{pn}^2}\, p_{n,\alpha}^{j*}(\boldsymbol{q}_{||}, x_3)\, p_{n,\alpha}^{i}(\boldsymbol{q}_{||}, x_3) = \delta_{ij}\,, \tag{17}$$

it is equivalent to assume that, after integrating the above expression with respect to x_3, the results obtained do not depend on $\boldsymbol{q}_{||}$. Evidently, this is not quite reasonable. If the orthonormalized expression is taken in the form

$$\sum_\alpha \sum_n \int_n \mathrm{d}x_3 \, \frac{\theta_n^{1/2}(\omega_j)\, \theta_n^{1/2}(\omega_i)}{\omega_{pn}^2}\, p_{n,\alpha}^{j*}(\boldsymbol{q}_{||}, x_3)\, p_{n,\alpha}^{i}(\boldsymbol{q}_{||}, x_3) = F(\boldsymbol{q}_{||})\, \delta_{ij}\,,$$

after integrating with respect to x_3, the results obtained continue to have the natural dependence of $\boldsymbol{q}_{||}$. We can prove (Appendix A) $F(\boldsymbol{q}_{||})$ to be $(L_3^0 q_{||})^{-1}$, where L_3^0 is unit length of the sample in x_3-direction. Thus, the orthonormalized relation should be

$$\sum_\alpha \sum_n \int_n \mathrm{d}x_3 \, \frac{\theta_n^{1/2}(\omega_j)\, \theta_n^{1/2}(\omega_i)}{\omega_{pn}^2}\, p_{n,\alpha}^{j*}(\boldsymbol{q}_{||}, x_3)\, p_{n,\alpha}^{i}(\boldsymbol{q}_{||}, x_3) = (L_3^0 q_{||})^{-1}\, \delta_{ij}\,. \tag{18}$$

In what follows, we shall use this orthonormalized relation to derive the expression of the Hamiltonian and discuss some concrete problems.

3. The Hamiltonian of the Polarization Eigenmodes

The Hamiltonian function of the polarization eigenmodes can be denoted in the form [6]

$$H_{\mathrm{p}} = \frac{1}{2A} \sum_{\boldsymbol{q}_{\|}} \sum_{\alpha} \sum_{n} \int \mathrm{d}x_3 \, \frac{\theta_n}{\varepsilon_0 \omega_{\mathrm{p}n}^2} \{ p^*_{n,\alpha}(\boldsymbol{q}_{\|}, x_3) \, p_{n,\alpha}(\boldsymbol{q}_{\|}, x_3) + \\ + \omega^2 p^*_{n,\alpha}(\boldsymbol{q}_{\|}, x_3) \, p_{n.\alpha}(\boldsymbol{q}_{\|}, x_3) \} \, , \tag{19}$$

where A is the area of the bilayer system parallel to the x_1–x_2 plane, and

$$\int \mathrm{d}\boldsymbol{q}_{\|} \to \frac{4\pi^2}{A} \sum_{\boldsymbol{q}_{\|}} ; \qquad \delta(\boldsymbol{q}_{\|} - \boldsymbol{q}'_{\|}) \to \frac{A}{4\pi^2} \delta_{\boldsymbol{q}_{\|}, \boldsymbol{q}'_{\|}} \, .$$

If the polarization $\boldsymbol{p}_n(\boldsymbol{q}_{\|}, x_3)$ is represented in terms of the complete set of the orthonormal polarization eigenmodes $\boldsymbol{p}_n^j(\boldsymbol{q}_{\|}, x_3)$, i.e.

$$\hat{\boldsymbol{p}}_n(\boldsymbol{q}_{\|}, x_3) = \sum_j \left[\frac{\varepsilon_0 \hbar A}{2\omega_j(\boldsymbol{q}_{\|})} \right]^{1/2} [\hat{a}_j^+(-\boldsymbol{q}_{\|}) + \hat{a}_j(\boldsymbol{q}_{\|})] \, \boldsymbol{p}_n^j(\boldsymbol{q}_{\|}, x_3) \, , \tag{20a}$$

$$\hat{\dot{\boldsymbol{p}}}_n(\boldsymbol{q}_{\|}, x_3) = \sum_j \left[\frac{\varepsilon_0 \hbar A \omega_j(\boldsymbol{q}_{\|})}{2} \right]^{1/2} [\hat{a}_j^+(-\boldsymbol{q}_{\|}) - \hat{a}_j(\boldsymbol{q}_{\|})] \, \boldsymbol{p}_n^j(\boldsymbol{q}_{\|}, x_3) \, . \tag{20b}$$

where the cap $\hat{}$ in $\boldsymbol{p}$ and $\dot{\boldsymbol{p}}$ refers the corresponding physical quantities to be considered as the quantum field operators. Substituting the above expressions into (19), and using the orthonormalized relation (18), we have the following commutation relation for the operators a and a_j:

$$[\hat{a}_j(\boldsymbol{q}_{\|}), \hat{a}_i^+(\boldsymbol{q}_{\|})] = (L_3^0 q_{\|}) \, \delta_{\boldsymbol{q}_{\|}, \boldsymbol{q}'_{\|}} \delta_{ij} \, , \tag{21a}$$

$$[\hat{a}_j^+(\boldsymbol{q}_{\|}), \hat{a}_i^+(\boldsymbol{q}_{\|})] = [\hat{a}_j(\boldsymbol{q}_{\|}), \hat{a}_i(\boldsymbol{q}_{\|})] = 0 \, , \tag{21b}$$

where $\hat{a}_j^+$ and $\hat{a}_j$ are, respectively, the creation and annihilation operators of long optical phonons. In the next section, we will see that there are three kinds of phonons corresponding to the p-polarized wave. They are, respectively, the surface optical phonon (SO), longitudinal optical phonon (LO) transverse, optical phonon (TO). The phonons corresponding to the s-polarized wave are the transverse optical ones. Because the electrons do not interact with TO phonons, we only write the Hamiltonian corresponding to SO and LO phonons. They are

$$H_{\mathrm{p}}^{\mathrm{SO}} = \sum_j \sum_{\boldsymbol{q}_{\|}} \hbar\omega_{\mathrm{SO},j}(\boldsymbol{q}_{\|}) \left[\left(\frac{1}{L_3^0 q_{\|}} \right) \hat{a}^+_{\mathrm{SO},j}(\boldsymbol{q}_{\|}) \, \hat{a}_{\mathrm{SO},j}(\boldsymbol{q}_{\|}) + \frac{1}{2} \right], \tag{22a}$$

$$H_{\mathrm{p}}^{\mathrm{LO}} = \sum_j \sum_{\boldsymbol{q}_{\|}} \hbar\omega_{\mathrm{LO},j}(\boldsymbol{q}_{\|}) \left[\left(\frac{1}{L_3^0 q_{\|}} \right) \hat{a}^+_{\mathrm{LO},j}(\boldsymbol{q}_{\|}) \, \hat{a}_{\mathrm{LO},j}(\boldsymbol{q}_{\|}) + \frac{1}{2} \right]. \tag{22b}$$

Introducing

$$\hat{a}^+(\boldsymbol{q}_{\|}) = \hat{b}^+(\boldsymbol{q}_{\|}) \, (L_3 q_{\|})^{1/2}; \qquad \hat{a}(\boldsymbol{q}_{\|}) = \hat{b}(\boldsymbol{q}_{\|}) \, (L_3^0 q_{\|})^{1/2} \, , \tag{23}$$

the Hamiltonian for SO and LO phonons can be rewritten as

$$H_{\mathrm{p}}^{\mathrm{SO}} = \sum_j \sum_{\boldsymbol{q}_{\|}} \hbar\omega_{\mathrm{SO},j}(\boldsymbol{q}_{\|}) \, [\hat{b}^+_{\mathrm{SO},j}(\boldsymbol{q}_{\|}) \, \hat{b}_{\mathrm{SO},j}(\boldsymbol{q}_{\|}) + \tfrac{1}{2}] \, , \tag{24a}$$

$$H_{\mathrm{p}}^{\mathrm{LO}} = \sum_{\boldsymbol{q}} \hbar\omega_{\mathrm{LO}}(\boldsymbol{q}_{\|}) \, \{\hat{b}^+_{\mathrm{LO}}(\boldsymbol{q}_{\|}) \, \hat{b}_{\mathrm{LO}}(\boldsymbol{q}_{\|}) + \tfrac{1}{2}\} \, . \tag{24b}$$

Evidently, the new operators $\hat{b}_j^+$ and $\hat{b}_j$ defer to the commutation relation

$$[\hat{b}_j^+(\boldsymbol{q}_{||}), \hat{b}_j(\boldsymbol{q}'_{||})] = \delta_{\boldsymbol{q}_{||}, \boldsymbol{q}'_{||}}\delta_{ij} \,. \tag{25}$$

Analogously, for the transverse phonons of the p-polarized and s-polarized waves we can also obtain the same relations.

Now, we turn to consider the interaction of the charged particles with SO and LO phonons. Assuming the electron to be at the position $(\boldsymbol{x}_{||}^{\mathrm{e}}, x_3^{\mathrm{e}})$, the interaction of the electron with the polarizable medium is

$$H_{\mathrm{ep}} = -\int \boldsymbol{D}(\boldsymbol{x} - \boldsymbol{x}^{\mathrm{e}}) \cdot \boldsymbol{p}(\boldsymbol{x}, t)\, \mathrm{d}\boldsymbol{x} \,, \tag{26}$$

where $\boldsymbol{D}(\boldsymbol{x} - \boldsymbol{x}^{\mathrm{e}})$ is the electric induction at $\boldsymbol{x}$ caused by the electron at $(\boldsymbol{x}_{||}^{\mathrm{e}}, x_3^{\mathrm{e}})$. Making use of the scalar potential representation, the above expression changes to

$$\begin{aligned} H_{\mathrm{ep}} &= \frac{e}{4\pi\varepsilon_0}\int \left\{\nabla_{\boldsymbol{x}} \frac{1}{|\boldsymbol{x} - \boldsymbol{x}^{\mathrm{e}}|}\right\} \cdot \boldsymbol{p}(\boldsymbol{x}, t)\, \mathrm{d}\boldsymbol{x} \\ &= \frac{e}{4\pi\varepsilon_0}\int \frac{1}{|\boldsymbol{x} - \boldsymbol{x}^{\mathrm{e}}|} \nabla_{\boldsymbol{x}} \cdot \boldsymbol{p}(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x} - \\ &\quad - \frac{e}{4\pi\varepsilon_0} \sum_k \int \frac{1}{|\boldsymbol{x}_k - \boldsymbol{x}^{\mathrm{e}}|} \boldsymbol{N}_k \cdot \boldsymbol{p}(\boldsymbol{x}_{k,||}, x_{k,3})\, \mathrm{d}s_k \,. \end{aligned} \tag{27}$$

Substituting the Fourier form of $\boldsymbol{p}(\boldsymbol{x})$ and $1/|\boldsymbol{x} - \boldsymbol{x}^{\mathrm{e}}|$ into this expression and making use of the operator representation for the polarization eigenmodes $\boldsymbol{p}(\boldsymbol{q}_{||}, x_3)$, the Hamiltonian of the electron–phonon interaction has finally the following form:

$$\begin{aligned} H_{\mathrm{ep}} &= \sum_j \sum_{\boldsymbol{q}_{||}} \mathrm{e}^{i\boldsymbol{q}_{||}\cdot\boldsymbol{x}_{||}^{\mathrm{e}}} \left(\frac{\hbar e^2}{8\varepsilon_0 A\omega_j}\right)^{1/2} \sum_n \left\{\int_n \mathrm{d}x_3\, \mathrm{e}^{-q_{||}|x_3 - x_3^{\mathrm{e}}|} \frac{1}{q_{||}} \times \right. \\ &\quad \times \left(\boldsymbol{e}_{||} i q_{||} - \boldsymbol{e}_3 \frac{\partial}{\partial x_3}\right) \cdot \boldsymbol{p}_n^j(\boldsymbol{q}_{||}, x_3) + \sum_k \frac{\mathrm{e}^{-q_{||}|x_{k,3} - x_3^{\mathrm{e}}|}}{q_{||}} \times \\ &\quad \left. \times \boldsymbol{N}_k \cdot \boldsymbol{p}_n^j(\boldsymbol{q}_{||}, x_{k,3})\right\} [\hat{b}_j^+(-\boldsymbol{q}_{||}) + \hat{b}_j(\boldsymbol{q}_{||})]\, (L_3^0 q_{||})^{1/2} = \\ &= \sum_j \sum_{\boldsymbol{q}} \mathrm{e}^{i\boldsymbol{q}_{||}\cdot\boldsymbol{x}_{||}}\, V_j(\boldsymbol{q}_{||}, x_3)\, [\hat{b}_j^+(-\boldsymbol{q}_{||}) + \hat{b}_j(\boldsymbol{q}_{||})] \,, \end{aligned} \tag{28}$$

where

$$\begin{aligned} V_j(\boldsymbol{q}_{||}, x_3^{\mathrm{e}}) &= \left(\frac{\hbar e^2}{8\varepsilon_0 A\omega_j}\right)^{1/2} \sum_n \left\{\int_n \mathrm{d}x_3 \frac{\mathrm{e}^{-q_{||}|x_3 - x_3^{\mathrm{e}}|}}{q_{||}} \left(\boldsymbol{e}_{||} i q_{||} - \boldsymbol{e}_3 \frac{\partial}{\partial x_3}\right) \cdot \boldsymbol{p}_n^j(\boldsymbol{q}_{||}, x_3) + \right. \\ &\quad \left. + \sum_k \frac{\mathrm{e}^{-q_{||}|x_{k,3} - x_3^{\mathrm{e}}|}}{q_{||}} \boldsymbol{N}_k \cdot \boldsymbol{p}_n^j(\boldsymbol{q}_{||}, x_{k,3})\, (L_3^0 q_{||})^{1/2}\right\} \end{aligned} \tag{29}$$

is called the potential function of the interaction.

In the next section, we shall meet the situation where the polarization is not only a function of $\boldsymbol{q}_{||}$, but also of m, where m takes the values 1, 2, 3, ... For this case the polarization $\boldsymbol{p}(\boldsymbol{q}_{||}, x_3)$ can be regarded as the superposition of a number of polarization components $\boldsymbol{p}(\boldsymbol{q}_{||}, m, x_3)$, i.e.

$$\boldsymbol{p}(\boldsymbol{q}_{||}, x_3) = \sum_m C^m(\boldsymbol{q}_{||})\, \boldsymbol{p}(\boldsymbol{q}_{||}, m, x_3) \,, \tag{30}$$

where $C^m(\boldsymbol{q}_{||})$ has the meaning of the normalized coefficient that will be taken into consideration in the next section.

4. Electron–Phonon Interaction

Because the electron does not couple to TO phonons, we only consider the interaction of the electron with p-polarized SO and LO phonons in this section. However, in order to simplify the calculations, we assume the two different dielectric media to be filled in the half-space of $x_3 < 0$ and $x_3 > 0$ respectively, i.e. according to the geometry illustrated in Fig. 1, we take $a \to \infty$ and $b \to \infty$.

4.1 p-polarized SO phonon

If $\epsilon_n(\omega) \neq 0$ and $\chi_n^{-1}(\omega)\,\epsilon_n(\omega) \neq 0$, from (16a) and (16b) we have

$$\frac{\mathrm{d}^2}{\mathrm{d}x_3^2} p_{||}^j(\boldsymbol{q}_{||}, x_3) = q_{||}^2 p_{||}^j(\boldsymbol{q}_{||}, x_3)\,, \tag{31a}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}x_3^2} p_3^j(\boldsymbol{q}_{||}, x_3) = q_{||}^2 p_3^j(\boldsymbol{q}_{||}, x_3)\,. \tag{31b}$$

The solutions of both equations are

$$p_{||}^j(q_{||}, x_3) = iC_s^j[F_n^j\,\mathrm{e}^{q_{||}x_3} - G_n^j\,\mathrm{e}^{-q_{||}x_3}]\,, \tag{32a}$$

$$p_3^j(q_{||}, x_3) = C_s^j[F_n^j\,\mathrm{e}^{q_{||}x_3} + G_n^j\,\mathrm{e}^{-q_{||}x_3}]\,, \tag{32b}$$

where C_s^j is the normalized coefficient, the index $j = 1, 2, \ldots$ correspond to different eigenmodes, the symbol $n = 1$ or 2, $n = 1$ refers the half-space of $x_3 < 0$, $n = 2$ to that of $x_3 > 0$. Because the solutions must approach zero when $x_3 \to \infty$,

$$p_{||}^j(\boldsymbol{q}_{||}, x_3) = +iC_s^j F_1^j\,\mathrm{e}^{q_{||}x_3}\,, \quad p_3^j(\boldsymbol{q}_{||}, x_3) = C_s^j F_1^j\,\mathrm{e}^{q_{||}x_3}\,, \quad \text{when} \quad x_3 < 0\,, \tag{33a}$$

$$p_{||}^j(\boldsymbol{q}_{||}, x_3) = -iC_s^j G_2^j\,\mathrm{e}^{-q_{||}x_3}\,, \quad p_3^j(\boldsymbol{q}_{||}, x_3) = C_s^j G_2^j\,\mathrm{e}^{-q_{||}x_3}\,, \quad \text{when} \quad x_3 > 0\,. \tag{33b}$$

From the boundary conditions at $x_3 = 0$ and the condition for the existence of non-trivial solutions, we get

$$\epsilon_1(\omega_j) + \epsilon_2(\omega_j) = 0\,, \tag{34}$$

and the relation between F_1^j and G_2^j,

$$G_2^j = \frac{\epsilon_1(\omega_j)\,\chi_2(\omega_j)}{\epsilon_2(\omega_j)\,\chi_1(\omega_j)}\,F_1^j\,. \tag{35}$$

From the dispersion relations (34) and (14), the vibration frequencies are found to be

$$\omega_{s,\pm} = 2(\varepsilon_{\infty 1} + \varepsilon_{\infty 2})^{-1/2}\,[B_1 + B_2^{1/2}]^{1/2}\,, \tag{36a}$$

where

$$B_1 = \varepsilon_{\infty 1}(\omega_{\mathrm{L}1}^2 + \omega_{\mathrm{T}2}^2) + \varepsilon_{\infty 2}(\omega_{\mathrm{L}2}^2 + \omega_{\mathrm{T}1}^2)\,, \tag{36b}$$

$$B_2 = [\varepsilon_{\infty 1}(\omega_{\mathrm{L}1}^2 + \omega_{\mathrm{T}2}^2) + \varepsilon_{\infty 2}(\omega_{\mathrm{L}2}^2 + \omega_{\mathrm{T}1}^2)]^2 - 4(\varepsilon_{\infty 1} + \varepsilon_{\infty 2})\,(\varepsilon_{\infty 1}\omega_{\mathrm{L}1}^2\omega_{\mathrm{T}2}^2 + \varepsilon_{\infty 2}\omega_{\mathrm{L}2}^2\omega_{\mathrm{T}1}^2)\,. \tag{36c}$$

Substituting (33) into (18) and making use of (35), the normalized coefficient is obtained to be

$$C_s^j = \left\{\left[\frac{\theta_1(\omega_j)}{\omega_{\mathrm{p}1}^2} + \frac{\theta_2(\omega_j)\,\chi_2(\omega_j)}{\omega_{\mathrm{p}2}^2\chi_1(\omega_j)}\right](F_1^j)^2\right\}^{-1/2}\left(\frac{1}{L_3^0}\right)^{1/2}. \tag{37}$$

Because of $\nabla \cdot \boldsymbol{p}(\boldsymbol{x}) = \boldsymbol{0}$, the bulk polarization charges associated with these polarization eigenmodes disappear. However, the interface polarization charges are present between the two dielectric layers. They are

$$\sigma_s^{\mathrm{pol}(j)} = C_s^j [F_1^j - G_2^j] \,. \tag{38}$$

4.2 The interaction of the electron with p-polarized SO phonons

Assuming the electron to be located at $(\boldsymbol{x}_{||}^{\mathrm{e}}, x_3^{\mathrm{e}})$ of the half-space $x_3 > 0$, from (29) the potential function $V_j(\boldsymbol{q}_{||}, x_3^{\mathrm{e}})$ is given by

$$V_j(\boldsymbol{q}_{||}, x_3^{\mathrm{e}}) = \left(\frac{\hbar e^2}{8\varepsilon_0 A \omega_j}\right)^{1/2} \mathrm{e}^{-q_{||} x_3^{\mathrm{e}}} \frac{[\chi_1(\omega_j) + \chi_2(\omega_j)]\, q_{||}^{-1/2}}{\{\chi_1^2(\omega_j)\,[\theta_1(\omega_j)/\omega_{\mathrm{p}1}^2]\,\chi_2^2(\omega_j)\,[\theta_2(\omega_j)/\omega_{\mathrm{p}2}^2]\}^{1/2}} \,. \tag{39}$$

From the elementary relations (14) and (9b), we have

$$\chi_n^2(\omega_j)\,\frac{\theta_n(\omega_j)}{\omega_{\mathrm{p}n}^2} = \frac{(\varepsilon_{\infty n} + 2)^2\,(\epsilon_n - \varepsilon_{\infty n})^2\,\omega_{\mathrm{p}n}^2}{9\varepsilon_{\infty n}^2(\omega_{\mathrm{L}n}^2 - \omega_{\mathrm{T}n}^2)} = \frac{\varepsilon_{\infty n}(\omega_{\mathrm{L}n}^2 - \omega_{\mathrm{T}n}^2)}{(\omega_{\mathrm{T}n}^2 - \omega_j^2)^2} \,. \tag{40}$$

Substituting this result into (39) gives

$$V_j(\boldsymbol{q}_{||}, x_3^{\mathrm{e}}) = \left(\frac{\hbar e^2}{8\varepsilon_0 A \omega_j}\right)^{1/2} q_{||}^{-1/2}\, \mathrm{e}^{-q_{||} x_3^{\mathrm{e}}} \times$$

$$\times \frac{2(\omega_{\mathrm{T}1}^2 - \omega_j^2)\,(\omega_{\mathrm{T}2}^2 - \omega_j^2)}{\{\varepsilon_{\infty 1}(\omega_{\mathrm{L}1}^2 - \omega_{\mathrm{T}1}^2)\,(\omega_{\mathrm{T}2}^2 - \omega_j^2)^2 + \varepsilon_{\infty 2}(\omega_{\mathrm{L}2}^2 - \omega_{\mathrm{T}2}^2)\,(\omega_{\mathrm{T}1}^2 - \omega_j^2)^2\}^{1/2}} \,. \tag{41}$$

In order to more clearly gain an insight into the significance of this potential function, we take into account the dispersion relations of the dielectric layer. As calculated by Wendler for GaAs/GaP [6], the dielectric functions $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ of GaAs and GaP in the case of $\omega_{\mathrm{T}1} < \omega_{\mathrm{L}1} < \omega_{\mathrm{T}2} < \omega_{\mathrm{L}2}$ are given by Fig. 2. If we change one of the two materials or both, there is nothing to do but to displace the dispersion curves $\epsilon_2(\omega)$ relative to $\epsilon_1(\omega)$. Thus, if we gradually displace the dispersion curve $\epsilon_2(\omega)$ to the left relative to curve $\epsilon_1(\omega)$, we have the following cases:

1. $\omega_{\mathrm{L}2} > \omega_{\mathrm{T}2} < \omega_{\mathrm{L}1} > \omega_{\mathrm{T}1}$, $\quad \epsilon_1(\omega_+) > 0$, $\quad \epsilon_2(\omega_-) > 0$;
2. $\omega_{\mathrm{L}2} > \omega_{\mathrm{L}1} < \omega_{\mathrm{T}2} > \omega_{\mathrm{T}1}$, $\quad \epsilon_1(\omega_+) > 0$, $\quad \epsilon_2(\omega_-) > 0$;
3. $\omega_{\mathrm{L}2} > \omega_{\mathrm{L}1} < \omega_{\mathrm{T}1} > \omega_{\mathrm{T}2}$, $\quad \epsilon_1(\omega_+) > 0$, $\quad \epsilon_2(\omega_-) < 0$;
4. $\omega_{\mathrm{L}2} > \omega_{\mathrm{L}1} > \omega_{\mathrm{T}2} = \omega_{\mathrm{T}1}$, $\quad \epsilon_1(\omega) > 0$, $\quad$ only one solution;
5. $\omega_{\mathrm{L}2} = \omega_{\mathrm{L}1} > \omega_{\mathrm{T}2} > \omega_{\mathrm{T}1}$, $\quad \epsilon_2(\omega) > 0$, $\quad$ only one solution.

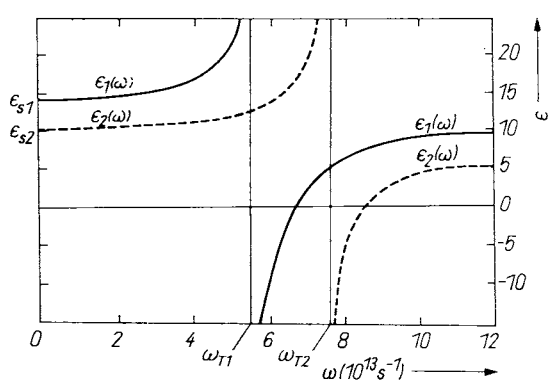

Fig. 2. The dielectric functions $\epsilon_1(\omega)$ (———) and $\epsilon_2(\omega)$ (– – –) of GaAs and GaP in the case $\omega_{\mathrm{T}1} < \omega_{\mathrm{L}2} < \omega_{\mathrm{T}2} < \omega_{\mathrm{L}2}$ (after [6])

Inversely, the cases $\omega_{L1} > \omega_{L2}$ are completely similar to the above ones, only the symbols 1 and 2 need to be interchanged. The cases 1 and 2 are identical, so we only need to consider case 1. For cases 3, 4, 5, there are also no essential differences from case 1. Their results can be obtained from that of case 1 through some simple procedures.

For case 1, the positions of $\omega_{s,\pm}$ on the ω-axis are $\omega_+ > \omega_{T2}$ and $\omega_{T1} < \omega_- < \omega_{T2}$, respectively. The dielectric function corresponding to the frequency ω_+ has the values $\epsilon_1(\omega_+) > 0$, $\epsilon_2(\omega_+) < 0$, but $\epsilon_1(\omega_+) < \varepsilon_{\infty 1}$. In this case, $V_j(\boldsymbol{q}_{||}, x_3)$ is rewritten as (denoted by V_+)

$$V_+(_{||}\boldsymbol{q}, x_3) = \left(\frac{\hbar e^2}{2\varepsilon_0 A\omega_+}\right)^{1/2} q_{||}^{-1/2}\, \mathrm{e}^{-q_{||}x_3^{\mathrm{e}}} \times \cdot$$

$$\times \frac{\varepsilon_{\infty 1}\varepsilon_{\infty 2}^{1/2}(\omega_{L2}^2 - \omega_{T2}^2)^{1/2}\,(\omega_{L1}^2 - \omega_{T1}^2)^{1/2}}{[\varepsilon_{\infty 2}(\epsilon_1 - \varepsilon_{\infty 1})^2\,(\omega_{L2}^2 - \omega_{T2}^2) + \varepsilon_{\infty 1}(\epsilon_2 - \varepsilon_{\infty 2})^2\,(\omega_{L1}^2 - \omega_{T1}^2)]^{1/2}}.$$

Because of $(\omega_{L2}^2 - \omega_{T2}^2) \approx (\omega_{L1}^2 - \omega_{T1}^2)$, the difference of $(\omega_{L2}^2 - \omega_{T2}^2)$ from $(\omega_{L1}^2 - \omega_{T1}^2)$ in the denominator can be neglected. Then, $V_+(\boldsymbol{q}, x_3)$ can be changed to

$$V_+(\boldsymbol{q}, x_3) = \left(\frac{\hbar e^2}{2\varepsilon_0 A}\right)^{1/2} \omega_+^{1/2} q_{||}^{-1/2}\, \mathrm{e}^{-q_{||}x_3^{\mathrm{e}}} \frac{\varepsilon_{\infty 1}\varepsilon_{\infty 2}^{1/2}(\omega_{L1}^2 - \omega_{T1}^2)^{1/2}}{\omega_+^{1/2}[\varepsilon_{\infty 2}(\epsilon_1 - \varepsilon_{\infty 1})^2 + \varepsilon_{\infty 1}(\epsilon_1 + \varepsilon_{\infty 2})^2]^{1/2}}.$$

Because of $(\epsilon_1 + \varepsilon_{\infty 2})^2 \gg (\epsilon_1 - \varepsilon_{\infty 1})^2$, the term $(\epsilon_1 - \varepsilon_{\infty 1})^2$ containing in the denominator of the above expression can be neglected. According to the dispersion relation (14), ω_+ can also be expressed as $(\varepsilon_{\infty 1} - \epsilon_1)^{-1/2}\,(\varepsilon_{\infty 1}\omega_{L1}^2 - \epsilon_1\,\omega_{T1}^2)^{1/2}$, thus $V_+(\boldsymbol{q}_{||}, x_3)$ can be rewritten as

$$V_+(\boldsymbol{q}_{||}, x_3) = \left(\frac{\hbar e^2}{2\varepsilon_0 A q_{||}}\right)^{1/2} \omega_+^{1/2}\, \mathrm{e}^{-q_{||}x_3^{\mathrm{e}}} \frac{[\varepsilon_{\infty 2}(\varepsilon_{\infty 1} + \varepsilon_{\infty 2})\,(\omega_{L1}^2 - \omega_{T1}^2)]^{1/2}}{[(\epsilon_1 + \varepsilon_{\infty 2})\,(\varepsilon_{\infty 1}\omega_{L1}^2 - \epsilon_1\omega_{T1}^2)]^{1/2}} \times$$

$$\times \left[\frac{\varepsilon_{\infty 1} - \epsilon_1}{(\epsilon_1 + \varepsilon_{\infty 2})\,(\varepsilon_{\infty 1} + \varepsilon_{\infty 2})}\right]^{1/2}. \tag{42}$$

For this case, in spite of $\epsilon_1(\omega_+) < \varepsilon_{\infty 1} < \epsilon_{s1}$ (the symbol s refers the static dielectric constant), we may suitably take $\epsilon_1(\omega_+) \approx \epsilon_{s1}$ or $\epsilon_1(\omega_+) \approx \varepsilon_{\infty 1}$. Then, (42) can be interpreted as the potential function of the interaction between the electron and the phonon with effective frequency

$$\omega_{\mathrm{eff},+}^{\mathrm{SO}} = \omega_+ \frac{\varepsilon_{\infty 2}(\varepsilon_{\infty 1} + \varepsilon_{\infty 2})\,(\omega_{L1}^2 - \omega_{T1}^2)}{(\epsilon_1 + \varepsilon_{\infty 2})\,(\varepsilon_{\infty 1}\omega_{L1}^2 - \epsilon_1\omega_{T1}^2)} \approx \frac{\varepsilon_{\infty 2}}{\varepsilon_{\infty 1}}\omega_+ . \tag{43}$$

Because $(\varepsilon_{\infty 1} - \epsilon_1)$ can approximately be substituted by $-(\epsilon_{s1} - \varepsilon_{\infty 1})$, if the Fröhlich-like coupling constant α_+^{SO} characterizing the strength of the interaction is defined as

$$\alpha_+^{\mathrm{SO}} = \frac{e^2\beta_s}{2\hbar\omega_{\mathrm{eff},+}^{\mathrm{SO}}}\left[\frac{1}{\varepsilon_{\infty 1} + \varepsilon_{\infty 2}} - \frac{1}{\epsilon_{s1} + \varepsilon_{\infty 2}}\right], \qquad \beta_s = \left(\frac{2m^*\omega_{\mathrm{eff},+}^{\mathrm{SO}}}{\hbar}\right)^{1/2}, \tag{44}$$

where m^* is the band mass of the electron, the interaction energy between the electron and SO phonon with the frequency ω^+ can be expressed as

$$H_{\mathrm{eff},+}^{\mathrm{SO}} = \sum_{\boldsymbol{q}_{||}} V_+(\boldsymbol{q}_{||})\, \mathrm{e}^{i\boldsymbol{q}_{||}\cdot\boldsymbol{x}_{||}^{\mathrm{e}} - q_{||}x_3^{\mathrm{e}}}\,[\hat{b}_+^+(-\boldsymbol{q}_{||}) + \hat{b}_+(\boldsymbol{q}_{||})]\,,$$
$$V_+(\boldsymbol{q}_{||}) = i\left[\frac{\alpha_+^{\mathrm{SO}}(\hbar\omega_{\mathrm{eff},+}^{\mathrm{SO}})}{\varepsilon_0 A q_{||}\beta_s}\right]^{1/2}. \tag{45}$$

Analogously, for the case of $\omega_{T1} < \omega_- < \omega_{T2}$, the dielectric functions corresponding to ω_- have the values $\epsilon_2(\omega_-) > 0$, but $\epsilon_2(\omega_-) > \epsilon_{s2} > \varepsilon_{\infty 2}$. Then, by use of the same procedures as the derivation of $V_+(\boldsymbol{q}_{||}, x_3^e)$, we easily get

$$V_-(\boldsymbol{q}_{||}, x_3^e) = \left(\frac{\hbar e^2}{2\varepsilon_0 A q_{||}}\right)^{1/2} e^{-q_{||}x_3^e} \omega_-^{1/2} \left[\frac{\varepsilon_{\infty 1}(\varepsilon_{\infty 1} + \varepsilon_{\infty 2})\,(\omega_{L2}^2 - \omega_{T2}^2)}{(\epsilon_2 + \varepsilon_{\infty 1})\,(\epsilon_2 \omega_{T2}^2 - \varepsilon_{\infty 2}\omega_{L2}^2)}\right]^{1/2} \times$$
$$\times \left[\frac{\epsilon_2 - \varepsilon_{\infty 2}}{(\varepsilon_{\infty 1} + \varepsilon_{\infty 2})\,(\epsilon_2 + \varepsilon_{\infty 1})}\right]^{1/2}. \tag{46}$$

Similar to the situation of ω_+, the above expression may also be regarded as the potential function of the interaction between the electron and the phonon with effective frequency

$$\omega_{\text{eff},-}^{SO} = \omega_- \frac{\varepsilon_{\infty 1}(\varepsilon_{\infty 1} + \varepsilon_{\infty 2})\,(\omega_{L2}^2 - \omega_{T2}^2)}{(\epsilon_2 + \varepsilon_{\infty 1})\,(\epsilon_2 \omega_{T2}^2 - \varepsilon_{\infty 2}\omega_{L2}^2)} \approx \frac{\varepsilon_{\infty 1}}{\varepsilon_{\infty 2}} \omega_- . \tag{47}$$

If the Fröhlich-like coupling constant α_-^{SO} is defined as

$$\alpha_-^{SO} = \frac{e^2 \beta_s}{2\hbar \omega_{\text{eff},+}^{SO}} \left[\frac{1}{\varepsilon_{\infty 1} + \varepsilon_{\infty 2}} - \frac{1}{\epsilon_2 + \varepsilon_{\infty 1}}\right], \qquad \beta_s = \left(\frac{2m^* \omega_{\text{eff},-}^{SO}}{\hbar}\right)^{1/2}, \tag{48}$$

the interaction energy between the electron and SO phonon with the frequency ω_- can be expressed as

$$H_{\text{eff},-}^{SO} = \sum_{\boldsymbol{q}_{||}} V_-(\boldsymbol{q})\, e^{i\boldsymbol{q}_{||}x_{||}^e - \boldsymbol{q}_{||}x_3^e} [\hat{b}_-^+(-\boldsymbol{q}_{||}) + \hat{b}_-(\boldsymbol{q}_{||})], \tag{49}$$

where

$$V_-(q) = i\left[\frac{\alpha_-^{SO}(\hbar\omega_{\text{eff},-}^{SO})}{A q_{||} \beta_s}\right]^{1/2}, \qquad \beta_s = \left(\frac{2m^* \omega_{\text{eff},-}^{SO}}{\hbar}\right)^{1/2}. \tag{50}$$

It is important to note that $\omega_{\text{eff},\pm}^{SO}$ may be negative value because the dominator in this expression may become negative in some case. If it is the case, the denominator in $\omega_{\text{eff},\pm}^{SO}$ should take the absolute value, and $V_\pm(\boldsymbol{q})$ does not contain imaginary spin. For cases 3, 4, 5, the results are similar with that above, here we do not repeat the calculations for saving space.

4.3 p-polarized LO phonon

When $\epsilon_n(\omega) = 0$, but $\epsilon_t(\omega) \neq 0$ $(t \neq n)$, from (14) we have $\omega_n = \omega_{Ln}$. This phonon with the vibration frequency ω_{Ln} is called p-polarized LO phonon. In this case, from (16) the equation of the polarization eigenmodes for the layer n is

$$\frac{d}{dx_3} p_{n,||}^m(\boldsymbol{q}_{||}, x_3) = i q_{||} p_{n,3}^m(\boldsymbol{q}_{||}, x_3), \tag{51}$$

for the layer t

$$\frac{d^2}{dx_3^2} p_{t,||}(\boldsymbol{q}_{||}, x_3) = q^2 p_{t,||}(\boldsymbol{q}_{||}, x_3). \tag{52}$$

The solution of the latter is still given by (33). However, the boundary condition at $x_3 = 0$ gives $\boldsymbol{p}_t$, $\boldsymbol{E}_t$, and $\boldsymbol{D}_t$ all to be zero. Inside the layer n, when the length of this layer in x_3-direction is L_3, the solution of (51) is

$$\boldsymbol{p}_n^m(q', x_3) = C_n^m(q)\left[\boldsymbol{e}_{||} i \sin\left(\frac{m\pi}{L_3} x_3\right) + \boldsymbol{e}_3 \frac{(m\pi/L_3)}{q_{||}} \cos\left(\frac{m}{L_3} x_3\right)\right]. \tag{53}$$

Substituting this solution into the left-hand side of (18) gives

$$\sum_m \frac{\theta_n(\omega_{Ln})}{\omega_{pn}^2} (C_{Ln}^m)^2 \left(\frac{L_3}{2}\right) \frac{q_{||}^2 + (m\pi/L_3)^2}{q_{||}^2} . \tag{54}$$

According to the orthonormalized expression (18), after summing up the above expression over m, it ought to equal $(L_3^0 q_{||})^{-1}$. Since L_3 is large, the summation may be substituted by the integral. The integrand is just the normalization value which we wish to find. Evidently, if the integrand is taken in the following form:

$$\frac{2}{L_3^0}\left[q_{||}^2 + \left(\frac{m\pi}{L_3}\right)^2\right]^{-1}, \tag{55}$$

after integrating with respect to m the result is just $(L_3^0 q_{||})^{-1}$. Then,

$$C_{L,n}^m(\boldsymbol{q}_{||}) = \frac{\omega_{pn}}{\theta_n^{1/2}(\omega_{Ln})} \frac{2q_{||}}{(L_3 L_3^0)^{1/2}} \left[q_{||}^2 + \left(\frac{m\pi}{L_3}\right)^2\right]^{-1} . \tag{56}$$

However, when L_3 is not large, the summation with respect to m cannot be changed to the integral. For this case, (55) may be understood as the general term of a summable series. Thus, (55) is also the desired expression corresponding to m.

Assuming $n = 1$ refers to the half-space $x_3 < 0$, and because of $\nabla \cdot \boldsymbol{p}(\boldsymbol{x}) \neq \boldsymbol{0}$ for this case, there exist the bulk polarization charges

$$\varrho_{L,1}^{m,\mathrm{pol}} = C_{L,1}\left[q_{||} + \frac{(m\pi/L_3)^2}{q_{||}}\right] \sin\left(\frac{m\pi}{L_3} x_3\right) \tag{57}$$

and the surface polarization charges

$$\sigma_{L,1}^{m,\mathrm{pol}} = C_{L,1}^m q_{||}^{-1} \left(\frac{m\pi}{L_3}\right) \quad \text{at} \quad x_3 = 0 , \tag{58a}$$

$$\sigma_{L,1}^{m,\mathrm{pol}} = -(-1)^m C_{L,1}^m q_{||}^{-1} \left(\frac{m\pi}{L_3}\right) \quad \text{at} \quad x_3 = -b , \tag{58b}$$

if the thickness of the dielectric layer is b.

Inversely, if n refers to the half-space $x_3 > 0$, i.e. $n = 2$, (57) is still hold only with the change of symbol 1 to 2, L_3 change to L_3' corresponding the thickness of the dielectric layer 2. On the corresponding boundary the surface polarization charges are

$$\sigma_{L,2}^{m,\mathrm{pol}} = -C_{L,2}^m q_{||}^{-1} \left(\frac{m\pi}{L_3'}\right) \quad \text{at} \quad x_3 = 0 , \tag{59a}$$

$$\sigma_{L,2}^{m,\mathrm{pol}} = (-1)^m C_{L,2}^m q_{||}^{-1} \left(\frac{m\pi}{L_3'}\right) \quad \text{at} \quad x_3 = a . \tag{59b}$$

4.4 The interaction of the electron with p-polarized LO phonons

Assuming the electron to be located at $\boldsymbol{x}^e$ of the dielectric 2 ($x_3 > 0$ half-space), substituting (53) into (29) and taking into consideration that the factor $(L_3^0 q_{||})^{1/2}$ in this expression should be substituted by $(L_3^0/2)^{1/2}\,[q_{||}^2 + (m\pi/L_3)^2]^{1/2}$, the potential function

of the interaction between the electron and the LO phonon of the dielectric medium 1 is

$$V_{\mathrm{L},1}(\boldsymbol{q}_{||}, x_3) = \left(\frac{\hbar e^2}{8\varepsilon_0 A\omega_{\mathrm{L}1}}\right)^{1/2} C^m_{\mathrm{L},1}\, \mathrm{e}^{-q_{||}x_3^{\mathrm{e}}} \left(\frac{L_3}{2}\right)^{1/2} \left(\frac{m\pi}{L_3}\right) \frac{[q_{||}^2 + (m\pi/L_3)^2]^{1/2}}{q_{||}^2} \times$$
$$\times [1 - (-1)^m\, \mathrm{e}^{-q_{||}b}] + \left(\frac{\hbar e^2}{8\varepsilon_0 A\omega_{\mathrm{L}1}}\right)^{1/2} C^m_{\mathrm{L}1}\, \mathrm{e}^{-q_{||}x_3^{\mathrm{e}}} \times$$
$$\times \left(\frac{L_3^0}{2}\right)^{1/2} \frac{[q_{||}^2 + (m\pi/L_3)^2]^{3/2}}{q_{||}^2} \int_{-b}^{0} \mathrm{e}^{q_{||}x_3} \sin\left(\frac{m\pi}{L_3} x_3\right) \mathrm{d}x_3 = 0\,.$$

Analogously, the potential function of the interaction between the electron and the LO phonon of the dielectric 2 (in which the electron is located) is

$$V_{\mathrm{L},2}(\boldsymbol{q}, x_3) = \left(\frac{\hbar e^2}{8\varepsilon_0 A\omega_{\mathrm{L}2}}\right)^{1/2} C^m_{\mathrm{L},2} \left(\frac{L_3^0}{2}\right)^{1/2} \left(\frac{m\pi}{L_3}\right) \frac{[q_{||}^2 + (m\pi/L_3)^2]^{1/2}}{q_{||}^2} \times$$
$$\times [-\mathrm{e}^{-q_{||}x_3} + (-1)^m\, \mathrm{e}^{-q_{||}(a-x_3)}] + \left(\frac{\hbar e^2}{8\varepsilon_0 A\omega_{\mathrm{L}2}}\right)^{1/2} C^m_{\mathrm{L},2} \left(\frac{L_3^0}{2}\right)^{1/2} \times$$
$$\times \frac{[q_{||}^2 + (m\pi/L_3)^2]^{3/2}}{q_{||}^2}\, \mathrm{e}^{-q_{||}x_3^{\mathrm{e}}} \int \mathrm{e}^{q_{||}x_3} \sin\left(\frac{m\pi}{L} x_3\right) \mathrm{d}x_3 +$$
$$+ \left(\frac{\hbar e^2}{8\varepsilon_0 A\omega_{\mathrm{L}2}}\right)^{1/2} C^m_{\mathrm{L},2} \left(\frac{L_3^0}{2}\right)^{1/2} \frac{[q_{||}^2 + (m\pi/L_3)^2]^{3/2}}{q_{||}^2} \times$$
$$\times\, \mathrm{e}^{q_{||}x_3^{\mathrm{e}}} \int \mathrm{e}^{-q_{||}x_3} \sin\left(\frac{m\pi}{L_3} x_3\right) \mathrm{d}x_3 = \left(\frac{\hbar e^2}{2\varepsilon_0 A\omega_{\mathrm{L}1}}\right)^{1/2} \left(\frac{\omega_{\mathrm{p}2}}{\theta_2^{1/2}}\right) \times$$
$$\times \frac{1}{[q_{||}^2 + (m\pi/L_3)^2]^{1/2}} \sin\left(\frac{m\pi}{L} x_3^{\mathrm{e}}\right). \tag{60}$$

This result shows that the electron interacts only with LO phonons of the dielectric layer in which the electron is located, and this interaction is weakened by the surface effects. According to the basic relations (9 b) and (14), and making use of the Lyddane-Sachs-Teller relation, we have

$$\frac{\omega_{\mathrm{p}n}}{\theta_{n'}^{1/2}} = \frac{1}{\varepsilon_{\infty n}} \omega_{\mathrm{LO}} \left[1 - \left(\frac{\omega_{\mathrm{TO}}}{\omega_{\mathrm{LO}}}\right)^2\right]^{1/2} = \omega_{\mathrm{LO}} \left(\frac{\epsilon_{\mathrm{s}n} - \varepsilon_{\infty n}}{\epsilon_{\mathrm{s}n}\varepsilon_{\infty n}}\right)^{1/2}.$$

Substituting this result into (60) gives

$$V_{\mathrm{LO}}(\boldsymbol{q}, x_3^{\mathrm{e}}) = \left(\frac{\hbar e^2}{2\varepsilon_0 A}\right)^{1/2} \omega_{\mathrm{LO}}^{1/2} \left(\frac{\epsilon_{\mathrm{s}} - \varepsilon_\infty}{\epsilon_{\mathrm{s}}\varepsilon_\infty}\right)^{1/2} \frac{1}{[q_{||}^2 + (m\pi/L_3)^2]^{1/2}} \sin\left(\frac{m\pi}{L_3} x_3^{\mathrm{e}}\right). \tag{61}$$

Thus, the Hamiltonian of the interaction between electron and LO phonon is

$$H_{\mathrm{ep,LO}} = \sum_{\boldsymbol{q}_{||}} \sum_m V_{\mathrm{LO}}(\boldsymbol{q}_{||}, m)\, \mathrm{e}^{i\boldsymbol{q}_{||}\cdot\boldsymbol{x}_{||}^{\mathrm{e}}} \sin\left(\frac{m\pi}{L_3} x_3\right) [b_m^+(-\boldsymbol{q}_{||}) + b_m(\boldsymbol{q}_{||})]\,, \tag{62}$$

where

$$V_{\mathrm{LO}}(\boldsymbol{q}_{||}, m) = \left(\frac{\hbar e^2}{2\varepsilon_0 A}\right)^{1/2} \omega_{\mathrm{LO}}^{1/2} \left(\frac{\epsilon_{\mathrm{s}} - \varepsilon_\infty}{\epsilon_{\mathrm{s}}\varepsilon_\infty}\right)^{1/2} \frac{1}{[q_{||}^2 + (m\pi/L_3)^2]^{1/2}}. \tag{63}$$

For a very thick slab $H_{\mathrm{ep,LO}}$ becomes

$$H_{\mathrm{ep,LO}} = \sum_{\boldsymbol{q}_{||}} \sum_{q_3 > 0} \mathrm{e}^{i\boldsymbol{q}_{||}\cdot\boldsymbol{x}_{||}^{\mathrm{e}}} \sin(q_3 x_3^{\mathrm{e}})\, V_{\mathrm{LO}}(\boldsymbol{q}_{||}, q_3)\, [b^+(\boldsymbol{q}_{||}, q_3) + b(\boldsymbol{q}_{||}, q_3)]\,, \tag{64}$$

where

$$V_{\mathrm{LO}}(\boldsymbol{q}_{\|}, q_3) = \left(\frac{\hbar e^2}{2\varepsilon_0 A}\right)^{1/2} [q_{\|}^2 + q_3^2]^{-1/2} \omega_{\mathrm{LO}}^{1/2} \left(\frac{\epsilon_s - \varepsilon_\infty}{\epsilon_s \varepsilon_\infty}\right)^{1/2}. \tag{65}$$

From the results of this section one can see that, making use of the new orthonormalized relation (18), the Hamiltonian of the interaction between electron and SO, LO phonon are identically with that obtained by Wendler [6]; however, the values of the bulk and surface polarization charges obtained here are very different.

5. Discussion

According to the results obtained above, in a dielectric bilayer system the Hamiltonian of charged particle and phonon including their interaction can be written as

$$\begin{aligned} H = & -\frac{\hbar^2}{2m^*}\nabla^2 + \sum_j \sum_{\boldsymbol{q}_{\|}} \hbar\omega_j^{\mathrm{SO}} b_j^+(\boldsymbol{q}_{\|})\, b_j(\boldsymbol{q}_{\|}) + \sum_j \sum_{\boldsymbol{q}} \hbar\omega_{\mathrm{LO}} b_j^+(\boldsymbol{q}_{\|})\, b_j(\boldsymbol{q}_{\|}) + \\ & + \sum_j \sum_{\boldsymbol{q}} V_j(\boldsymbol{q}_{\|})\, \mathrm{e}^{i\boldsymbol{q}_{\|}\cdot\boldsymbol{x}_{\|}^{\mathrm{e}} - q_{\|}x_3^{\mathrm{e}}} [b_j^+(-\boldsymbol{q}_{\|}) + b_j(\boldsymbol{q}_{\|})] + \\ & + \sum_{\boldsymbol{q}} \sum_m V_{\mathrm{LO}}(\boldsymbol{q}_{\|}, m)\, \mathrm{e}^{i\boldsymbol{q}_{\|}\cdot\boldsymbol{x}_{\|}^{\mathrm{e}}} \sin\left(\frac{m\pi}{L_3} x_3^{\mathrm{e}}\right) [b_m^+(-\boldsymbol{q}_{\|}) + b_m(\boldsymbol{q}_{\|})], \end{aligned} \tag{66}$$

where the first term is the electron kinetic energy, the second and third terms are the energies of the surface and bulk phonon (SO and LO) field, respectively, the last two terms come from the interaction of the electron with SO and LO phonons, respectively. In this Hamiltonian, $j = 1, 2, 3, 4$. They refer to four different SO phonon modes, respectively. According to the geometry of the bilayer illustrated in Fig. 1, if the surface phonon modes near $x_3 = a$ is denoted by $j = 1$, near $x_3 = -b$ by $j = 2$, and the interface phonon modes near $x_3 = 0$ by $j = 3, 4$, this form of the Hamiltonian is also suitable for a single dielectric layer.

The interaction energies of the electron with SO and LO phonons all are negative. Thus, there always exist tendencies of attracting the charged particles towards the interface for any two media being in contact with each other. (For a single dielectric layer, the interface should be explained as the contact surface with another nonpolar material, e.g., vacuum). In fact, as well known from electrostatics, when the distance of the charged particle from the interface is x_3^{e}, always an image potential is present which is proportional to $(\varepsilon_{\infty 1} - \varepsilon_{\infty 2})$. This potential has the positive value when $\varepsilon_{\infty 1} > \varepsilon_{\infty 2}$ and negative when $\varepsilon_{\infty 2} > \varepsilon_{\infty 1}$. From the theoretical viewpoint, the image potential undoubtedly comes from the interaction between electron and surface phonon. However, the interaction energy having the properties of the image potential cannot be obtained from the electron–SO phonon interaction. Thus, there are some confusions for the use of the image potential. For example, in the discussion of the charged-particle behavior near the interface, the author and Beril et al. explicitly took into account the effect of the image potential [8, 9], some other authors did not take it into consideration [10, 11]. In the calculation of the extra interaction between the solid and a charge Q outside, some authors pointed out that the surface modes are solely responsible for the image potential [2, 12]. The author believes that the image potential comes from the electron–SO phonon interaction; but the interface between two media cannot be regarded as ideal, i.e. the interface is not precipitous. In fact, there exists a transition layer between two media. The dielectric properties of this transition layer are, in average, different from that of the media on both sides of the transition layer. Thus, it is as if two interfaces were present: one is the exterior interface, the other the interior interface. If assuming the electron to be located in the