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Cyclotron resonance of a polaron in a realistic heterojunction and its pressure effect

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Abstract. The Larsen perturbation method is adopted to study the influence of magnetic fields on polarons in realistic heterojunctions in a quasi-two-dimension approximation. The interaction between an electron and both the bulk longitudinal optical phonons and the two branches of interface optical phonons is taken into account to show the influence of magnetic fields at different ranges on the polaron cyclotron mass due to the coupling of the electron with each branch of phonon modes. The result indicates that not only do the bulk phonons influence the polaron cyclotron mass, but the interface phonons do as well. The pressure effect on the cyclotron mass is also discussed.

PACS. 71.38.Fp Large or Frohlich polarons – 73.20.-r Electron states at surfaces and interfaces – 73.40.Kp III-V semiconductor-to-semiconductor contacts – 62.50.+p High-pressure and shock wave effects in solids and liquids (for high pressure apparatus and techniques)

1 Introduction

Since the sixties of last century, some authors have studied the surface phonon modes [1,2] and surface polarons [3,4] to indicate that the properties of phonon modes and polarons in a quasi-2D system are obviously different from that in three-dimension bulk materials. The fast development of man-made layered semiconductors gave a strong impetus in study of the properties of polarons in heterostructures, such as heterojunctions and quantum wells (QWs), both theoretically and experimentally. Some authors [5–7] adopted an approximation about the interaction between an electron and 2D bulk longitudinal optical (LO) phonons to simplify the complicated electron-phonon interaction. But these works over exaggerated the influences of bulk LO phonons due to the dimensional effect of polarons. Some authors derived the electron-optical-phonon interaction in heterostructures [8] and QWs [9], respectively. Chen et al. [10] studied the interface polarons in heterojunctions consisting of polar and non-polar crystals under magnetic fields of arbitrary strength. Gu et al. [11,12] discussed the ground states and cyclotron resonance of interface magnetopolarons in heterojunctions by considering the effect of bulk LO phonons and a single branch of effective interface optical (IO) phonons. However, the effect of IO phonons is weakened since only an image potential, which has been proved to be neglectable later on, was considered to restrict the electron near the interface. They ignored a more important restriction effect of energy band bending. Ban et al. [13,14] pointed out that the single branch approximation of IO phonons should be improved and a detailed structure of IO phonons should be considered for heterojunctions. In an early paper, Hai et al. [15] investigated the cyclotron resonance of polarons in QWs taking into account the electron-phonon interaction for all specific phonon modes.

Up to now, there are lots of experimental and theoretical works studying the basic properties of bulk material and low dimensional semiconductors under pressure [16–20], such as the effect of pressure on crystal constants, dielectric constants and effective electronic masses, etc. In literatures, Murnaghan equation [21] was commonly used to describe crystal constants under pressure. On the other hand, a variety of static dielectric constant is determined by the ionizabilities of materials. As usual, the ionizability of a covalent crystal is less and its static dielectric constant reduces as pressure increases. Contrarily, the ionizability of an ionic crystal is bigger and its static dielectric constant increases as pressure increases. Unfortunately, GaAs is an exception to this rule. The band masses of electrons and holes under pressure can be obtained by the relation between band gap and pressure [22]. Sukumar et al. [23] firstly adopted a perturbation method to study the binding energies of excitons in quantum wells under pressure without electron-phonon interaction. Guo [24] and Zhao et al. [20] also discussed the pressure effect of the binding energies by considering this interaction. The result indicates that both the phonon effect and pressure effect are remarkable. However, so far as we know that there is still a lack of works on cyclotron

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resonance of polarons in such a kind of heterostructures under pressure.

Under consideration of a realistic interface potential [25] in this paper, an improved perturbation method proposed by Larsen et al. [26] is adopted to study polarons in semiconductor heterojunctions in magnetic fields taking into account of the interaction between an electron and both the bulk LO and the two branches of IO phonons. The relation of polaronic properties dependent on the external magnetic fields is obtained by discussing the transition energies between the ground state and first excited state of Landau levels for a polaron. The polaron cyclotron mass (PCM) and pressure effect are studied for weak, strong and resonant magnetic fields, respectively. The numerical results for semiconductor heterojunctions consisting of III–V group show that the contribution from IO phonons with higher frequency can not be neglected in weak field limit, although the bulk LO phonons are more important to influence the PCM. As increase of a magnetic field, the contribution from the two branches of IO phonons tends to be comparable with that from the bulk LO phonons. It becomes more and more important that the contribution to the PCM from the two branches of IO phonons as the magnetic field increases under pressure of 40 kbar. At the same time, both of the contributions from bulk LO and IO phonons are important. The properties of the contributions to the PCM from different branches of phonons varying with strong magnetic fields and their pressure effect are the same and negative with that for weak magnetic fields. The pressure effect of LO and IO phonons on the PCM are important when the cyclotron resonance happens near the frequencies of different branches of phonons. The detailed IO phonon modes should be considered in the future work especially when ones study the pressure effects of cyclotron resonance of polarons.

2 Hamiltonian and perturbation calculation

Let us suppose a heterojunction (GaAs/AlAs) consisting of two semi-infinite polar semiconductors labeled 1 and 2, respectively, with an electron moving inside 1 near the interface ($x-y$ plane). A static uniform magnetic field with a symmetrical gauge transformation $B=(0,0,B_M)$ is applied perpendicular to the interface (z direction). The system of the electron, LO and IO phonons can be described by the following Hamiltonian

$$H = H_\perp + H_{||}, \tag{1a}$$

where,

$$H_\perp = \frac{P_z^2}{2m} + V_r(z), \tag{1b}$$

$$H_{||} = H_0 + H_{e-p}. \tag{1c}$$

Here, the first term of equation (1b) is the kinetic energy of electron in the z direction and the second term is the heterojunction potential [25]. The Hamiltonian without electron-phonon interaction in equation (1c) is [10,26]

$$H_0 = (P_x - \tilde{\beta}^2 y/4)^2/2m + (P_x + \tilde{\beta}^2 x/4)^2/2m + \sum_k \hbar\omega_{LO} a_k^+ a_k + \sum_{q,\xi} \hbar\omega_{IO\xi} b_{q,\xi}^+ b_{q,\xi}. \tag{1d}$$

In the above equation, $\vec{P}=(P_x,P_y,P_z)$ is the electronic momentum, $\tilde{\beta}^2 = 2eB_M/c$ ($c$is velocity of light), ω_{LO} and $\omega_{IO\xi}$ are the frequencies of bulk LO phonons and the ξ'th ($\xi=\pm$) branch of IO phonons. $a_k^+(a_k)$ is the creation (annihilation) operator of bulk LO phonons with wave vector $\vec{k}=(\vec{k}_{||},k_z)$ and $b_{q,\xi}^+(b_{q,\xi})$ the corresponding operators of the ξ'th branch of IO phonons with two-dimension wave vector $\vec{q}$. Here, the effective mass of an electron is chosen as that in material 1 to simplify the calculation since the probability of the electron penetrating into material 2 is small [25].

The Hamiltonian of interaction between an electron and LO, IO phonons in equation (1c) is written as [25]

$$H_{e-p} = H_{e-LO} + H_{e-IO}, \tag{1e}$$

where

$$H_{e-LO} = \sum_k [V_k^* \sin(zk_z)\exp(-i\vec{\rho}\cdot\vec{k}_{||})a_k^+ + H.C.], \tag{1f}$$

and

$$H_{e-IO} = \sum_{q,\xi} [C_{q,\xi}^* e^{-qz}\exp(-i\vec{\rho}\cdot\vec{q})b_{q,\xi}^+ + H.C.]. \tag{1g}$$

Here $\vec{r}=(\vec{\rho},z)$ is the electronic position vector. In (1f),

$$V_k^* = \frac{i}{k}\left[\frac{4\pi e^2}{\varepsilon V}\hbar\omega_{LO}\right]^{1/2}, \tag{2a}$$

and

$$C_{q,\xi}^* = i\left[\frac{\pi e^2}{q\varepsilon^* S}\hbar\omega_{IO\xi}\right]^{1/2}, \tag{2b}$$

in which, V is the volume of material 1 and S is the area of the interface. In addition,

$$\frac{1}{\varepsilon} = \frac{1}{\varepsilon_{\infty 1}} - \frac{1}{\varepsilon_{01}}, \tag{2c}$$

and

$$\frac{1}{\varepsilon^*} = \frac{2}{\varepsilon_{\infty 1}+\varepsilon_{\infty 2}} - \frac{2}{\varepsilon_{01}+\varepsilon_{02}}, \tag{2d}$$

where, $\varepsilon_{0i}(\varepsilon_{\infty i}, i=1,2)$ is the static (high) frequency dielectric constant of material i.

The ξ'th branch of IO phonons modes with frequency $\omega_{IO\xi}$ can be obtained by

$$\omega_{IO\pm}^2 = \frac{b \pm \sqrt{b^2-4ac}}{2a}, \tag{2e}$$

with

$$a = \varepsilon_{\infty 1}+\varepsilon_{\infty 2},$$
$$b = \varepsilon_{\infty 1}(\omega_{L1}^2+\omega_{T2}^2)+\varepsilon_{\infty 2}(\omega_{L2}^2+\omega_{T1}^2),$$
$$c = \varepsilon_{\infty 1}\omega_{L1}^2\omega_{T2}^2+\varepsilon_{\infty 2}\omega_{L2}^2\omega_{T1}^2,$$

where ω_{Ti} and ω_{Li} are the frequencies of transverse optical and bulk LO phonons, respectively.

We introduce one-dimensional harmonic oscillator operators [10,26]

$$A = \frac{1}{\sqrt{\hbar}\tilde{\beta}}\left[\left(P_x - \tilde{\beta}^2\frac{y}{4}\right) - i\left(P_y + \tilde{\beta}^2\frac{x}{4}\right)\right], \tag{3a}$$

and

$$B = A^+ - i\frac{\tilde{\beta}}{2\sqrt{\hbar}}(x+iy), \tag{3b}$$

which satisfy the following commutation relations

$$[A, A^+] = [B, B^+] = 1, [A, B] = [A, B^+] = 0. \tag{3c}$$

Inserting (3a) into (1d), one obtains

$$H_0 = \frac{\hbar\tilde{\beta}^2}{2m}(AA^+ + 1/2) + \sum_k \hbar\omega_{LO}a_k^+ a_l + \sum_{q\xi}\hbar\omega_{IO\xi}b_{q\xi}^+ b_{q\xi}, \tag{4a}$$

$$H_{e-LO} = \sum_k (V_k^* L_k M_k a_k^+ + H.c.), \tag{4b}$$

and

$$H_{e-IO} = \sum_{q\xi}(C_{q,\xi}^* L_q M_q b_q^+ + H.c.), \tag{4c}$$

where

$$L_k = \exp\left[\frac{\sqrt{\hbar}}{\tilde{\beta}}(k_x + ik_y)A - \frac{\sqrt{\hbar}}{\tilde{\beta}}(k_x - ik_y)A^+\right], \tag{4d}$$

$$M_k = \exp\left[\frac{\sqrt{\hbar}}{\tilde{\beta}}(k_x - ik_y)B - \frac{\sqrt{\hbar}}{\tilde{\beta}}(k_x + ik_y)B^+\right], \tag{4e}$$

$$L_q = \exp\left[\frac{\sqrt{\hbar}}{\tilde{\beta}}(q_x + iq_y)A - \frac{\sqrt{\hbar}}{\tilde{\beta}}(q_x - iq_y)A^+\right], \tag{4f}$$

and

$$M_q = \exp\left[\frac{\sqrt{\hbar}}{\tilde{\beta}}(q_x - iq_y)B - \frac{\sqrt{\hbar}}{\tilde{\beta}}(q_x + iq_y)B^+\right]. \tag{4g}$$

A quasi-adiabatic approximation [10] is adopted here to seek for the expected value of H, which depends on parameter "z". Then the expected value is added as an adiabatic potential to $H_\perp$ so as to obtain the effective Hamiltonian. H_0 can be treated as an unperturbed Hamiltonian and H_{e-p} as a perturbed one in calculation of $H_{||}$. It should be pointed out that the quasi-adiabatic approximation is valid only in the case when the characteristic extent for the motion of a polaron along the z direction is much large than the magnetic length. This corresponds the magnetic field is not very weak for a given interface potential. The unperturbed eigenstates are denoted by

$$|n\rangle_A |M\rangle_B |N_k\rangle |N_q\rangle \equiv |n, M, N_k, N_q\rangle. \tag{5}$$

At zero-temperature limit, the energy of unperturbed ground state is

$$E_n^{(0)} = \langle n, M, 0, 0| H_0 |n, M, 0, 0\rangle = \left(n + \frac{1}{2}\right)\hbar\omega_c, \tag{6a}$$

and the energy correction in the second order is

$$\Delta E_n^{(2)}(z) = \sum_k |V_k^*|^2 [\sin(zk_z)]^2 \times \sum_{n'} \frac{|_A\langle n'|L_k^{-1}|n\rangle_A|^2}{E_n^{(0)} - E_{n'}^{(0)} - \hbar\omega_{LO}} + \sum_{q\xi}|C_{q\xi}^*|^2\exp(-2qz) \times \sum_{n'}\frac{|_A\langle n'|L_q^{-1}|n\rangle_A|^2}{E_n^{(0)} - E_{n'}^{(0)} - \hbar\omega_{IO\xi}}. \tag{6b}$$

Then, one obtains the effective Hamiltonian to the second order for the state with Landau quantum number n:

$$H_{n,eff}(z) = H_\perp + \left(n + \frac{1}{2}\right)\hbar\omega_c + \Delta E_n^{(2)}(z). \tag{7}$$

The following trial function in the z direction can be chosen for the ground state:

$$\zeta(z) = \begin{cases} \zeta_A(z) = Bb^{1/2}(bz+\beta)e^{-bz/2} & \text{for } z > 0 \\ \zeta_B(z) = B'b'^{1/2}e^{b'z/2} & \text{for } z < 0 \end{cases}, \tag{8}$$

in which, $\beta = 2b/(b'+b)$, $B = [\beta(1+b/b') + 2\beta + 2]^{-1/2}$ and $B' = B\beta(b/b')^{1/2}$. Here b and b' are variational parameters [19].

The realistic heterojunction potential in equation (1b) can be obtained by using the above function as

$$V_r(z) = V_d(z) + V_s(z) + V_0\theta(-z),$$

and its average value is

$$V_r = \langle V_r(z)\rangle = \langle V_d(z)\rangle + \langle V_s(z)\rangle + \langle V_0\theta(-z)\rangle, \tag{9}$$

where V_d is the depletion charge contribution, V_s is the electron contribution to the potential and V_0 is the potential barrier height. $\theta(z)$ is a step function. In equation (9),

$$\langle V_d(z)\rangle = 4\pi e^2 N_d\{-B'^2/b'\varepsilon_{02} + B^2[(6+4\beta+\beta^2)/b\varepsilon_{01}]\},$$
$$\langle V_s(z)\rangle = 4\pi e^2 N_s[B'^2(1 - B'^2/2)b'\varepsilon_{02} + B^4(33 + 50\beta + 34\beta^2 + 12\beta^3 + 2\beta^4)/4b\varepsilon_{01}],$$

and $\langle V_0\theta(-z)\rangle = V_0B'^2$,

where N_s is the areal electron density and N_d is the donor concentration.

At last, the energy of Landau levels with quantum number n can be given by

$$E_n(b, b') = \langle\varsigma(z)|\, H_{n,eff}\,|\varsigma(z)\rangle, \tag{10a}$$

for which b and b' can be determined by

$$\frac{\partial E_n}{\partial b} = 0, \frac{\partial E_n}{\partial b'} = 0. \tag{10b}$$

$$E_0 = \frac{1}{2}\hbar\omega_c + \frac{\hbar^2 b^2}{2m}\left[\frac{1}{4} - (\beta+1)B^2\right] + V_r - \frac{\sqrt{\pi}\hbar\omega_{LO}}{2}\alpha_L\lambda_L\int_0^\infty \frac{e^{-t}}{(1-e^{-\lambda_L^2 t})^{1/2}}dt + B^2 b\left(\frac{\sqrt{\hbar}}{\beta}\right)\hbar\omega_{LO}\alpha_L\lambda_L\int_0^\infty\int_0^\infty e^{-t}\left[\frac{1}{(1+u)^3}\right.$$
$$\left.+\frac{1}{(1+u)^2}+\frac{\beta^2}{2(1+u)}\right]\exp\left[\frac{-\hbar^2}{\beta^2}\left(\frac{b}{2}\right)^2 u^2\left(1-e^{-\lambda_L^2 t}\right)\right]dudt - B'^2 b'\beta^2\left(\frac{\sqrt{\hbar}}{\beta}\right)\hbar\omega_{LO}\alpha_L\lambda_L\int_0^\infty\int_0^\infty\frac{e^{-t}}{2(1+u)}\exp\left[\frac{-\hbar^2}{\beta^2}\right.$$
$$\left.\times\left(\frac{b}{2}\right)^2 u^2(1-e^{-\lambda_L^2 t})\right]dudt + B^2 b\left(\frac{\sqrt{\hbar}}{\beta}\right)\hbar\omega_{IO\xi}\alpha_{I\xi}\lambda_{I\xi}\int_0^\infty\int_0^\infty e^{-t}\left[\frac{1}{(1+u)^3}+\frac{1}{(1+u)^2}+\frac{\beta^2}{2(1+u)}\right]\exp\left[\frac{-\hbar^2}{\beta^2}\left(\frac{b}{2}\right)^2\right.$$
$$\left.\times u^2\left(1-e^{-\lambda_{I\xi}^2 t}\right)\right]dudt - B'^2 b'\beta'^2\left(\frac{\sqrt{\hbar}}{\beta}\right)\hbar\omega_{IO\xi}\alpha_{I\xi}\lambda_{I\xi}\int_0^\infty\int_0^\infty\frac{e^{-t}}{2(1+u)}\exp\left[\frac{-\hbar^2}{\beta^2}\left(\frac{b}{2}\right)^2 u^2\left(1-e^{-\lambda_{I\xi}^2 t}\right)\right]dudt \quad (11)$$

$$E_1 = \frac{1}{2}\hbar\omega_c + \hbar^2\frac{b^2}{2m}\left[\frac{1}{4} - (\beta+1)B^2\right] + V_r - \sqrt{\pi}\frac{\hbar\omega_{LO}}{4}\alpha_L\lambda_L\int_0^\infty\frac{e^{-(1-\lambda_L^2 t)}(1+e^{-\lambda_L^2 t})}{(1-e^{-\lambda_L^2 t})^{1/2}}dt$$
$$+ B^2 b\left(\frac{\sqrt{\hbar}}{\beta}\right)\hbar\omega_{LO}\alpha_L\lambda_L\int_0^\infty\int_0^\infty e^{-(1-\lambda_L^2 t)}\left[\frac{1}{(1+u)^3}+\frac{1}{(1+u)^2}+\frac{\beta^2}{2(1+u)}\right]\exp\left[\frac{-\hbar}{\beta^2}\left(\frac{b}{2}\right)^2 u^2\left(1-e^{-\lambda_L^2 t}\right)\right]$$
$$\times\left[e^{-\lambda_L^2 t}+(1-e^{-\lambda_L^2 t})^2\frac{\hbar}{\beta^2}\left(\frac{b}{2}\right)^2 u^2\right]dudt - B'^2 b'\beta^2\left(\frac{\sqrt{\hbar}}{\beta}\right)\hbar\omega_{LO}\alpha_L\lambda_L\int_0^\infty\int_0^\infty\frac{e^{-(1-\lambda_L^2 t)}}{2(1+u)}\exp\left[\frac{-\hbar}{\beta^2}\left(\frac{b}{2}\right)^2 u^2(1-e^{-\lambda_L^2 t})\right]$$
$$\times\left[e^{-\lambda_L^2 t}+\left(1-e^{-\lambda_L^2 t}\right)^2\frac{\hbar}{\beta^2}\left(\frac{b}{2}\right)^2 u^2\right]dudt + B^2 b\left(\frac{\sqrt{\hbar}}{\beta}\right)\hbar\omega_{IO\xi}\alpha_{I\xi}\lambda_{I\xi}\int_0^\infty\int_0^\infty e^{-(1-\lambda_{I\xi}^2 t)}\left[\frac{1}{(1+u)^3}+\frac{1}{(1+u)^2}+\frac{\beta^2}{2(1+u)}\right]$$
$$\times\exp\left[\frac{-\hbar}{\beta^2}\left(\frac{b}{2}\right)^2 u^2\left(1-e^{-\lambda_{I\xi}^2 t}\right)\right]\left[e^{-\lambda_{I\xi}^2 t}+(1-e^{-\lambda_{I\xi}^2 t})^2\frac{\hbar}{\beta^2}\left(\frac{b}{2}\right)^2 u^2\right]dudt - B'^2 b'\beta^2\left(\frac{\sqrt{\hbar}}{\beta}\right)\hbar\omega_{IO\xi}\alpha_{I\xi}\lambda_{I\xi}$$
$$\times\int_0^\infty\int_0^\infty\frac{e^{-(1-\lambda_{I\xi}^2 t)}}{2(1+u)}\exp\left[\frac{-\hbar}{\beta^2}\left(\frac{b}{2}\right)^2 u^2(1-e^{-\lambda_{I\xi}^2 t})\right]\left[e^{-\lambda_{I\xi}^2 t}+(1-e^{-\lambda_{I\xi}^2 t})^2\frac{\hbar}{\beta^2}\left(\frac{b}{2}\right)^2 u^2\right]dudt. \quad (15)$$

3 Cyclotron resonance

The cyclotron frequency is defined by $\omega_c = \frac{\tilde{\beta}^2}{2m}$ for a free electron in magnetic fields and the cyclotron frequency ω_c^* for a polaron in magnetic fields can be determined by the difference of energies between the first state and the ground excited state, i.e. $E_1 - E_0 = \hbar\omega_c^*$. The PCM m^* can be determined by $\omega_c^* = eB_M/m^*c$.

If one defines

$$\lambda_L^2 = \frac{\omega_c}{\omega_{LO}}, \quad \lambda_{I\xi}^2 = \frac{\omega_c}{\omega_{IO\xi}},$$

then the ground-state energy for a polaron can be obtained from (6) by taking $n = 0$:

see equation (11) above

where

$$\alpha_L = \frac{e^2}{2\hbar^2}\left(\frac{2m}{\hbar\omega_{LO}}\right)^{1/2}\frac{1}{\varepsilon}, \quad (12)$$

and

$$\alpha_{I\xi} = \frac{e^2}{2\hbar^2}\left(\frac{2m}{\hbar\omega_{IO\xi}}\right)^{1/2}\frac{1}{\varepsilon^*} \quad (13)$$

are the coupling constants of interaction between the electron, bulk-LO and IO phonons, respectively. The following subsections are given to discuss ω_c^* for different intensities of magnetic fields.

3.1 Weak magnetic field ($\omega_c < \omega_{LO}, \omega_{IO}$)

In the case of $\omega_c < \omega_{LO}, \omega_{IO}$, the denominator in equation (6b) is obviously negative for every non-negative n', i.e.

$$E_1^{(0)} - E_{n'}^{(0)} - \hbar\omega_{LO} = (1-n')\hbar\omega_c - \hbar\omega_{LO} < 0, \quad (14a)$$

and

$$E_1^{(0)} - E_{n'}^{(0)} - \hbar\omega_{IO\xi} = (1-n')\hbar\omega_c - \hbar\omega_{IO\xi} < 0, \quad (14b)$$

with $n' = 1, 2, 3, ...$

Then, the energy of the first excited state for a polaron can be obtained from equation (6) by taking $n = 1$ and is given by

see equation (15) above

Then the cyclotron frequency ω_c^* can be obtained. Meanwhile, ω_c^* and the PCM m^* satisfy $m^*/m = \omega_c/\omega_c^*$. As discussed in Section 2, the quasi-adiabatic approximation is invalid for weak field limit corresponding to $\lambda_L^2, \lambda_{I\xi}^2 \ll 1$ so that equation (15) does not given correct result. On the other hand, the harmonic oscillator description for the motion of an electron in the $x-y$ plane is incorrect.

3.2 Strong magnetic field ($\omega_c \gg \omega_{LO}, \omega_{IO}$)

For this case, the denominators in equation (6b) can be rewritten as

$$E_1^{(0)} - E_{n'}^{(0)} - \hbar\omega_{LO} = \hbar\omega_{LO}[(1-n')\lambda_L^2 - 1], \qquad (16)$$

and

$$E_1^{(0)} - E_{n'}^{(0)} - \hbar\omega_{IO\xi} = \hbar\omega_{IO\xi}[(1-n')\lambda_{I\xi}^2 - 1]. \qquad (17)$$

Since $\lambda_L^2, \lambda_{I\xi}^2 \gg 1$ in the process of summing up n', one obtains

$$\begin{aligned} E_1 = {} & \frac{3}{2}\hbar\omega_c + \hbar^2\frac{b^2}{2m}\left[\frac{1}{4} - (\beta+1)B^2\right] \\ & + V_r - \frac{3}{8}\sqrt{\pi}\hbar\omega_{LO}\alpha_L\lambda_L \\ & + B^2 b\left(\frac{\sqrt{\hbar}}{\beta}\right)\hbar(\omega_{LO}\alpha_L\lambda_L + \omega_{IO\xi}\alpha_{I\xi}\lambda_{I\xi})\left[\frac{1}{(1+u)^3}\right. \\ & \left. + \frac{1}{(1+u)^2} + \frac{\beta^2}{2(1+u)}\right]\int_0^\infty \frac{(1-\hbar b^2u^2/\beta^2)^2}{\exp\left[\frac{\hbar}{\beta^2}b^2u^2\right]}du \\ & - B'^2 b'\beta^2\left(\frac{\sqrt{\hbar}}{\beta}\right)\hbar(\omega_{LO}\alpha_L\lambda_L \\ & + \omega_{IO\xi}\alpha_{I\xi}\lambda_{I\xi})\int_0^\infty \frac{du}{2(1+u)}\frac{(1-\hbar b^2u^2/\beta^2)^2}{\exp\left[\frac{\hbar}{\beta^2}b^2u^2\right]}. \end{aligned} \qquad (18)$$

3.3 Resonant magnetic fields

Replacing $E_1^{(0)} - E_{n'}^{(0)}$ by $E_1 - E_{n'}$ in (6b), one can easily obtain the polaron energy for the first excited Landau level. The following three situations should be discussed for the interaction between an electron and phonons:

(i) When the frequency of magnetic field satisfies $|(\omega_c - \omega_{IO-})/(\omega_c - \omega_{IO+})| \ll 1$ and $\omega_c \cong \omega_{IO-}$, the two-fold splitting of PCM also happens. One obtains

$$\begin{aligned} E_1 = {} & \frac{1}{2}\hbar\omega_c + \hbar^2\frac{b^2}{2m}\left[\frac{1}{4} - (\beta+1)B^2\right] + V_r \\ & + \frac{\hbar^{2/3}}{\beta^3}\left(\frac{b}{2}\right)^3\frac{(\hbar\omega_{IO-})^2\alpha_{I-}\lambda_{I-}}{E_1 - E_0 - \hbar\omega_{IO-}} \\ & \times\left[B^2 b\int_0^\infty u^2\left[\frac{1}{(1+u)^3} + \frac{1}{(1+u)^2}\right.\right. \\ & \left. + \frac{\beta^2}{2(1+u)}\right]\exp\left[-\frac{\hbar}{\beta^2}\left(\frac{b}{2}\right)^2u^2\right]du \\ & \left. - B'^2 b'\beta^2\int_0^\infty \frac{u^2}{2(1+u)}\exp\left[-\frac{\hbar}{\beta^2}\left(\frac{b}{2}\right)^2u^2\right]du\right], \end{aligned} \qquad (19)$$

where E_0 is given by equation (11). A two-fold splitting of polaron cyclotron frequency can be obtained from the two solutions $E_{1,\pm}$ of the above equation:

$$\omega_{c,\pm}^* = (E_{1,\pm} - E_0)/\hbar. \qquad (20)$$

The corresponding PCM $m_\pm^*$ reads

$$\frac{m_\pm^*}{m} = \frac{\hbar\omega_c}{E_{1,\pm} - E_0}. \qquad (21)$$

(ii) When the frequency of magnetic field satisfies $|(\omega_c - \omega_{IO+})/(\omega_c - \omega_{IO-})| \ll 1$ and $\omega_c \cong \omega_{IO+}$, the two-fold splitting of PCM also happens. Equation (18) can be rewritten as

$$\begin{aligned} E_1 = {} & \frac{1}{2}\hbar\omega_c + \hbar^2\frac{b^2}{2m}\left[\frac{1}{4} - (\beta+1)B^2\right] + V_r \\ & + \frac{\hbar^{2/3}}{\beta^3}\left(\frac{b}{2}\right)^3\frac{(\hbar\omega_{IO+})^2\alpha_{I+}\lambda_{I+}}{E_1 - E_0 - \hbar\omega_{IO+}} \\ & \times\left[B^2 b\int_0^\infty u^2\left[\frac{1}{(1+u)^3} + \frac{1}{(1+u)^2} + \frac{\beta^2}{2(1+u)}\right]\right. \\ & \times\exp\left[-\frac{\hbar}{\beta^2}\left(\frac{b}{2}\right)^2u^2\right]du \\ & \left. - B'^2 b'\beta^2\int_0^\infty \frac{u^2}{2(1+u)}\exp\left[-\frac{\hbar}{\beta^2}\left(\frac{b}{2}\right)^2u^2\right]du\right], \end{aligned} \qquad (22)$$

and equations (20) and (21) are also available.

(iii) When the frequency of magnetic field satisfies $|(\omega_c - \omega_{LO})/(\omega_c - \omega_{IO\xi})| \ll 1$ and $\omega_c \cong \omega_{LO}$, the coupling between the electron and a bulk LO phonon causes another two-fold splitting for the PCM. For

this case,

$$E_1 = \frac{1}{2}\hbar\omega_c + \hbar^2\frac{b^2}{2m}\left[\frac{1}{4} - (\beta+1)B^2\right] + V_r + \frac{(\hbar\omega_{LO})^2\alpha_L\lambda_L}{E_1 - E_0 - \hbar\omega_{LO}}\left[\sqrt{\pi}/4 - \frac{\hbar^{3/2}}{\tilde{\beta}^3}\left(\frac{b}{2}\right)^3\int_0^\infty\left[\frac{1}{(1+u)^3} + \frac{1}{(1+u)^2} + \frac{\beta^2}{2(1+u)}\right]u^2\exp\left[-\frac{\hbar}{\beta^2}\left(\frac{b}{2}\right)^2u^2\right]du - B'^2b'\beta^2\int_0^\infty\frac{u^2}{2(1+u)}\exp\left[-\frac{\hbar}{\beta^2}\left(\frac{b}{2}\right)^2u^2\right]du\right], \quad (23)$$

where E_0 can be obtained by equation (11). One can find the cyclotron frequency from the two solutions $E^L_{1,\pm}$ of the above equation:

$$\omega^*_{c,\pm} = (E^L_{1,\pm} - E_0)/\hbar. \quad (24)$$

4 Pressure effect

The relation between pressure and crystal constant of bulk material can be obtained by Murnaghan equation [21]

$$a(P) = a(0)\left(1 + P\frac{B'}{B}\right)^{-1/3B'}, \quad (25)$$

where B is the bulk elastomeric modulus, and satisfies $B' = dB/dP$. Under low-pressure condition, equation (25) can be simplified as

$$a(P) = a(0)(1 - P/3B). \quad (26)$$

The relation of high-frequency dielectric constant varying with pressure [27,28] can be obtained from the dependence of band gap on pressure, i.e.

$$\varepsilon_\infty = 1 + DA\omega_p^2/\bar{E}_g^2, \quad (27)$$

with

$$\bar{E}_g^2 = E_h^2 + C^2. \quad (28)$$

Here, ω_p is the frequency of a valence electron and depends on volume as $\omega_p \sim V^{1/2}$. $\bar{E}_g$ is the average optical gap (or Penn gap), which can be divided as a homopolar (covalent) contribution $\bar{E}_h$ and an ionic contribution C. Factor A is a constant ($A \cong 1$) and $D = N_{eff}/4$ indicates the probability of occupied d states transition between the interbands. It is generally assumed that $dC/dP \cong 0$. The volume dependence of E_h and D is estimated to be $E_h \sim V^{0.83}$ and $D - 1 \sim V^{4.3}$. The derivative of ε_∞ to volume can be written in terms of the Phillps-Van Veceten ionicity $f_i = C^2/E_g^2$:

$$\frac{\partial \ln\varepsilon_\infty}{\partial \ln V} \cong \frac{5(\varepsilon_\infty - 1)}{3\varepsilon_\infty}(0.9 - f_i). \quad (29)$$

Table 1. Parameters for III–V group semiconductors GaAs and AlAs.

Materials	ε_0	ε_∞	m	α_B	E_{LO}	E_{TO}
AlAs	10.06	8.16	0.109	0.1260	50.09	45.11
GaAs	12.83	10.90	0.0655	0.0681	36.70	33.83

Table 2. Calculated parameters for GaAs/AlAs heterojunction.

Materials	α_{IO}	E_{IO}	α_{IO+}	E_{IO+}	α_{IO-}	E_{IO-}
GaAs/AlAs	0.0862	37.07	0.0469	47.56	0.0308	35.17

The pressure dependence of volume can be written as $\partial P/\partial V = -B/V$. One can obtain the dielectric constant as following form:

$$\varepsilon_\infty(P) = 1 + [\varepsilon_\infty(0) - 1]e^{-\frac{5}{3B}(0.9 - f_i)P}. \quad (30)$$

In order to obtain the effects of the electron-phonon interaction coupling constant dependent on hydrostatic pressure for heterojunction structures, one needs to know the dependence of the bulk optical phonons on pressure. The Grüneisen-mode parameters under low pressure should be introduced as [29]

$$\gamma_j = -\left.\frac{\partial \ln\omega_j}{\partial \ln V}\right|_{V=V_0} = B\left.\frac{\partial\omega_j}{\partial P}\right|_{P=0}, \quad (31)$$

where $j = LO, TO$ labels the LO- and TO-phonons, respectively. Since γ_j is nearly a constant at low pressure for the two kinds of phonons, the modification of phonon energy due to pressure can be expressed as

$$\hbar\omega_j(P) = \hbar\omega_j(0)e^{\frac{\gamma_j}{B}P}, \quad (32)$$

In equation (32), parameter 0 denotes the condition without pressure effect ($P = 0$). Equation (32) shows that the phonon frequency increases as pressure. This conclusion agrees with the calculation of the self-consistent density-functional perturbation theory [29].

At low pressure, one can fit the band gap $E_g(p)$ to a quadratic function

$$E_g(P) = E_g(0) + bP + cP^2. \quad (33)$$

The pressure dependence of electron band mass can be expressed as

$$\frac{m_0}{m^*(P)} = 1 + \frac{A}{E_g(P)}. \quad (34)$$

5 Numerical results and discussion

The relative parameters used in calculation for semiconductor heterojunctions of the III–V group GaAs/AlAs are listed in Tables 1 and 2 and the results are shown by Figures 1–5.

For convenience, we choose λ^2 ($\lambda^2_{I+}/\lambda^2_{I-} = \omega_{IO-}/\omega_{IO+}$, $\lambda^2_L/\lambda^2_I = \omega_{IO}/\omega_{LO}$) to denote the strength of

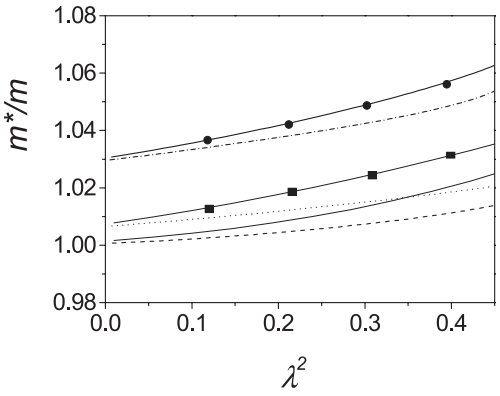

Fig. 1. Contributions to polaron cyclotron mass from different branches of phonons and their values under pressure (40 kbar) in weak magnetic fields. The dashed, dot and dot dashed lines correspond to the contributions from IO-phonons with lower frequency ω_{IO-}, higher frequency ω_{IO+} and LO-phonons with frequency ω_{LO}, respectively. The solid, square dot solid and dot solid lines correspond to their contributions under pressure (40 kbar).

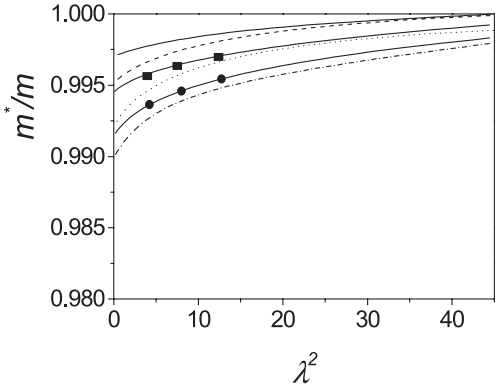

Fig. 2. Contributions to polaron cyclotron mass from different branches of phonons and their values under pressure (40 kbar) in strong magnetic fields. The dashed, dot and dot dashed lines correspond to the contributions from IO-phonons with lower frequency ω_{IO-}, higher frequency ω_{IO+} and LO-phonons with frequency ω_{LO}, respectively. The solid, square dot solid and dot solid lines correspond to their contributions under pressure (40 kbar).

magnetic fields. It should be pointed out that the abscissa λ^2 without pressure effect was adopted in Figures 1–5 so as to measure the magnetic strength with an equal-weight because it changes with pressure.

Figure 1 shows that the contribution from each branch of phonons to the PCM in weak magnetic fields and their pressure effects (40 kbar). One can see from the contributions of different phonons that the bulk LO phonons are most, while the IO phonons are lest important. The contribution from each branch of phonons increases nonlinearly with magnetic strength and the magnetic effect of bulk LO phonons is strongest. Here, we do not show the result for very small λ^2 since equation (15) is incorrect as discussed in Section 3.1.

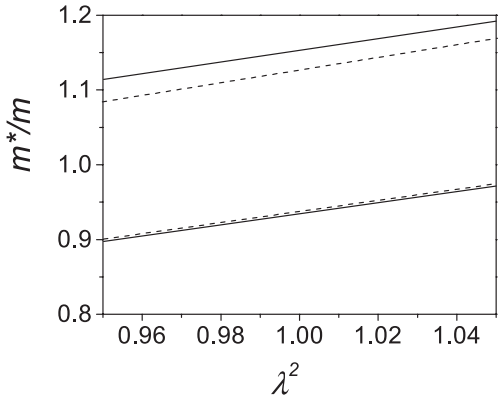

Fig. 3. he splitting of polaron cyclotron mass and its pressure effect (40 kbar) around ω_{IO-}. The solid and dashed lines correspond to with and without pressure, respectively.

At zero pressure, the contribution from bulk LO phonons plays a main role at the limit of weak magnetic field. Meanwhile, the contribution from IO phonons with lower frequency can be neglected and that from IO phonons with higher frequency can not be neglected. As increase of the strength of magnetic fields, the contributions from both branches of IO phonons also increase, but that from IO phonons with lower frequency increases much faster and can not be neglected. The contributions from bulk LO and IO phonons are both important and that from LO and IO phonons are comparable. The physical reason is that the electron tunnels into well far from the interface so as to couple with bulk LO phonons more strongly because of the confinement of interface potential and band bending to the electron in a realistic heterojunction. The electron moves on the quantized orbits (Landau levels) in the $x-y$ plane due to the static magnetic field in the z direction. On the one hand, the cyclotron frequency ω_c of an electron increases with magnetic fields, accordingly the confinement to the electron becomes stronger and the electronic wave functions are localized more obviously. On the other hand, the average electronic number on each Landau level increases whereas the number of Landau levels filled by electrons decreases as the magnetic field increases and the electronic wave function is confined within a narrower region. Both of the above localizations lead to strengthening of the coupling between the electron and IO phonons. These conclusions are more general than that given in reference [14] because a realistic heterojunction potential is taken into account here.

Under pressure, the contribution from each branch of phonons is similar to that at zero pressure. The contributions from the two branches of IO phonons increase with magnetic fields faster than that from LO phonons, the increase of that from IO phonons with higher frequency is fastest, and that from bulk LO phonons slowest. At this moment, the contributions from bulk LO and IO phonons are both important, the contributions from the two branches of IO phonons tend to be stronger than that at zero pressure. It can be easily understood from equations (33) and (9) that the pressure effect enhances the

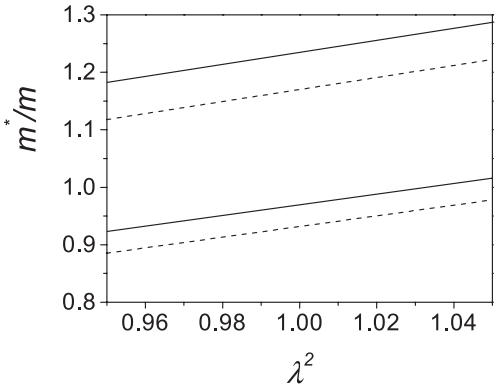

Fig. 4. The splitting of polaron cyclotron mass and its pressure effect (40 kbar) around ω_{IO+}. The solid and dashed lines correspond to with and without pressure, respectively.

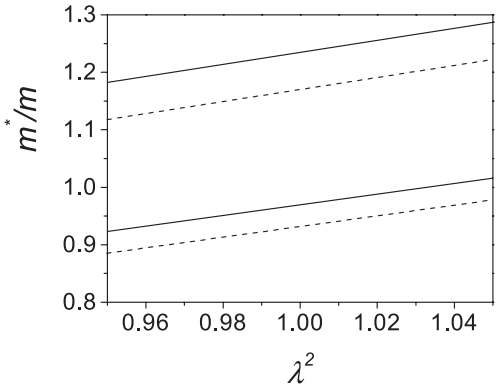

Fig. 5. The splitting of polaron cyclotron mass and its pressure effect (40 kbar) around ω_{LO}. The solid and dashed lines correspond to with and without pressure, respectively.

confinement of the electron as well as broadens the band gap E_g and enhances the band bending. As a result, the electron moves in the well nearer the interface and couples more strongly with IO phonons. On the other hand, equations (34) and (32) indicate respectively that the electronic band mass increases with E_g and the frequencies of phonons increase with pressure. The collaborating effect together with the influence of pressure on the dielectric constant strengthens the interaction between an electron and different kinds of phonons.

Figure 2 gives the contributions to the PCM from different branches of phonons in strong magnetic fields and their pressure effects (40 kbar). The properties of the contributions as magnetic fields increasing are the same but negative with that as decreasing of weak magnetic fields.

Figures 3 and 4 describe the two-fold splitting of PCM due to IO phonons with lower frequency ($\omega_c \cong \omega_{IO-}$, $\lambda^2_{I-} \cong 1$) and higher frequency ($\omega_c \cong \omega_{IO+}$, $\lambda^2_{I+} \cong 1$), respectively. It is obvious that the two-fold splitting increases linearly with magnetic fields for both branches of phonons with lower and higher frequencies. Since the splitting width increases with the coupling between the electron and phonons, and the pressure effect leads to the strengthening of the coupling, the splitting width of the PCM increases with pressure effects due to the contributions from the two branches of IO phonons, in which that from the branch of phonons with higher frequency is much obvious. The position of the PCM after splitting is determined mainly by the electron-phonon coupling constant (increases with electron mass and phonon frequency), and phonon frequency. Pressure makes both of them increase. Then, the contributions from two branches of IO phonons broaden the splitting of the PCM, and the splitting caused by the branch with higher frequency is more obvious. It should be pointed out that in Figure 3 the two-fold splitting caused by the branch with lower frequency locates at two sides of that without pressure effects, which needs to be discussed further about its physical property.

Figure 5 gives the two-fold splitting of the PCM ($\omega_c \cong \omega_{LO}, \lambda^2_{LO} \cong 1$) due to the contribution of bulk LO phonons. It can be seen that the splitting increases nonlinearly with magnetic fields. This is similar to the results derived in a previous paper [11]. It is obvious that the splitting width is narrower than that from IO phonons. However, the pressure effect is important although the contribution of bulk LO phonons due to pressure effect is less than that of IO phonons.

6 Conclusion

In conclusions, the cyclotron resonance of polarons in realistic heterojunctions and its pressure effect are discussed by considering the influences of LO and two branches of IO phonons. The numerical computation for semiconductor heterojunctions of the III–V group GaAs/AlAs indicates that the contribution to the polaron resonant mass from the branch of IO phonons with higher frequency can not be neglected at weak magnetic fields although that from LO phonons is more important. As the increase of the magnetic fields, the contributions from LO and two branches of IO phonons are comparable. The contributions from two branches of IO phonons become more and more obviously as the increase of magnetic fields under pressure, and both LO and IO phonons are important. In strong magnetic fields, the contributions from different branches of phonons varying with magnetic fields and pressure are similar but negative with that in weak fields. The pressure effect of cyclotron resonance appearing near the frequencies of different branches of phonons is obvious.

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