Eur. Phys. J. B **5**, 153–158 (1998)

THE EUROPEAN PHYSICAL JOURNAL B

© EDP Sciences
Springer-Verlag 1998

Interface polarons in a heterojunction with triangular bending-band

S. Ban and X.X. Liang[a]

CCAST (World Laboratory), P.O. Box 8730, Beijing 100080, P.R. China[b]
and
Laboratory of Solid State Physics, Department of Physics, Inner Mongolia University, Hohhot, 010021, P.R. China

Received: 4 November 1997 / Revised and Accepted: 9 March 1998

Abstract. The interface polaron states in a heterojunction are discussed by considering an energy-band bending near the interface and the influence of an image potential. The ground state energy and the effective mass of a polaron are variationally calculated. The numerical results for the GaAs/$Al_xGa_{1-x}As$ ($x \geq 0.3$) heterojunction are given. It is shown that even though the influences from bulk longitudinal optical (LO) phonons are more important for the heterojunctions with lower Al composition, the contributions from two branches of interface optical (IO) phonons are not negligible. For the heterojunctions with higher Al composition, both the influences from LO phonons and two branches of IO phonons are important. The band-bending plays an important role for the interface localization of polarons, but the influence of the image potential is not essential.

PACS. 71.38.+I Polarons and electron phonon interactions – 73.40.Lq Other semiconductor-to-semiconductor contacts, *p-n* junctions, and heterojunctions – 63.20.kr Phonon-electron and phonon-phonon interactions

1 Introduction

The appearance of artificially fabricated semiconductor heterojunctions and quantum wells brought about a fast development for modern electronic and photo-electronic devices. To clarify, in physics, the novel phenomena in these materials due to the presence of interfaces may give a significant impetus to their application. The polaron problems in semiconductor heterostructures have attracted many author's attentions in recent years, owing to the establishment of the detailed interaction mechanism between electrons and optical phonons in layered materials [1–5]. It has been found that the influence of interface optical (IO) phonons on electron states is important for quantum wells with narrow widths [6,7]. The magnetphonon resonance results in single GaAs/$Al_xGa_{1-x}As$ heterojunctions [8] demonstrated that the frequencies of the optical phonons coupling with electrons lower than that of the bulk longitudinal optical (LO) phonons in GaAs. This may indicate that the presence of the IO phonons and their interaction with the electrons should be taken into account in considering the heterojunction problems.

On the other hand, semiconductor heterojunctions exhibit an abrupt discontinuity in the local band structure and electrons from the higher bandedges tend to accumulate in the lower bandedges at the interfaces. For example, in a GaAs/$Al_xGa_{1-x}As$ heterojunction, the electrons transfer from the donor energy levels of wide forbid-band $Al_xGa_{1-x}As$ into the narrow forbid-band GaAs. This Hartree-Fock potential brings about a energy band bending and form a potential well binding electrons to the interface in GaAs, which form a so-called quasi 2D electron gas (2DEG) at equilibrium states [9]. When the concentration of the electrons near the interface is not large enough, one can study the single polaron problem by neglecting the screening effect [10].

The previous works studied the interface polaron problems involving the effects from both the bulk LO- and the IO-phonon modes. The early works treated the electron IO-phonon interactions by using a single-branch effective IO phonon model [11]. Lately, Pokatilov *et al.* have investigated surface polarons at the contact of two polar crystals in detail [12]. They considered the interactions between the electron and two branches of SO-phonon modes besides the bulk LO-phonon and calculated the ground-state energies and the effective masses of the surface polarons in a weak coupling approximation. Some other authors investigated these problems by using a quasi two-dimensional (2D) [13,14] or pure 2D [15,16] model, which include the interactions between the electrons and the two branches of IO phonon modes. A 2D model was also adopted to study the polaron ground states and the polaron cyclotron resonance for GaAs/AlAs heterojunction [16]. The results shown that both the two branches of IO phonon modes

[a] e-mail: `xxliang@nmg2.imu.edu.cn`
[b] Mailing address

should be considered to investigate the properties of interface polarons.

The quasi 2D results for the electrons moving in AlAs, under the influence of a strong electric field near the GaAs/AlAs interface [13], indicated that the bulk LO phonons and IO phonons make competitive contribution to the polarons. The studies improves the previous single-branch effective phonon method. However, most of them only attributed the interface localization of the polarons to the image potential (IP) and electron-phonon interaction, without taking the band-bending potential near the interface into account.

In this paper a detail investigation for the interface polarons in a heterojunction is presented. Out of the previous works an energy-band bending and induced intrinsic interface states of electrons are considered together with the influences of the image potential and electron-phonon interaction. The ground-state energy and effective mass of an interface polaron are variationally calculated by using an LLP-like method [13]. As an example we discuss the $GaAs/Al_xGa_{1-x}As$ system. A triangular potential is used here to describe the bent energy-band in GaAs since the electrons can be presumed in the lowest subband for the polaron ground state [9,17]. Contrarily the image potential for this system is repulsive. In the other side of the interface, an infinite barrier into $Al_xGa_{1-x}As$ at the interface are also considered. The interactions of the electrons with both of the half-space bulk LO phonons and two branches of IO phonon modes are included in consideration of the electron-phonon coupling. An effective LO phonon mode approximation [18,19], which has been proved to be reasonable for ternary mixed crystals with the weak electron-LO phonon coupling such as the $Al_xGa_{1-x}As$ material [19] and also used to investigate the electron IO-phonon interaction in the $GaAs/Al_xGa_{1-x}As$ quantum well. To sum the above competitive influences up, the slow moving electrons in a $GaAs/Al_xGa_{1-x}As$ heterojunction still can be confined near the interfaces in GaAs. The numerical variation about the ground-state energies and effective masses is performed for the practically realizable $GaAs/Al_xGa_{1-x}As$ heterojunction with composition of $x \geq 0.3$. It is found that both the contributions from the bulk LO-phonons and the two branches of IO-phonons to the polaronic energies are important for the heterojunctions with higher Al composition, specially for the extreme case of $x = 1$. The influences of the IO phonons can not be neglected, even for the heteojunctions with lower Al composition, where the contribution from bulk LO phonons is more important.

2 Model and variational calculation

Let us consider a heterojunction consisting of two semi-infinite polar semiconductors denoted respectively by materials "1" filling in the half space of $z < 0$ and "2" in $z > 0$ with the interface in the $x{-}y$ plane ($z = 0$). As mentioned above, the previous authors have discussed the surface or interface polarons bound by an image potential and electron-phonon interaction [11–16] without including the intrinsic interface states caused by a band-bending potential. However the image potential sometimes, such as in the $GaAs/Al_xGa_{1-x}As$ heterojunction, appears as repulsive and detrimental to localize of the polarons on the interface in GaAs. Here we deal with a real heterojunction, where is an energy-band bending near the interface in material "1", which localizes the electrons on the interface whereas an image potential tend to repelling it moving far from the interface. On the other hand, the potential barrier height on the interface can be presumed as infinite for electrons in the lowest subband which corresponds to the polaron ground states. Considering the effects of half space bulk LO phonons and IO phonons, we write the Hamiltonian of the single electron and phonon system as

$$H = H_1 + H_2, \tag{1}$$

where

$$H_1 = \frac{p_z^2}{2m} + V(z) + \frac{e^2\left(\varepsilon_{\infty 2} - \varepsilon_{\infty 1}\right)}{4\varepsilon_{\infty 1}\left(\varepsilon_{\infty 2} - \varepsilon_{\infty 1}\right)z} \tag{1a}$$

and

$$\begin{aligned} H_2 = \frac{p_t^2}{2m} &+ \sum \hbar\omega_{L1} a_k^+ a_k + \sum_{q,\,\sigma} \hbar\omega_\sigma b_{q\sigma}^+ b_{q\sigma} \\ &+ \sum_k \left[\frac{B\sin(k_z z)}{k} e^{-i\mathbf{k}_t\cdot\boldsymbol{\rho}} a_k^+ + h.c.\right] \\ &+ \sum_{q\sigma}\left[\frac{G_\sigma}{\sqrt{q}} e^{-i\mathbf{q}\cdot\boldsymbol{\rho}} e^{-q|z|} b_{q\sigma}^+ + h.c.\right]. \end{aligned} \tag{1b}$$

Here $\mathbf{r} = (\boldsymbol{\rho}, z)$, $\mathbf{p} = (\mathbf{p}_t, p_z)$, in which $\boldsymbol{\rho}$ and $\mathbf{p}_t$ are the $x{-}y$ plane components of the electron coordinates and momenta and z and p_z the z-component, respectively. m is the band mass of the electron in material "1". A triangular potential $V(z)$ is adopted to describe the potential well caused by the energy-band bending as

$$V(z) = \begin{cases} -eF_z z & z \leq 0, \\ \infty & z > 0. \end{cases} \tag{1c}$$

where F_z is chosen as a typical value $F_z = 20$ kV/cm for GaAs in the $GaAs/Al_xGa_{1-x}As$ heterojunction system. $\varepsilon_{\infty 1}$ and $\varepsilon_{\infty 2}$ are respectively the optical dielectric constants of the media "1" and "2". $a_k^+(a_k)$ denotes the creation (annihilation) operator of a half-space bulk LO phonon with wave-vector $\mathbf{k} = (\mathbf{k}_t, k_z)$ and frequency ω_{L1}, while $b_{q\sigma}^+(b_{q\sigma})$ the corresponding operator for an IO phonon with a 2D wave-vector $\mathbf{q}$ and frequency $\omega_{q\sigma}$. $\sigma = +$ and $\sigma = -$ represent respectively the two branches of IO phonon modes with the higher and lower frequencies:

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

with

$$a = \varepsilon_{\infty 1} + \varepsilon_{\infty 2}, \tag{2a}$$

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

$$c = \varepsilon_{\infty 1}\omega_{L1}^2\omega_{T2}^2 + \varepsilon_{\infty 2}\omega_{L2}^2\omega_{T1}^2, \tag{2c}$$

$$
\begin{aligned}
H_2^* &= U_2^{-1}U_1^{-1}H_2U_1U_2 \\
&= \frac{1}{2m}\left(\mathbf{P}_t - \hbar\sum_k \mathbf{k}_t a_k^+ a_k - \hbar\sum_{q\sigma}\mathbf{q}b_{q\sigma}^+ b_{q\sigma}\right)^2 + \sum_k\left(\frac{\sin(k_z z)}{k}B^* f_k e^{-ik_z z} + h.c.\right) + \sum_{q\sigma}\left(\frac{G_\sigma^*}{\sqrt{q}}e^{-q|z|}g_{q\sigma} + h.c.\right) \\
&\quad + \sum_k \hbar\omega_{L1}a_k^+ a_k + \sum_{q\sigma}\hbar\omega_{q\sigma}b_{q\sigma}^+ b_{q\sigma} + \frac{\hbar^2}{2m}\left(\sum_k \mathbf{k}_t|f_k|^2 + \sum_{q\sigma}\mathbf{q}|g_{q\sigma}|^2\right)^2 + \sum_k |f_k|^2\left(\hbar\omega_{L1} + \frac{\hbar^2 k_t^2}{2m} - \frac{\hbar\mathbf{k}_t\cdot\mathbf{P}_t}{m}\right) \\
&\quad + \sum_{q\sigma}|g_{q\sigma}|^2\left(\hbar\omega_{q\sigma} + \frac{\hbar^2 q^2}{2m} - \frac{\hbar\mathbf{q}\cdot\mathbf{P}_t}{m}\right) + \frac{\hbar^2}{m}\sum_k a_k^+ a_k\left(\mathbf{k}_t\cdot\sum_{k'}\mathbf{k}'{}_t|f_{k'}|^2\right) + \frac{\hbar^2}{m}\sum_{q\sigma}b_{q\sigma}^+ b_{q\sigma}\left(\mathbf{q}\cdot\sum_{q'\sigma'}\mathbf{q}'|g_{q'\sigma'}|^2\right) \\
&\quad + \sum_k\left\{a_k\left[\frac{\sin(k_z z)}{k}B^* + f_k^* e^{ik_z z}\left(\hbar\omega_{L1} + \frac{\hbar^2 k_t^2}{2m} - \frac{\hbar\mathbf{k}_t\cdot\mathbf{P}_t}{m} + \frac{\hbar^2\mathbf{k}_t}{m}\cdot\left(\sum_{k'}\mathbf{k}'_t|f_{k'}|^2\right)\right)\right]h.c.\right\} \\
&\quad + \sum_{q\sigma}\left\{b_{q\sigma}\left[\frac{G_\sigma^*}{\sqrt{q}}e^{-q|z|} + g_{q\sigma}^*\left(\hbar\omega_\sigma + \frac{\hbar^2 q^2}{2m} - \frac{\hbar\mathbf{q}\cdot\mathbf{P}_t}{m} + \frac{\hbar^2\mathbf{q}}{m}\cdot\left(\sum_{q'\sigma'}\mathbf{q}'|g_{q'\sigma'}|^2\right)\right)\right]h.c.\right\}
\end{aligned}
\tag{7}
$$

where $\varepsilon_{0\lambda}(\lambda = 1, 2)$ is the static dielectric constant and $\omega_{T\lambda}$ the transverse optical (TO) phonon frequency of material "λ ", respectively.

The last two terms in H_2 denote the interaction between an electron and bulk LO and IO phonons respectively in which the parameters B and G_σ are given by

$$
B = -i\left[\frac{4\pi e^2\hbar\omega_{L1}}{V}\left(\frac{1}{\varepsilon_{\infty 1}} - \frac{1}{\varepsilon_{01}}\right)\right]^{1/2} \tag{3}
$$

and

$$
G_\sigma(k) = i\left(\delta_1^2 + \delta_2^2\right)^{-1/2}\left(\frac{2\pi\hbar e^2}{S\omega_\sigma}\right)^{1/2}, \tag{4}
$$

where

$$
\delta_\lambda = \frac{\left(\varepsilon_{0\lambda} - \varepsilon_{\infty\lambda}\right)^{1/2}\omega_{T\lambda}}{\left(\omega_{T\lambda}^2 - \omega_\sigma^2\right)} \qquad (\lambda = 1, 2), \tag{4a}
$$

In equations (3, 4), V and S refer to the volume of the medium "1" and the area of the interface, respectively.

Performing two unitary transformation

$$
U_1 = \exp\left[\frac{i}{\hbar}\left(\mathbf{P}_t - \hbar\sum_k \mathbf{k}_t a_k^+ a_k - \hbar\sum_{q\sigma}\mathbf{q}b_{q\sigma}^+ b_{q\sigma}\right)\cdot\boldsymbol{\rho}\right], \tag{5}
$$

where $\mathbf{P}_t$ is the eigenvalue of the total momentum operator and

$$
U_2 = \exp\left[\sum_k\left(f_k e^{-ik_z z}a_k^+ + h.c.\right) + \sum_{q\sigma}\left(g_{q\sigma}b_{q\sigma}^+ + h.c.\right)\right]\cdot \tag{6}
$$

The Hamiltonian H_2 in equation (1) is then transformed to be:

See equation (7) above

where the high order terms of $a_k^+,\ a_k$ and $b_{q\sigma}^+,\ b_{q\sigma}$ have been neglected because they have no contribution to the expectation value for the zero phonon states.

In equation (7), f_k and $g_{q\sigma}$ will be determined by the variational minimization with respect to the polaron ground state $|\psi\rangle$ which is chosen as the product of the zero phonon state $|0\rangle$ and the variational wave function $|\phi\rangle$ of the electron in z-direction:

$$
|\psi\rangle = |\phi\rangle|0\rangle = |\phi\rangle\prod_{kq\sigma}|0_k\rangle|0_{q\sigma}\rangle. \tag{8}
$$

The Hamiltonian H_2 in equation (1) changes nothing after the transformations. The polaron variational energy then can be written as

$$
E = \langle\psi|U_2^{-1}U_1^{-1}HU_1U_2|\psi\rangle = E_1 + E_2, \tag{9}
$$

with

$$
E_1 = \langle\phi|\frac{p_z^2}{2m} + V(z) + \frac{e^2\left(\varepsilon_{\infty 2} - \varepsilon_{\infty 1}\right)}{4\varepsilon_{\infty 1}\left(\varepsilon_{\infty 2} + \varepsilon_{\infty 1}\right)z}|\phi\rangle, \tag{10}
$$

and

$$
\begin{aligned}
E_2 &= \frac{p_t^2}{2m} \\
&\quad + \langle\phi|\sum_k\left[\frac{\sin(k_z z)}{k}B^* f_k e^{-ik_z z} + h.c.\right]|\phi\rangle \\
&\quad + \langle\phi|\sum_{q\sigma}\left[\frac{G_\sigma^*}{\sqrt{q}}e^{-q|z|}g_{q\sigma} + h.c.\right]|\phi\rangle \\
&\quad + \frac{\hbar^2}{2m}\left[\sum_k \mathbf{k}_t|f_k|^2 + \sum_{q\sigma}\mathbf{q}|g_{q\sigma}|^2\right]^2 \\
&\quad + \sum_k |f_k|^2\left[\hbar\omega_{L1} + \frac{\hbar^2\mathbf{k}_t^2}{2m} - \frac{\hbar\mathbf{k}_t\cdot\mathbf{P}_t}{m}\right] \\
&\quad + \sum_{q\sigma}|g_{q\sigma}|^2\left[\hbar\omega_\sigma + \frac{\hbar^2\mathbf{q}^2}{2m} - \frac{\hbar\mathbf{q}\cdot\mathbf{P}_t}{m}\right].
\end{aligned}
\tag{11}
$$

The displacement amplitudes f_k and $g_{q\sigma}$ read respectively

$$f_k = \frac{\phi_B(k_z)}{\hbar\omega_{L1} + \frac{\hbar^2 \mathbf{k}_t^2}{2m} - \frac{\hbar \mathbf{k}_t \cdot \mathbf{P}_t}{m}(1-\eta)}, \quad (12)$$

$$\text{and} \quad g_{q\sigma} = \frac{\phi_G(\sigma, q)}{\hbar\omega_\sigma + \frac{\hbar^2 q^2}{2m} - \frac{\hbar \mathbf{q} \cdot \mathbf{P}_t}{m}(1-\eta)}, \quad (13)$$

where

$$\phi_B(k_z) = \langle\phi| \frac{B \exp(ik_z z) \sin(k_z z)}{k} |\phi\rangle, \quad (12a)$$

$$\text{and} \quad \phi_G(\sigma, q) = \langle\phi| \frac{G_\sigma \exp(-q|z|)}{\sqrt{q}} |\phi\rangle \cdot \quad (13a)$$

In the above calculations, the electron is considered to be fixed on the lowest subband state (ground state) in the potential well of bending-band in z-direction, since the probabilities of the subband transitions due to the electron-phonon interaction are second-order small.

In equations (12, 13) the parameter η can be derived by using the following relation

$$\eta \mathbf{P}_t = \sum_k \hbar \mathbf{k}_t |f_k|^2 + \sum_{q\sigma} \hbar \mathbf{q} |g_{q\sigma}|^2. \quad (14)$$

It gives

$$\eta = \frac{\sum_\sigma \Delta m_{I\sigma} + \Delta m_{LO}}{1 + \sum_\sigma \Delta m_{I\sigma} + \Delta m_{LO}}, \quad (15)$$

where $\Delta m_{I\sigma}$ and Δm_{LO} are related respectively to IO and LO phonons and defined as follows

$$\Delta m_{I\sigma} = \frac{2\hbar^2}{m} \sum_q \frac{|\phi_G(\sigma, q)|^2 q^2 \cos^2\vartheta}{\left(\hbar\omega_\sigma + \frac{\hbar^2 q^2}{2m}\right)^3}, \quad (15a)$$

and

$$\Delta m_{LO} = \frac{2\hbar^2}{m} \sum_k \frac{|\phi_B(k_z)|^2 k_t^2 \cos^2\vartheta}{\left(\hbar\omega_{L1} + \frac{\hbar^2 k_t^2}{2m}\right)^3} \cdot \quad (15b)$$

In equation (15) ϑ denotes the angle between the in-plane wave-vectors $\mathbf{k}_t$ or $\mathbf{q}$ and the total momentum $\mathbf{P}_t$. Inserting equations (12, 13, 15) into (11), we finally obtain

$$\begin{aligned} E_2 &= \frac{\mathbf{P}_t^2}{2m^*} - \sum_\sigma E_{I\sigma} - E_{LO} \\ &= \frac{\mathbf{P}_t^2}{2m^*} - \sum_{\sigma q} \frac{|\phi_G(\sigma, q)|^2}{\hbar\omega_\sigma + \frac{\hbar^2 q^2}{2m}} \\ &\quad - \sum_k \frac{|\phi_B(k_z)|^2}{\hbar\omega_{L1} + \frac{\hbar^2 {k_t}^2}{2m}} + O(\mathbf{P}_t^4). \end{aligned} \quad (16)$$

The last term in equation (16) stands for the higher order terms over fourth power of the total momentum $\mathbf{P}_t$, which can be neglected for the slow-moving polarons. m^* is the polaron effective mass along the direction parallel to $x-y$ plane and given by

$$m^* = m\Big(1 + \sum_\sigma \Delta m_{I\sigma} + \Delta m_{LO}\Big). \quad (17)$$

The trial wave-function $|\phi\rangle$ for the interface state of the electron is chosen as following form [9,13]

$$|\phi\rangle = \begin{cases} -\left(\beta^3/2\right)^{1/2} z \exp(\beta z/2), & z \le 0 \\ 0, & z > 0 \end{cases} \quad (18)$$

where β is a variational parameter which will be determined by minimizing the expectation value of the polaron energy E in equation (9).

Changing the summations in equations (15, 16) into integrals by using the following relations

$$\sum_k \to \frac{V}{(2\pi)^3} \int d\mathbf{k}, \qquad \sum_q \to \frac{S}{(2\pi)^2} \int d\mathbf{q},$$

the polaron variational energy terms E_1 and E_2 can be rewritten as

$$E_1 = \frac{\hbar^2\beta^2}{8m} + \frac{3eF_z}{\beta} - \frac{\beta e^2 (\varepsilon_{\infty 2} - \varepsilon_{\infty 1})}{8\varepsilon_{\infty 1} (\varepsilon_{\infty 2} + \varepsilon_{\infty 1})}, \quad (19)$$

$$\begin{aligned} E_2 = \frac{\mathbf{P}_t^2}{2m^*} &- \sum_\sigma \alpha_\sigma \hbar\omega_\sigma \int_0^\infty dq \frac{u_\sigma \beta^6}{(q+\beta)^6 (u_\sigma^2 + q^2)} \\ &- \alpha_{L1} \hbar\omega_{L1} \int_0^\infty dz \int_0^\infty d\rho \frac{u_{L1}\beta^6 \rho}{\pi(\rho^2 + K^2)(u_{L1}^2 + \rho^2)} \\ &\times \left[\frac{4k^2 \left(3\beta^2 - 4k^2\right)^2}{(\beta^2 + 4k^2)^6} + \left(\frac{1}{\beta^3} - \frac{\beta\left(\beta^2 - 12k^2\right)}{(\beta^2 - 4k^2)^3}\right)^2\right], \end{aligned} \quad (20)$$

where

$$\alpha_{L1} = \left(\frac{1}{\varepsilon_{\infty 1}} - \frac{1}{\varepsilon_{01}}\right) \frac{me^2}{\hbar^2 u_{L1}}, \quad (20a)$$

$$\text{and} \quad \alpha_\sigma = \frac{2me^2}{\left(\delta_1^2 + \delta_2^2\right) \hbar^2 \omega_\sigma^2 u_\sigma}, \quad (20b)$$

are respectively the dimensionless coupling constants of the interaction between the electron and half space bulk LO phonons in material "1" and that between the electron and the σth branch of the IO phonon modes.

$$u_{L1} = \left(\frac{2m\omega_{L1}}{\hbar}\right)^2, \ \text{and} \ u_\sigma = \left(\frac{2m\omega_\sigma}{\hbar}\right)^2.$$

In the similar way, equation (17) can be reduced to be

$$\begin{aligned} \frac{m^*}{m} = 1 &+ \sum_\sigma \alpha_\sigma \int_0^\infty dq \frac{2u_\sigma^3 \beta^6 q^2}{(q+\beta)^6 \left(u_\sigma^2 + q^2\right)^3} \\ &+ \alpha_{L1} \int_0^\infty dz \int_0^\infty d\rho \frac{u_{L1}^3 \beta^6 \rho^3}{\pi(\rho^2 + K^2)\left(u_{L1}^2 + \rho^2\right)^3} \\ &\times \left[\frac{4k^2 \left(3\beta^2 - 4k^2\right)^2}{(\beta^2 + 4k^2)^6} + \left(\frac{1}{\beta^3} - \frac{\beta\left(\beta^2 - 12k^2\right)}{(\beta^2 - 4k^2)^3}\right)^2\right]. \end{aligned} \quad (21)$$

Table 1. Parameters used in the numerical calculation. Energy is in unit of meV and mass in unit of the bare electron.

	GaAs	$Al_xGa_{1-x}As$
m	0.067	
$\hbar\omega_{LO}$	36.25	$36.25 + 1.83x + 17.12x^2 - 5.11x^3$
$\hbar\omega_{TO}$	33.29	$33.29 + 10.70x + 0.03x^2 - 0.86x^3$
ε_0	13.18	$13.18 - 3.12x$
ε_∞	10.89	$10.89 - 2.73x$

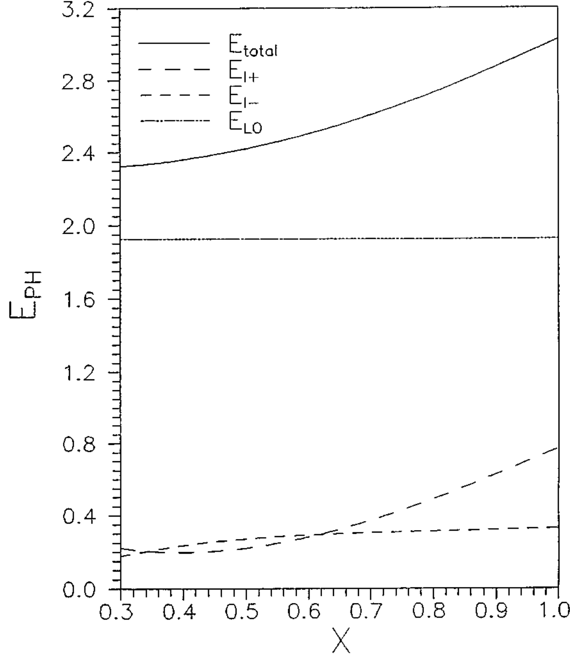

Fig. 1. Contributions (in unit of meV) of bulk LO phonons and two branches of IO phonon modes to the polaron ground state energies as functions of the Al composition x for GaAs/$Al_xGa_{1-x}As$ heterojunction.

In equations (20, 21), the last two terms describe respectively the contribution from the IO and bulk LO phonons.

3 Numerical results and discussion

The energy of the polaron should be calculated by a numerically variation of the energy (Eq. (9)) for specific systems. As an example we consider the GaAs/$Al_xGa_{1-x}As$ heterojunction, where GaAs is refereed as material "1" and $Al_xGa_{1-x}As$ as material "2". We have performed the numerical variation for the practically realizable system with the Al composition $x \geq 0.3$. An effective phonon mode approximation for the electron-LO-phonon interaction in the ternary mixed crystal $Al_xGa_{1-x}As$ is adopted here to obtain the IO phonon modes [18,19]. The parameters used in the computations are listed in Table 1 [18].

Inserting equations (19, 20) into (9) and performing the numerical variation, one can obtain the ground state energies of interface polarons. We choose $F_s = 20$ kV/cm

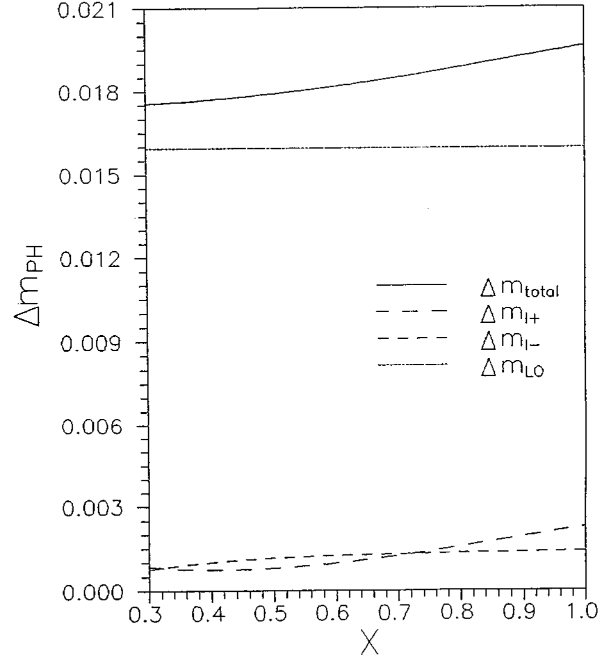

Fig. 2. Contributions (in unit of the bare electron mass) of bulk LO phonons and two branches of IO phonon modes to the polaron effective mass as functions of the Al composition for GaAs/$Al_xGa_{1-x}As$.

for the triangular potential describing the energy-band bending in GaAs. The variational results show that the polaron average distance from the interface is around 50 Å which is in good agreement with the result of electron distribution given by Ando [9]. This indicates that our approximation is reasonable. The phonon contributions to the polaron ground state energies display in two aspects: (1) self-trapping terms, *i.e.* the last two terms in equations (20), and (2) mass renormalization (Eq. (21)). The numerical results for the two kinds of contributions are shown in Figures 1 and 2.

From equation (16), the self-trapping energy can be written as the summation of the contributions from three different branches of phonon modes

$$E_{total} = E_{I+} + E_{I-} + E_{LO},$$

whose curves as functions of the Al composition x are plotted in Figure 1. It is seen that the contribution E_{I+} from the IO phonon mode of frequency ω_+ decreases with increasing the Al composition x at beginning. It reaches a minimum value around $x = 0.4$ then increases with x, and finally tends to the maximum when $x = 1$. On the contrary, the contribution E_{I-} from the mode of ω_- increases monotonously with increasing x. There is a intersection of E_{I+} and E_{I-} in the middle range of x. It is caused by $\alpha_+ < \alpha_-$. The contribution from bulk LO phonon mode keeps independent on x because the electrons do not penetrate into the $Al_xGa_{1-x}As$ layers in our model. The typical values of the ratio $\sum_\sigma E_{I\sigma}/E_{LO}$ of the total IO-phonon contribution to the LO-phonon contribution are 0.207 for

$x = 0.3$ and 0.572 for $x = 1$. This indicates that the contributions of IO phonons to the polaron ground-state energies are comparable with that of LO phonons for higher Al composition $Al_xGa_{1-x}As$ systems. The influences of IO phonons can not be neglected even for the lower Al composition cases, although the bulk LO phonons make more important contributions. It follows that the two branches of IO phonon modes should be considered in dealing with the interface states of electrons as pointed out by our previous papers [15,16].

The relative shifts of the polaronic effective mass due to the influence of phonons can be written as (see Eqs. (17, 21))

$$\Delta m_{total} = \Delta m_{I+} + \Delta m_{I-} + \Delta m_{LO},$$

where the three terms denote the contributions from two branches of IO phonons with frequencies ω_+ and ω_- and a bulk LO phonon branch with frequency ω_{LO}. The computed results as functions of x are given in Figure 2. The characteristics of the curves of Δm_{I+}, m_{I-}, m_{LO} and Δm_{ph} are respectively similar to that of the corresponding curves in Figure 1. However, the IO phonon influence on the polaron effective mass is negligible weak (about $0.1 \sim 0.3\%$) and the ratio $\sum_\sigma \Delta m_{I\sigma}/\Delta m_{LO}$ of the IO-phonon influence to the LO-phonon influence, such as values 0.101 for $x = 0.3$ and 0.230 for $x = 1$, is also smaller than that on the self-trapping energy (Fig. 1). The variations of the contributions of IO phonons to the relative shift of the effective mass with the composition x are also gentler than that in Figure 1. In short the IO phonon influence on the effective mass of the interface polaron is not important.

Moreover the numerical result also indicates that the influence of image potential on the polaronic states is very weak. If the band-bending potential is removed, the polaron may move into the inside of GaAs far from the interface and the result approaches approximately to the result of three dimensional polarons. At the limit of $\beta \to \infty$, our model gives the result of 2D interface polarons.

In conclusion, we have varationally investigated the interface polaron problem in a heterojunction system. Out of the previous works a bending energy band near the interface, which is verified essential to bind the electron in the vicinity of the interface, is considered together with the influences of image potential and electron-phonon interaction. A triangular potential is reasonably adopted to describe band bending potential well. The binary crystal-ternary mixed crystal heterojunction system $GaAs/Al_xGa_{1-x}As$ is concretely considered and an effective phonon mode approximation is used to describe the optical phonon modes in a ternary mixed crystal. The computed result of the ground state energy and the effective mass of the interface polaron for $GaAs/Al_xGa_{1-x}As$ heterojunction shows that the influence of the IO phonons is not negligible, in special for the higher Al composition cases both of the bulk LO and IO phonons is important. In addition we have used an infinite barrier on the interface which will be improved to consider the wave functions of the electrons penetrating through the interface later on. This may enhance the influence of interface phonons.

This work was supported by the National Natural Science Foundation (Project 19474027) of P.R. China and the Found for Excellent Young University Teachers of the State Education Commission of China.

References

1. L. Wendler, R. Pechestedt, Phys. Stat. Sol. (b) **141**, 129 (1987).
2. L. Wendler, R. Haupt, Phys. Stat. Sol. (b) **143**, 487 (1987).
3. N. Mori, T. Ando, Phys. Rev. B **40**, 6175 (1989).
4. X.X. Liang, X. Wang, Phys. Rev. B **43**, 5155 (1991).
5. X.X. Liang, J. Phys. Condens. Matter. **41**, 9769 (1992).
6. G.Q. Hai, F.M. Peeters, J.T. Devreese, Phys. Rev. B **48**, 4666 (1993).
7. R.S. Zheng, S.L. Ban, X.X. Liang, Phys. Rev. B **49**, 1796 (1994).
8. M.A. Brummell, R.J. Nicholas, M.A. Hopkins, J.J. Harris, C.T. Foxon, Phys. Rev. Lett. **58**, 77(1987).
9. A. Ando, J. phys. Soc. Jpn **51**, 3893 (1982); 3900 (1982).
10. X. Wu, F.M. Peeters, J.T. Devreese, Phys. Rev. B **40**, 4090 (1989).
11. X.X. Liang, Solid State Commun. **55**, 215 (1985).
12. E.P. Pokatilov, S.I. Beril, V.M. Formin, G.Yu. Riabukhin, Phys. Stat. Sol. (b) **156**, 225 (1989).
13. M.H. Degani, G.A. Farias, Phys. Rev. B **41**, 3572 (1990).
14. G.A. Farias, M.H. Degani, O. Hipolito, Phys. Rev. B **43**, 4113 (1991).
15. S.L. Ban, X.X. Liang, R.S. Zheng, Phys. Lett. A **192**, 110 (1994).
16. S.L. Ban, X.X. Liang, R.S. Zheng, Phys. Rev. B **51**, 2351 (1995).
17. W. Xu, F.M. Peeters, J.T. Devreese, Phys. Rev. B **48**, 1562 (1993).
18. S. Adachi, J. Appl. Phys. **58**, R1 (1985).
19. X.X. Liang, J.S. Yang, Solid State Commun. **100**, 629 (1996).
20. S. Das Sarma, A. Madhukar, Phys. Rev. B **22**, 2823 (1980).