Temperature dependence of the effective mass of the interface polaron

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Abstract. The temperature dependences of the effective mass and the self-energy of the interface polaron are investigated by means of the Lee–Low–Pines variation method. The influence of the electron interaction with both the bulk longitudinal optical (LO) and the surface optical (SO) phonons on the temperature characteristic of the interface polaron is discussed. Numerical calculation, for GaAs–GaSb as an example, illustrates that both the effective mass and the self-energy will decrease with increasing temperature. Near the interface of crystals, the electron–SO phonon interaction will play the main role in determining the temperature behaviour of the interface polaron.

1. Introduction

Recently, there have been some new works on the investigation of the temperature dependence of the polaron mass [1–7]. In these theoretical studies, the different mechanisms of the electron–phonon interaction and the different theoretical approximation methods have provided two completely contrary conclusions. In early studies, Yokota [8] found that the polaron mass would decrease with increasing temperature by using the Hartree approximation. However, using the Gurari variation method, Fulton [9] reached the opposite conclusion. Up to now, the conclusions have not been identical. At low lattice temperature, some theories [1, 2] predicted the same result as did Yokota, while others [3, 4] led to a polaron mass that would increase with increasing temperature.

The polaron mass in crystals is usually determined by cyclotron resonance experiments in a weak magnetic field. For different materials the experimental results also showed the same two contrary conclusions. The experimental data in the silver halides illustrated that the mass would increase as the lattice temperature went up [10]. In the cyclotron resonance measurements on GaAs–Ga$_{1-x}$Al$_x$As heterojunctions, Brummell *et al* [11] reported an anomalous case, i.e. the mass would increase with temperature up to about 100 K and start to decrease for higher temperature.

With the wide application of heterojunctions and superlattices to technology, the electron–phonon interaction as the main factor to determine the temperature behaviour of the polaron has given rise to great interest. But only the temperature dependence of

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Crystal   Crystal
'2' (GaSb)   '1' (GaAs)

0 ├─────────────────────► z
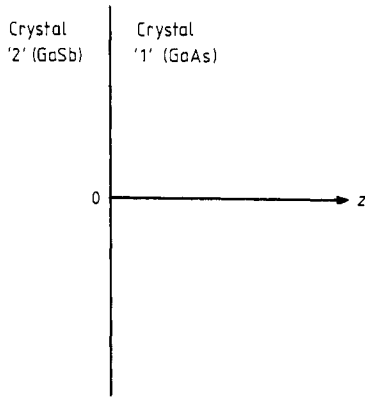
Figure 1. Geometry of the interface between two polar crystals.

the interaction between the quasi-free electron and the bulk longitudinal optical (LO) phonons has been investigated [6, 12, 13]. The magnetophonon resonance results in [11] also produced phonon frequencies significantly below LO mode values. So, it could be suggested that the interaction between the electron and other phonon modes associated with the presence of the interface should be considered.

Since the 1970s, the behaviour of the electron–phonon interaction near the surface or interface of the dielectric layer has been studied. For the first time, Lucas *et al* [14] took the electron–phonon interaction into account in their study on the bilayer system. Then Evans and Mills [15], by using the variation method, investigated the case where the electron interacted with both the surface and bulk LO waves and the phonons were considered as the only electric-dipole-active excitations. The importance of the electronic polarisability was first pointed out by Licari and Evrard [16]. Recently, with the consideration of the effect of electronic polarisability, Wendler [17] and Pen [18] deduced the equations for the polarisation eigenmodes of the dielectric bilayer system respectively from the microscopic dynamical equation and from the microscopic electrostatic potential. In these works, the authors developed the models of the electron–phonon interaction in the dielectric bilayer system and some of them also calculated the effective mass and interaction energies of the interface polaron in the limit of zero temperature.

The purpose of this present paper is to explore the effect of the electron–phonon interaction on the temperature behaviour of the interface polaron. With both the electron–bulk LO phonon and the electron–SO phonon interactions included, we obtain the expressions of the effective mass and the self-energy as functions of finite temperature by using the Lee–Low–Pines variation technique [19]. From the calculations, for GaAs–GaSb as an example, it is found that the effective mass and self-energies will both decrease with increasing temperature. It is also learnt that when the electron approaches the surface or interface of crystals the temperature dependence of these quantities will be entirely determined by the SO mode effect. The results presented here give one the main features of the contribution of the electron–phonon interaction to the temperature characteristic of the interface polaron. The variation method used here provides a reasonable approximation for weakly and intermediately coupled polarons.

2. The Hamiltonian

Figure 1 gives an illustration of the problem we wish to consider. An interface between two polar crystals (such as GaAs–GaSb) is perpendicular to the z axis; the semi-infinite

space $z > 0$ is occupied by the crystal (GaAs) represented by label '1', whereas the space $z < 0$ is full of another crystal (GaSb) represented by label '2'. A slow electron is placed inside the polar crystal '1', a distance z ($z > 0$) from the interface. We assume the effective-mass approximation to be valid and, for the slowly moving electron, the effect of small and finite penetration of the electron through the interface to be negligible. Because our interest is directly to study the polaron's temperature behaviour quali-tatively, for simplicity we only consider the interaction between the electron and long-wave optical phonons without the influence of the electronic polarisability. With the above considerations, the Hamiltonian of the electron–phonon system in explicit form can be written as

$$H = \frac{p_z^2}{2m^*} + \frac{\hbar^2 K_\parallel^2}{2m^*} - \frac{e^2(\varepsilon_{\infty 1} - \varepsilon_{\infty 2})}{4z\varepsilon_{\infty 1}(\varepsilon_{\infty 1} + \varepsilon_{\infty 2})} + \sum_w \hbar\omega_l a_w^+ a_w$$

$$+ \sum_q \hbar\omega_s b_q^+ b_q + \sum_w \frac{\sin(w_z z)}{w} (V^* \, e^{-i w_\parallel \cdot r_\parallel} a_w^+ + \text{HC})$$

$$+ \sum_q \frac{e^{-qz}}{\sqrt{q}} (C^* \, e^{-iq\cdot r_\parallel} b_q^+ + \text{HC}). \tag{1}$$

In equation (1), the first two terms are the kinetic energies of the electron in the directions perpendicular and parallel to the interface of the crystals, where m^* is the band mass of the electron and K is its wavevector (in equation (1) the subscript $\parallel$ denotes the projection of a given vector onto a plane parallel to the interface). The third term represents the energy of the image potential, in which ε_∞ is the optical dielectric constant. From the theoretical viewpoint, undoubtedly, the image potential comes from the interaction between electron and surface phonons, which may be regarded as the macroscopical description of the complicated electron–SO interaction near the transition layer between the two media and cannot be directly obtained from the electron–SO interaction [18]. The image potential is proportional to $(\varepsilon_{\infty 1} - \varepsilon_{\infty 2})$; when $\varepsilon_{\infty 1} > \varepsilon_{\infty 2}$ the positive value indicates repulsion, and when $\varepsilon_{\infty 1} < \varepsilon_{\infty 2}$ the negative value represents attraction. Since we are interested in discussing the polaron in a bound state near the interface, in this paper we only consider the case with $\varepsilon_{\infty 1} < \varepsilon_{\infty 2}$. The fourth and fifth terms in equation (1) stand for the energy of the bulk LO and SO phonon field, respectively. The last two terms describe the electron–bulk LO phonon and electron–SO phonon interaction energies. In these expressions, a_w^+ (a_w) is the creation (annihilation) operator of the bulk LO phonon with frequency ω_l and wavevector w, b_q^+ (b_q) is the corresponding operator for the SO phonon with frequency ω_s and wavevector q. The coefficients V^* and C^* are given by

$$V^* = i \left(\frac{4\pi\hbar\omega_l e^2}{\varepsilon V} \right)^{1/2}$$

$$C^* = i \left(\frac{\pi\hbar\omega_s e^2}{\varepsilon^* A} \right)^{1/2} \tag{2}$$

and

$$\frac{1}{\varepsilon} = \frac{1}{\varepsilon_{\infty 1}} - \frac{1}{\varepsilon_0}$$

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

where ε_0 is the static dielectric constant, and A and V are the interface area and the volume of crystal '1', respectively.

According to the variation treatment of Lee, Low and Pines [9], we begin by introducing the first canonical transformation U_1, which removes the coordinate $r_\parallel$ from the Hamiltonian

$$U_1 = \exp\left(-i\sum_w a_w^+ a_w \boldsymbol{w}_\parallel \cdot \boldsymbol{r}_\parallel - i\sum_q b_q^+ b_q \boldsymbol{q} \cdot \boldsymbol{r}_\parallel \right). \tag{3}$$

The transformed Hamiltonian is obtained

$$H' = U_1^{-1} H U_1$$

$$= \frac{p_z^2}{2m^*} + \frac{e^2(\varepsilon_{\infty1} - \varepsilon_{\infty2})}{4z\varepsilon_{\infty1}(\varepsilon_{\infty1} + \varepsilon_{\infty2})} + \sum_w \hbar\omega_l a_w^+ a_w + \sum_q \hbar\omega_s b_q^+ b_q$$

$$+ \frac{\hbar^2}{2m^*}\left(\boldsymbol{K}_\parallel - \sum_w \boldsymbol{w}_\parallel a_w^+ a_w - \sum_q \boldsymbol{q} b_q^+ b_q \right)^2$$

$$+ \sum_w \frac{1}{w}\sin(w_z z)(V^* a_w^+ + V a_w) + \sum_q \frac{e^{-qz}}{\sqrt{q}}(C^* b_q^+ + C b_q). \tag{4}$$

Then we perform the second canonical transformation U_2

$$U_2 = \exp\left(\sum_w (a_w^+ f_w - a_w f_w^*) + \sum_q (b_q^+ g_q - b_q g_q^*) \right). \tag{5}$$

The operator U_2 describes the displacements of the lattice oscillators, in which the parameters f_w, f_w^*, g_q and g_q^* are treated as variational parameters, to be determined by the requirement that the energy of the system should be minimised. After some tedious but straightforward algebra, the transformed Hamiltonian is written in three parts

$$H^* = U_2^{-1} H' U_2 = H_0^* + H_1^* + H_2^*$$

$$H_0^* = U_2^{-1}\frac{p_z^2}{2m^*} U_2 + \frac{\hbar^2}{2m^*}\left(\boldsymbol{K}_\parallel - \sum_w a_w^+ a_w \boldsymbol{w}_\parallel - \sum_q b_q^+ b_q \boldsymbol{q} \right)^2$$

$$+ \frac{e^2(\varepsilon_{\infty1} - \varepsilon_{\infty2})}{4z\varepsilon_{\infty1}(\varepsilon_{\infty1} + \varepsilon_{\infty2})} + \frac{\hbar^2}{2m^*}\left[\left(\sum_w |f_w|^2 \boldsymbol{w}_\parallel \right)^2 + \left(\sum_q |g_q|^2 \boldsymbol{q} \right)^2 \right]$$

$$+ \sum_w \frac{\sin(w_z z)}{w}(V^* f_w^* + V f_w) + \sum_q \frac{e^{-qz}}{\sqrt{q}}(C^* g_q^* + C g_q)$$

$$+ \sum_w |f_w|^2\left(\hbar\omega_l - \frac{\hbar^2}{m^*}\boldsymbol{w}_\parallel \cdot \boldsymbol{K}_\parallel + \frac{\hbar^2}{2m^*}\boldsymbol{w}_\parallel^2 \right) + \sum_q |g_q|^2$$

$$\times \left(\hbar\omega_s - \frac{\hbar^2}{m^*}\boldsymbol{q} \cdot \boldsymbol{k}_\parallel + \frac{\hbar^2}{2m^*}\boldsymbol{q}^2 \right) + \sum_w \hbar\omega_l a_w^+ a_w + \sum_q \hbar\omega_s b_q^+ b_q$$

$$+ \frac{\hbar^2}{m^*}\left(\sum_w a_w^+ a_w |f_w|^2 \boldsymbol{w}_\parallel^2 + \sum_q b_q^+ b_q |g_q|^2 \boldsymbol{q}^2 \right)$$

$$+ \sum_w \left\{ a_w^+ \left[\frac{V^* \sin(w_z z)}{w} + f_w\left(\hbar\omega_l - \frac{\hbar^2}{m^*}\boldsymbol{w}_\parallel \cdot \boldsymbol{K}_\parallel \right. \right.\right.$$

$$\left.\left.\left. + \frac{\hbar^2}{2m^*}\boldsymbol{w}_\parallel^2 + \frac{\hbar^2}{m^*}\boldsymbol{w}_\parallel \sum_{w'} |f_w|^2 \boldsymbol{w}_\parallel' \right) \right] + HC \right\} + \sum_q \left\{ b_q^+ \left[\frac{e^{-qz}}{\sqrt{q}} C^* \right.\right.$$

$$+ g_q \left(\hbar \omega_s - \frac{\hbar^2}{m^*} \boldsymbol{q} \cdot \boldsymbol{K}_\parallel + \frac{\hbar^2}{2m^*} \boldsymbol{q}^2 + \frac{\hbar^2}{m^*} \boldsymbol{q} \sum_{q'} |g_q|^2 \boldsymbol{q}' \right) \Bigg] + \text{HC} \Bigg\}. \tag{6a}$$

$$H_1^* = \frac{\hbar^2}{2m^*} \sum_{h,w'} \boldsymbol{w}_\parallel \cdot \boldsymbol{w}'_\parallel (a_w a_{w'} f_w^* f_{w'}^* + a_w^+ a_{w'}^+ f_w f_{w'} + 2 a_w a_{w'}' f_w^* f_{w'})$$

$$+ \frac{\hbar^2}{m^*} \sum_{w,w'} \boldsymbol{w}_\parallel \cdot \boldsymbol{w}'_\parallel (a_w^+ a_w a_{w'} f_{w'}^* + a_w^+ a_w a_{w'}^+ f_{w'})$$

$$+ \frac{\hbar^2}{2m^*} \sum_{q,q'} \boldsymbol{q} \cdot \boldsymbol{q}' (b_q b_{q'} g_q^* g_{q'}^* + b_q^+ b_{q'}^+ g_q g_{q'} + 2 b_q b_{q'}^+ g_q^* g_{q'})$$

$$+ \frac{\hbar^2}{m^*} \sum_{q,q'} \boldsymbol{q} \cdot \boldsymbol{q}' (b_q^+ b_q b_{q'} g_{q'}^* + b_q^+ b_q b_{q'}^+ g_{q'}) \tag{6b}$$

$$H_2^* = \frac{\hbar^2}{m^*} \Bigg(\sum_{w,q} \boldsymbol{w}_\parallel \cdot \boldsymbol{q} [a_w^+ a_w b_q g_q^* + a_w^+ a_w b_q^+ g_q + a_w^+ a_w |q_q|^2 + a_w b_q^+ b_q f_w^*$$

$$+ a_w b_q f_w^* g_q^* + a_w b_q^+ f_w^* g_q + a_w f_w^* |g_q|^2 + a_w^+ b_q b_q^+ f_w$$

$$+ a_w^+ b_q f_w g_q^* + a_w^+ b_q^+ f_w g_q + a_w^+ f_w |g_q|^2 + b_q^+ b_q |f_w|^2$$

$$+ b_q g_q^* |f_w|^2 + b_q^+ g_q |f_w|^2 + |f_w|^2 |g_q|^2] \Bigg). \tag{6c}$$

We choose $|\{N_l(w)\}, \{N_s(q)\}\rangle$ as the wavefunction to describe the phonon state, in which $\{N_l(w)\}$ and $\{N_s(q)\}$ represent the number of bulk LO and SO phonons, respectively. In our study, the temperature is restricted to the range lower than room temperature. So, even though the phonon frequencies will decrease with increasing temperature, we approximately take them as constants due to their very small relative change ($|\Delta\omega|/\omega \sim 1\%$) [11]. On the other hand, for the weakly and intermediately coupled cases, because the interaction energies between the electron and phonons are much smaller than the phonon energies ($\hbar\omega_l$ and $\hbar\omega_s$), we will omit them from the total energy of the phonons. As a result of these approaches, the eigenvalues of $a_w^+ a_w$ and $b_q^+ b_q$ in the phonon state at finite temperature can be approximately expressed by the thermal equilibrium values

$$N_1 = \langle a_w^+ a_w \rangle = [\exp(\hbar\omega_1/k_B T) - 1]^{-1} \tag{7a}$$

$$N_2 = \langle b_q^+ b_q \rangle = [\exp(\hbar\omega_s/k_B T) - 1]^{-1} \tag{7b}$$

where k_B is the Boltzmann constant.

Finally, the expected value of H^* referring to the phonon state is found as

$$\overline{H^*} = \langle \{N_l(w)\}, \{N_s(q)\} | H^* | \{N_s(q)\}, \{N_l(w)\} \rangle$$

$$= \frac{p_z^2}{2m^*} + \frac{\hbar^2 K_\parallel^2}{2m^*} - \frac{\hbar^2}{m^*} \left(\sum_w N_1 \boldsymbol{w}_\parallel \cdot \boldsymbol{K}_\parallel + \sum_q N_2 \boldsymbol{q} \cdot \boldsymbol{K}_\parallel \right)$$

$$+ \frac{e^2 (\varepsilon_{\infty 1} - \varepsilon_{\infty 2})}{4z \varepsilon_{\infty 1} (\varepsilon_{\infty 1} + \varepsilon_{\infty 2})} + \frac{\hbar^2}{2m^*} \left[\left(\sum_w |f_w|^2 \boldsymbol{w}_\parallel \right)^2 + \left(\sum_q |g_q|^2 \boldsymbol{q} \right)^2 \right]$$

$$+ \sum_w N_1 \hbar\omega_l + \sum_g N_2 \hbar\omega_s + \frac{\hbar^2}{m^*} \left(\sum_w N_1 |f_w|^2 w_\parallel^2 + \sum_q N_2 |g_q|^2 \boldsymbol{q}^2 \right)$$

$$+ \sum_w \frac{\sin(w_z z)}{w} (V^* f_w^* + V f_w) + \sum_q \frac{e^{-qz}}{\sqrt{q}} (C^* g_q^* + C g_q)$$

$$+ \sum_w |f_w|^2 \left(\hbar\omega_l - \frac{\hbar^2}{m^*} \mathbf{w}_\parallel \cdot \mathbf{K}_\parallel + \frac{\hbar^2}{2m^*} w_\parallel^2 \right)$$

$$+ \sum_q |g_q|^2 \left(\hbar\omega_s - \frac{\hbar^2}{m^*} \mathbf{q} \cdot \mathbf{K}_\parallel + \frac{\hbar^2}{2m^*} q^2 \right). \tag{8}$$

It should be noted that, at finite temperature, we still assume that the successive virtual phonons around the electron are emitted individually, i.e. the interaction between the phonons with different frequencies can be neglected. So, H_1^*, H_2^* and the terms in H_0^* expressing the different phonon interactions are omitted.

Because the direction of $\mathbf{K}_\parallel$ is the only preferred direction in the plane parallel to the interface, to simplify the deduction, one may express f_w and g_q in terms of the two quantities η_1 and η_2 defined by

$$\eta_1 \mathbf{K}_\parallel = \sum_w |f_w(\mathbf{w}_\parallel)|^2 \mathbf{w}_\parallel \qquad \eta_2 \mathbf{K}_\parallel = \sum_q |g_q(\mathbf{q})|^2 \mathbf{q}. \tag{9}$$

Inserting equation (9) into equation (8), the amplitudes f_w and g_q are determined by the variational condition that

$$\delta\bar{H}^*/\delta f_w = \delta\bar{H}^*/\delta g_q = 0. \tag{10}$$

One finds that

$$f_w = -\frac{V^*}{w} \sin(w_z z) \Big/ \left(\hbar\omega_l + \frac{\hbar^2}{2m^*} w_\parallel^2 (2N_1 + 1) - \frac{\hbar^2}{m^*} (1 - \eta_1) \mathbf{w}_\parallel \cdot \mathbf{K}_\parallel \right) \tag{11a}$$

$$g_q = -\frac{C^*}{\sqrt{q}} e^{-qz} \Big/ \left(\hbar\omega_s + \frac{\hbar^2}{2m^*} q^2 (2N_2 + 1) - \frac{\hbar^2}{m^*} (1 - \eta_2) \mathbf{q} \cdot \mathbf{K}_\parallel \right) \tag{11b}$$

and f_w^* and g_q^* are the corresponding conjugate expressions of equations (11a) and (11b).

From equations (9), (11a) and (11b), we obtain the following implicit equations for η_1 and η_2

$$\eta_1 \mathbf{K}_\parallel = \sum_w \frac{|V|^2 \mathbf{w}_\parallel}{w^2} \sin^2(w_z z) \Big/ \left(\hbar\omega_l + \frac{\hbar^2}{2m^*} w_\parallel^2 (2N_1 + 1) - \frac{\hbar^2}{m^*} (1 - \eta_1) \mathbf{w}_\parallel \mathbf{K}_\parallel \right)^2 \tag{12a}$$

$$\eta_2 \mathbf{K}_\parallel = \sum_q \frac{|C|^2 \mathbf{q}}{g} e^{-2qz} \Big/ \left(\hbar\omega_s + \frac{\hbar^2}{2m^*} q^2 (2N_2 + 1) - \frac{\hbar^2}{m^*} (1 - \eta_2) \mathbf{q} \cdot \mathbf{K}_\parallel \right)^2. \tag{12b}$$

Because we are interested only in the slow electron observed in experiments, we shall be content to calculate η_1 and η_2 to first order in an expansion in powers of $\mathbf{K}_\parallel$. On doing this, one readily obtains

$$\eta_1 = \alpha F_B(z)/[1 + \alpha F_B(z)] \tag{13a}$$

where

$$F_B(z) = \frac{4u_l^3}{\pi} \int_0^1 (1 - x^2) \, dx \int_0^\infty \frac{w^2[1 - \cos(2zxw)]}{[u_l^2 + (2N_1 + 1)(1 - x^2)w^2]^3} \, dw \tag{13b}$$

and

$$\eta_2 = \alpha F_S(z)/[1 + \alpha F_S(z)] \tag{14a}$$

where

$$F_S(z) = 4u_1 u_s^2 \left(\frac{1}{\varepsilon_{\infty 1} + \varepsilon_{\infty 2}} - \frac{1}{\varepsilon_{01} + \varepsilon_{02}} \right) \left(\frac{\varepsilon_{\infty 1} \varepsilon_{01}}{\varepsilon_{01} - \varepsilon_{\infty 1}} \right)$$

$$\times \int_0^\infty \frac{e^{-2qz} q^2}{[u_s^2 + (2N_2 + 1)q^2]^3} \, dq. \tag{14b}$$

In the above equations, the coupling constant α and the polaron wavevectors u_l and u_s are defined respectively by

$$\alpha = \frac{m^* e^2}{\hbar^2 u_l} \left(\frac{1}{\varepsilon_{\infty 1}} - \frac{1}{\varepsilon_{01}} \right) \tag{15a}$$

$$u_l = \left(\frac{2m^* \omega_l}{\hbar} \right)^{1/2} \qquad u_s = \left(\frac{2m^* \omega_s}{\hbar} \right)^{1/2}. \tag{15b}$$

These expressions of the variation parameters and η_1, η_2 may be substituted back into equation (8). By expanding relative terms to the first power of $K_{\parallel}$, we obtain the effective Hamiltonian, which is defined as the variational minimum of $\bar{H}^*$

$$H_{\text{eff}} = \text{Min } \bar{H}^*$$

$$= \frac{p_z^2}{2m^*} + \frac{e^2 (\varepsilon_{\infty 1} - \varepsilon_{\infty 2})}{4 z \varepsilon_{\infty 1} (\varepsilon_{\infty 1} + \varepsilon_{\infty 2})} + \frac{\hbar^2 K_{\parallel}^2}{2m^*} (1 - \eta_1 - \eta_2 + \eta_1^2 + \eta_2^2)$$

$$- \frac{\hbar^2}{m^*} \left(\sum_w N_1 w_{\parallel} \cdot K_{\parallel} + \sum_q N_2 q \cdot K_{\parallel} \right) + \sum_w N_1 \hbar \omega_l$$

$$+ \sum_q N_2 \omega_s \hbar - \sum_w \frac{|V|^2}{w^2} \sin^2 (w_z z) \bigg/ \left(\hbar \omega_l + \frac{\hbar^2}{2m^*} w_{\parallel}^2 (2N_1 + 1) \right)$$

$$- \sum_q \frac{|C|^2}{q} e^{-2qz} \bigg/ \left(\hbar \omega_s + \frac{\hbar^2}{2m^*} q^2 (2N_2 + 1) \right). \tag{16}$$

3. Effective mass and self-energies

According to the standard definition of the polaron effective mass [20], in equation (16) let

$$\frac{\hbar^2}{2M^*} K_{\parallel}^2 = \frac{\hbar^2}{2m^*} K_{\parallel}^2 (1 - \eta_1 - \eta_2 + \eta_1^2 + \eta_2^2).$$

Then we obtain the effective mass of the interface polaron as

$$M^*(z) = m^* (1 - \eta_1 - \eta_2 + \eta_1^2 + \eta_2^2)^{-1}. \tag{17}$$

For weakly and intermediately coupled polarons, we have $\alpha F_B(z) \ll 1$ and $\alpha F_S(z) \ll 1$. Then the effective mass can be approximately expressed as

$$M^*(z) \simeq m^* [1 + \alpha F_B(z) + \alpha F_S(z)]. \tag{18}$$

For higher moments, it is clear that the effective mass becomes $K_{\parallel}$-dependent, but we have here given only the $K_{\parallel} \simeq 0$ contribution, i.e. its value independent of $K_{\parallel}$. In the zero-temperature limit, N_1 and N_2 will obviously tend to zero and consequently $F_B(z)$ and $F_S(z)$ will also approach their values of zero temperature. So, the definition of the effective mass in the present paper is adequate because of no discrepancy between the expressions at zero and finite temperature.

The last two terms in H_{eff} (equation (16)) are self-energies E_s^B and E_s^S induced respectively by the electron–bulk LO phonon interaction and the electron–SO phonon

interaction. Both quantities are functions of $K_\parallel$, but for $K_\parallel \simeq 0$ their approach to limiting values will be independent of $K_\parallel$. Setting $K_\parallel = 0$ and transforming the summations into integrations, we obtain the expression of the self-energies

$$E_s^B(z) = - \frac{\alpha\hbar\omega_l}{\sqrt{(2N_1+1)}} \left(\frac{\pi}{2} - \int_0^\infty \frac{\exp[-2zu_ly/\sqrt{(2N_1+1)}]}{1+y^2} \, dy \right) \tag{19a}$$

$$E_s^S(z) = - \frac{2\alpha\hbar\omega_s}{\sqrt{(2N_2+1)}} \frac{u_l}{u_s} \left(\frac{1}{\varepsilon_{\infty 1}+\varepsilon_{\infty 2}} - \frac{1}{\varepsilon_{01}+\varepsilon_{02}} \right) \frac{\varepsilon_{01}\varepsilon_{\infty 1}}{\varepsilon_{01}-\varepsilon_{\infty 1}}$$

$$\times \int_0^\infty \frac{\exp[-2zu_sy/\sqrt{(2N_2+1)}]}{1+y^2} \, dy. \tag{19b}$$

The next step is to compute the expectation values of the effective mass and self-energies with reference to the wavefunction along the z coordinate. Just as mentioned earlier, we confine our attention only to a slow electron moving in crystal '1' ($z > 0$). Because the tunnelling of electrons through the interface is ignored for weak and intermediate coupling, we take the wavefunction of the electron equal to zero on the interface and close to zero in an exponential manner as the electron moves to the interface. We use a variational method of calculation and choose for our trial wavefunction

$$\varphi(z) = \begin{cases} 2\beta^{3/2} z\, e^{-\beta z} & z > 0 \\ 0 & z < 0 \end{cases} \tag{20}$$

where β is the variational parameter. This wavefunction is a special case of a more general form used in some papers [15].

Consequently, one readily finds the expectation value of energy referring to $\varphi(z)$

$$E(K_\parallel) = \langle \varphi(z)|H_{\text{eff}}|\varphi(z)\rangle. \tag{21}$$

For the slow-moving electron, the general expression for $E(K_\parallel)$ is cumbersome and of little general interest. We display explicitly only $E(0)$, the energy at $K_\parallel = 0$,

$$E(0) = \frac{\hbar^2\beta^2}{2m^*} + \frac{e^2(\varepsilon_{\infty 1}-\varepsilon_{\infty 2})\beta}{4\varepsilon_{\infty 1}(\varepsilon_{\infty 1}+\varepsilon_{\infty 2})} + \sum_w N_1\hbar\omega_l + \sum_q N_2\hbar\omega_s$$

$$- \frac{\alpha\hbar\omega_l}{\sqrt{(2N_1+1)}} \left(\frac{\pi}{2} - G(\lambda) \right) - \frac{\alpha_s\hbar\omega_s}{\sqrt{(2N_2+1)}} G(\sigma). \tag{22}$$

The last two terms are the expectation values of self-energies, $\langle E_s^B\rangle$ and $\langle E_s^S\rangle$, respectively. In these expressions, we have

$$G(x) = \frac{(x^3-3x^5)\ln x + 0.5(\pi x^6 + 5x^5 - 3\pi x^4 + 6x^6 + x)}{(1+x^2)^3} \tag{23a}$$

and

$$\lambda = \frac{\beta}{u_l}\sqrt{(2N_1+1)} \qquad \sigma = \frac{\beta}{u_s}\sqrt{(2N_2+1)}$$

$$\alpha_s = \frac{2\alpha u_l}{u_s} \left(\frac{1}{\varepsilon_{\infty 1}+\varepsilon_{\infty 2}} - \frac{1}{\varepsilon_{01}+\varepsilon_{02}} \right) \left(\frac{\varepsilon_{01}\varepsilon_{\infty 1}}{\varepsilon_{01}-\varepsilon_{\infty 1}} \right). \tag{23b}$$

By utilising the variational wavefunction $\varphi(z)$, the expectation value of effective mass can be directly obtained as

Table 1. Characteristic parameters of crystals. All the parameters are taken from [21]. Energies are in millielectronvolts and m_0 is the free-electron rest mass.

	ε_0	ε_∞	$\hbar\omega_s$ (meV)	$\hbar\omega_l$ (meV)	m^*/m_0	α
GaAs	12.83	10.9	35.03	36.7	0.0657	0.0681
GaSb	15.69	14.44	29.28	29.8	0.047	0.0256
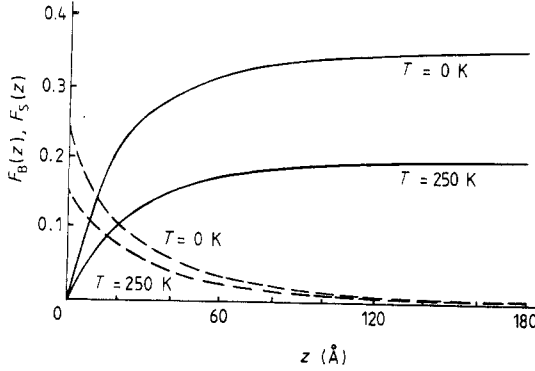
Figure 2. Effect of LO mode, $F_B(z)$ (——), and of SO mode, $F_S(z)$ (---), on the effective mass as a function of coordinate z at different temperatures.

$$\langle M^*(z)\rangle \simeq m^*[1 + \alpha\langle F_B(z)\rangle + \alpha\langle F_S(z)\rangle] \tag{24}$$

where

$$\langle F_B(z)\rangle = \frac{4u_1^3}{\pi}\int_0^1 (1-x^2)\,\mathrm{d}x \int_0^\infty \frac{w^2}{[u_1^2 + (2N_1+1)(1-x^2)w^2]^3}$$

$$\times \left(1 - \frac{\beta^4(\beta^2 - 3x^2w^2)}{(\beta^2 + x^2w^2)^3}\right)\,\mathrm{d}w \tag{25a}$$

$$\langle F_S(z)\rangle = 4u_lu_s^2 \left(\frac{1}{\varepsilon_{\infty1} + \varepsilon_{\infty2}} - \frac{1}{\varepsilon_{01} + \varepsilon_{02}}\right)\left(\frac{\varepsilon_{01}\varepsilon_{\infty1}}{\varepsilon_{01} - \varepsilon_{\infty1}}\right)$$

$$\times \int_0^\infty \frac{\beta^3 q^2}{[u_s^2 + (2N_2+1)q^2]^3(\beta+q)^3}\,\mathrm{d}q. \tag{25b}$$

4. Results and discussion

We have carried out a study of the effective mass and self-energies of the interface polaron at $K_\parallel \simeq 0$ by using the formulae obtained in § 3. Taking GaAs–GaSb as an example, we calculate these quantities and their expectation values at different temperatures.

The crystal characteristic parameters are related to the temperature. But for the temperature range ($T < 300$ K) we wish to study in this paper, their changes with temperature are very small [21]. In our calculation, these parameters are assumed as constants and taken as the values at low temperature. Table 1 shows the relative parameters of GaAs and GaSb crystals.

From equation (18), it is clear that the effective mass is determined by $F_B(z)$ and $F_S(z)$, which represent the effect of the electron–bulk LO phonon interaction and the electron–SO phonon interaction, respectively. Figure 2 gives a description of the variation of $F_B(z)$ and $F_S(z)$ with coordinate z at different temperatures. It is shown that the
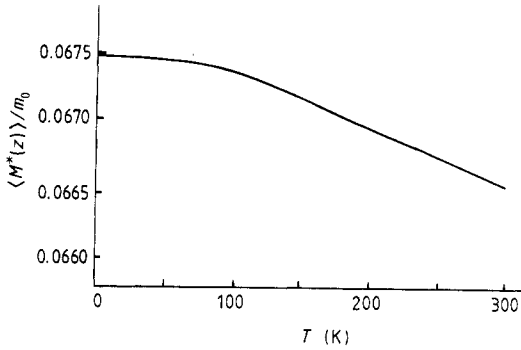
Figure 3. Expectation value of the effective mass $\langle M^*(z)\rangle/m_0$ versus finite temperature T (m_0 is the free-electron rest mass).
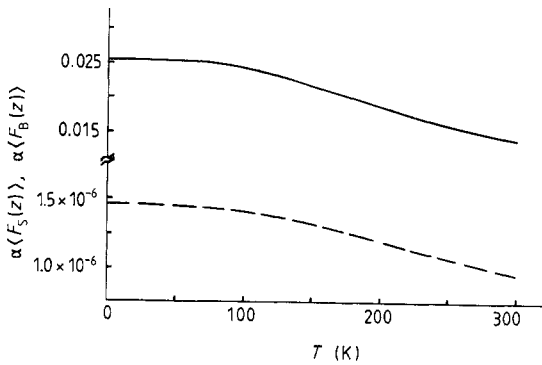

Figure 4. Comparison between the influence of electron–bulk LO phonon interaction and of electron–SO phonon interaction on the expectation value of the effective mass: (———) $\langle F_B(z)\rangle$, the contribution of LO mode; (– – – –) $\langle F_S(z)\rangle$, the contribution of SO mode.

polarised electric field produced by the bulk LO mode is very weak in the vicinity of the interface, so its effect on the effective mass will tend to zero as the electron approaches the interface. On departure of the electron from the interface, the bulk LO mode contribution will increase and become dominant rapidly. On the contrary, only when the electron is very close to the interface will the SO mode effect play the main role in influencing the effective mass. Thus, the temperature dependence of the effective mass will depend on the SO mode effect near the crystal interface and on the bulk LO mode effect far from the interface. With increasing temperature, the uncorrelated motion of phonons becomes an important factor and the coherence between the electron motion and the phonon motion becomes weaker. This results in the weakness of the electron–phonon interaction, namely in the decrease of the mass with increasing temperature. As seen in figure 2, both bulk LO and SO mode effects will be getting weaker when the temperature increases.

Figure 3 shows that, as a result of the temperature behaviour of the electron–phonon interaction, the expectation value of the effective mass $\langle M^*(z)\rangle/m_0$ will decrease with increasing temperature. As shown in figure 4, for the semi-infinite dielectric layer system, such a variation of $\langle M^*(z)\rangle/m_0$ will be determined entirely by the contribution of the bulk LO phonon, and the SO mode effect can be ignored.

In [11], for GaAs–Ga$_{1-x}$Al$_x$As heterojunctions, an anomalous increase in the polaron mass with increasing temperature was obtained. The experimental data also suggested that the dominant interaction of electrons would be with the modes associated with the presence of the interface. From the calculation of the polaron mass at finite temperature with the inclusion of full dynamical screening, Wu *et al* [6] theoretically obtained a temperature behaviour that qualitatively agreed with [11], but the results at 100 K are quantitatively a factor of almost 2 smaller. With the SO mode included in this
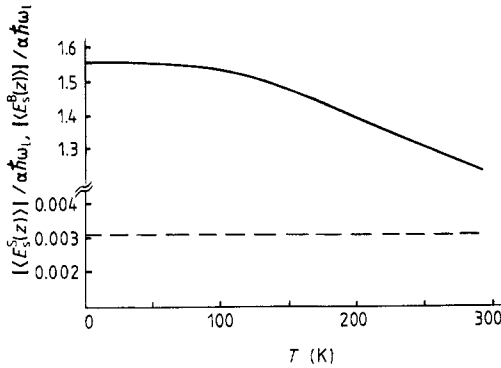
Figure 5. The expectation values of self-energies from the electron–LO phonon interaction and the electron–SO phonon interaction, respectively: (———) $\langle E_s^B \rangle$, LO self-energy; (- - - -) $\langle E_s^S \rangle$, SO self-energy.

paper, we find that in the two-dimensional limit ($z \rightarrow 0$) the temperature behaviour of the polaron mass is really attributed to the SO mode effect. Our numerical result is a bit smaller than the experimental data in [11], and, since we have not taken the screening of the electron–phonon interaction into account, there is no anomalous increase at low temperature obtained in this paper.

The self-energy consists of two parts, E_s^B and E_s^S, which are produced respectively by bulk LO mode effect and SO mode effect. We also calculate their expectation values with reference to $\varphi(z)$. Figure 5 gives us a comparison between the energy of electron–LO phonon interaction $\langle E_s^B \rangle$ and that of the electron–SO phonon interaction $\langle E_s^S \rangle$. Obviously, in such a system we consider that the value of $\langle E_s^S \rangle$ is very small and has almost no contribution to the temperature characteristic of the expectation value of the self-energy. So, the variation of $\langle E_s^B \rangle$ will represent the temperature dependence of the total self-energy, i.e. as shown in figure 5 the self-energy will decrease when the temperature goes up.

In our calculation, we have neglected the part of the Hamiltonian, namely H_1^* (equation ($6b$)), that represents the electron's recoil kinetic energy. The correlation between the emission of successive virtual phonons introduced by H_1^* will set a limit to the validity of our method. Since we have no dimensional arguments to fall back on for estimating corrections to our results, the validity of our calculation may best be estimated by calculating the lowest-order correction to the energy resulting from H_1^*. According to perturbation theory, the energy shift is given by

$$\Delta E_1 = - \sum_{n_2}{}' \frac{|\langle H_1^* \rangle_{n_1 n_2}|^2}{E_{n_2} - E_{n_1}} \tag{26}$$

where $\sum_{n_2}'$ is a sum over all the states in which H_1^* has non-vanishing matrix elements, i.e. in which there are two phonons more than the phonons in the phonon state: $|N_1, N_2\rangle$. From equation ($6b$), we readily find

$$\Delta E_1 = - \frac{\hbar^4}{4m^{*2}} \sum_{w_1, w_2} [N_1^2 (w_{1\parallel} \cdot w_{2\parallel})^2 \langle \varphi(z)| |f_{w_1}|^2 |f_{w_2}|^2 |\varphi(z)\rangle]/D_w$$

$$- \frac{\hbar^4}{4m^{*2}} \sum_{q_1, q_2} [N_2^2 (q_1 \cdot q_2)^2 \langle \varphi(z)| |g_{q_1}|^2 |g_{q_2}|^2 \varphi(z)]/D_q \tag{27}$$

where

$$D_w = 2\hbar\omega_1 - \frac{\hbar^2}{m^*}(w_{1\parallel} + w_{2\parallel}) \cdot K_\parallel(1 - \eta_1)$$

$$+ \frac{\hbar^2}{2m^*}(w_{1\parallel} + w_{2\parallel})^2 + \frac{\hbar^2}{m^*}(w_{1\parallel} + w_{2\parallel}) \cdot \sum_w n_1 w$$

and

$$D_q = 2\hbar\omega_s - \frac{\hbar^2}{m^*}(q_1 + q_2) \cdot K_\parallel(1 - \eta_2) + \frac{\hbar^2}{2m^*}(q_1 + q_2)^2 + \frac{\hbar^2}{m^*}(q_1 + q_2) \cdot \sum_q N_2 q$$

with f_w and g_q given by equations (11a) and (11b) and N_1 and N_2 given by equations (7a) and (7b). According to equations (26) and (27), our numerical calculations illustrate that the relative correction at $T = 0$ K may be the largest. So, we will only discuss the case in the limit of zero temperature to estimate the correction. Carrying out the indicated summations in equation (27) numerically up to order $\hbar^2 K_\parallel^2/2m^*$, at $T = 0$ K, we get

$$\Delta E_1 \simeq -0.0266\alpha^2\hbar\omega_l + 0.00441\left(\frac{\alpha}{1 + \alpha\langle F_B\rangle}\right)^2 \frac{\hbar^2 K_\parallel^2}{2m^*}. \tag{28}$$

From equations (16) and (21), the expectation value of the energy in the zero-temperature limit can be obtained as

$$E \simeq -1.566\alpha^2\hbar\omega_l + 1.026\left(\frac{1}{1 + \alpha\langle F_B\rangle}\right)\frac{\hbar^2 K_\parallel^2}{2m^*}. \tag{29}$$

Comparing the above numerical results, for $\alpha = 3$, we find the relative correction to the $K_\parallel$-independent term of approximately 5.1%; the relative correction to the $K_\parallel$-dependent term is only 1.9%. On the other hand, for the existence of the electron–phonon bound state near the surface, the value of α might be restricted to less than 2 [15]. On the whole, our variation method provides a reasonable approximation for the weakly and intermediately coupled interface polaron with $\alpha < 2$.

Acknowledgment

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