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Polaron Free Energy in GaAs Quantum Wells

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The polaron free energy in a GaAs/AlAs quantum well is calculated as a function of temperature and well width. The interaction considered is that between the conduction electrons and the GaAs-like polar optical oscillations. The calculation follows a perturbative scheme in the coupling constant for the thermodynamical potential in the one-particle limit. Phonons are described with the use of a long-wavelength dispersive electroelastic continuum model.

Zero temperature polaron properties in semiconducting heterostructures have been systematically investigated with the use of different model interaction Hamiltonians since the second half of the past decade (see, for instance [1 to 4]). However, the finite temperature polaron free energy does not seem to have been so far widely calculated in low-dimensional heterostructures may be due to the explicit difficulties for the application of the traditional scheme based on the Feynman path integral procedure [5 to 7] in systems bearing interfaces. An alternative way which is the use of the perturbative method coming from a Green‘s function approach to the thermodynamical potential appears to be appropriate in the case of semiconducting materials like the III–V and II–VI compounds, where the magnitudes of the electron–phonon coupling constants are small enough to allow for a perturbative treatment usually restricted – at most – to the second-order corrections (see, for instance [8]). Therefore, such a calculation process can be carried out as well in the case of semiconducting heterostructures made from those materials.

In this work, we are going to deal with a particular system, namely, a GaAs/AlAs double heterostructure (DHS), for which a Fröhlich-like interaction Hamiltonian has been recently put forward in the framework of a dispersive electroelastic continuum model (DECM) [9]. In all Fröhlich-like problems, the expansion for the electron–phonon correction to the electronic gas thermodynamical potential can be viewed as a series in the electron–phonon coupling constant α, in such a way that the n-th order term in the expansion for the one-electron Green‘s function is proportional to the n-th power of α [10]. This feature allows us to write the expression for the first-order correction (which is the usually evaluated in III–V arsenides) – equivalent to take into account the first "bubble" diagram in the expansion for the thermodynamical potential [10] – in the form

$$\Delta\Omega = \frac{1}{\beta}\int\limits_0^{\alpha}\frac{\mathrm{d}\alpha}{\alpha}\sum_{\mathbf{k},\zeta}\left\{\frac{G^{(1)}(\mathbf{k},\zeta;\tau)}{G^{(0)}(\mathbf{k},\zeta;\tau)}-1\right\}, \tag{1}$$

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where $G^{(1)}(\mathbf{k},\zeta;\tau)$ and $G^{(0)}(\mathbf{k},\zeta;\tau)$ are the first-order and unperturbed one-electron Green's functions, respectively, in the imaginary time representation, associated to electron states in the conduction band with effective mass m^*. $\mathbf{k}$ is the in-plane electron wavevector, and ζ is the quantum number labelling the energy states of the motion along the growth direction of the heterostructure, z. $\beta = 1/k_\mathrm{B}T$. We shall assume the non-degenerate situation and write, in the one-particle limit, the relation for the chemical potential μ as

$$\mathrm{e}^{\beta\mu} = \frac{2\pi}{S}\,\frac{\hbar^2\beta}{m^*}\left(\sum_{\zeta}\mathrm{e}^{-\beta E_\zeta}\right)^{-1} . \tag{2}$$

In our case, the conduction band electronic states in the GaAs/AlAs DHS are calculated using a finite barrier quantum-well model, explicitly considering the difference between the effective masses in both materials (see [1]). It will be also assumed that the electron is in the Γ-point even when really X is the lowest conduction band. This is done mostly in order to avoid the extra complication coming from the consideration of an indirect gap. The barrier height is taken to be $V_0 = 915$ meV. For that reason, we shall limit to consider only the discrete energy levels in the above expression ($\zeta = l$), avoiding the more intractable situation of the continuum part of the spectrum. On the other hand, we follow the usual procedure and use the so-called leading term approximation (LTA) [1], which means to consider only the intrasubband matrix elements corresponding to $l = 1$, the ground level.

The GaAs-like phonon modes in the DECM are neither purely confined slab modes nor interface modes [9]. There is a mixed character and certain modes are rather more interface-like than others. Furthermore, we only can say that the modes may be predominantly "longitudinal" (quasi-L) in some cases or predominantly "transversal" (quasi-T) in others because the polarization also exhibits a mixed character. The expression for the LTA electron–phonon matrix elements $I_{11}^{m}(q)$ within the DECM is reported in [4]. q is the phonon two-dimensional wavenumber, and m is a discrete index labelling the different modes appearing in the system.

With all this, it is possible to write for the LTA first-order polaron free energy correction in the DHS, the following expression [11]:

$$F^{(1)}(t) = -\frac{4\alpha\hbar\omega_\mathrm{LO}R}{d}\,\frac{\mathrm{e}^{-\beta\varepsilon_1}}{\sum\limits_{l}\mathrm{e}^{-\beta\varepsilon_l}}\sum_{m}\int\limits_{0}^{\infty}\mathrm{d}q\,\frac{qI_{11}^{\mathrm{m}}(q)}{\omega_{qm}}\int\limits_{0}^{t/2}\mathrm{d}x\,D_{qm}(x)\,\mathrm{e}^{-q^2R^2x(1-\frac{x}{t})} , \tag{3}$$

where $t = \hbar\omega_\mathrm{LO}\beta$ is a dimensionless temperature-dependent variable. ω_LO is the bulk GaAs longitudinal optical phonon frequancy, $\omega_{qm} = \omega_m(q)/\omega_\mathrm{LO}$, $\omega_m(q)$ being the dispersion relation of the m-th mode [4, 9], $R = (\hbar/2m^*\omega_\mathrm{LO})^{1/2}$ is the bulk polaron radius. The function $D_{mq}(x)$ is

$$D_{qm}(x) = \frac{\mathrm{e}^{\omega_{qm}x}}{\mathrm{e}^{\omega_{qm}t}-1} + \frac{\mathrm{e}^{-\omega_{mq}x}}{1-\mathrm{e}^{-\omega_{qm}t}} . \tag{4}$$

In the calculations, the values $\omega_\mathrm{LO} = 291.9\ \mathrm{cm}^{-1}$, $m^* = 0.0665m_0$, and $\alpha = 0.068$ were taken for GaAs. For the well barrier effective mass we used m^* (AlAs) = $0.15m_0$, m_0 being the bare electron mass.

In Fig. 1 the relative polaron free-energy F_r is shown as a function of the quantum well width d for different values of the temperature. F_r is defined as the ratio $F^{(1)}(t)/F^{(1)}_\mathrm{3D}(t)$;

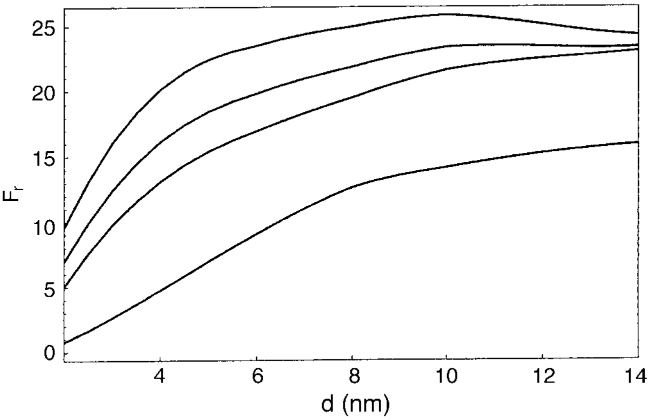

Fig. 1. Relative polaron free energy as a function of the GaAs quantum well width. Curves (in decreasing order) correspond to 613, 420, 300, and 0 K, respectively

where $F_{3D}^{(1)}(t)$, the polaron free-energy of first order for bulk GaAs is given by

$$F_{3D}^{(1)}(t) = -\frac{\alpha\hbar\omega_{LO}}{\sqrt{\pi}}\sqrt{t}\int_{0}^{t/2} dx\,\frac{D(x)}{\sqrt{x(t-x)}}\,, \tag{5}$$

where

$$D(x) = \frac{e^{x}}{e^{t}-1} + \frac{e^{-x}}{1-e^{-t}}\,. \tag{6}$$

In the limit $T = 0$ K ($t = \infty$), Eq. (5) gives precisely the bulk polaron binding energy value $-\alpha\hbar\omega_{LO}$.

The three upper curves in the figure correspond, from top to bottom, to the Debye temperature of GaAs ($T_D = 613$ K), the LO-phonon temperature of the material ($T_{ph} = \hbar\omega_{LO}/k_B = 420$ K), and to $T = 300$ K, respectively. Besides the room temperature value, the other two were chosen because they constitute significative temperatures for the material. For the sake of comparison, a lowest curve, corresponding to the $T = 0$ K polaron relative binding energy has been included. This curve is obtained from the expression resulting when taking the limit $t \to \infty$ of Eq. (3), which precisely coincides with the Rayleigh-Schrödinger-perturbation-theory equation presented in [4].

As expected, the polaron free energy raises with increasing quantum well width. The rate of increment varies for different temperatures indicating that the way by which the GaAs-like phonon modes contribute depends on the temperature as well. Nevertheless, it can be observed a tendency to change the monotony, which reverses towards a limiting bulk-value for d sufficiently large. This decreasing behavior will then be stronger at high temperatures – as it is shown in the curve corresponding to T_D – while is much more subtle for $T = 0$ K. Hence, the range of well width values selected represents the region of greater interest for the effect here studied. Furthermore, there exists another reason, this time of practical character: for higher values of d, the number of eigenmodes associated to the characterictics equations increases very rapidly, and the calculation process becomes really tedious [4, 9].

The relative polaron free energy is not reported for d below 2 nm because that region a macroscopic continuum model for the GaAs long-wavelength oscillations would certainly not work well, and its validity is doubtful. When $d \to 0$, only the bulk AlAs is present. However, in this study we have not considered so far the contribution to the electron–phonon interaction coming from the electric potential of the barrier modes. If taken into account, it will significantly change (by increasing) the polaronic correction for the smallest values of d; but in the case of well width around 10 nm and beyond the main contribution should come from GaAs-like polar optical modes.

The results obtained within this model indicate that the effect of the modification of the GaAs phonon spectrum due to the existence of interfaces is relevant only for layer thickness not larger than 100 Å. Significant differences with the 3D values are obtained for a GaAs-layer width of a few tens of angstroms. For wide enough wells, the use of the bulk Fröhlich Hamiltonian would provide correct results.

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