Electron-phonon interaction effects in a quasi-two-dimensional electron gas in the GaAs-$Ga_{1-x}Al_xAs$ heterostructure

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From a single-electron theory it is well established that the polaron effective mass in purely two-dimensional systems is larger than that in the corresponding three-dimensional case. On the other hand, recent cyclotron-resonance experiments have shown that the polaronic mass in two-dimensional GaAs heterostructures is a factor of 3 smaller than the three-dimensional results. In order to understand the discrepancy between the experiments and this simple theory we have improved the model by taking into account the electron interaction with both interface and longitudinal bulk phonons. We have also included in the calculation the effects of the electron screening within the random-phase-approximation formalism and the electron subband wave function. In contrast to previous works we have shown that the interface phonons give a significant contribution to the polaronic energy and effective mass and obviously cannot be neglected. The results of our calculations for the polaron mass correction are in excellent agreement with the experiment measurements.

Since the recent experimental observations of the magnetophonon resonance in quasi-two-dimensional systems there has been an increasing interest in the subject of surface polarons.[1-6] Most of the work is on weakly polar semiconductor materials of reduced dimensionality such as metal-oxide-semiconductor systems and semiconductor heterostructures and superlattices. By now it is well known that the polaronic effective mass in a purely two-dimensional system is larger than the corresponding three-dimensional one. Although this enhancement would be expected to occur because of the loss of a selection rule for the momentum perpendicular to the interface, cyclotron-resonance experiments on GaAs-$Ga_{1-x}Al_xAs$ heterojunctions have revealed a polaronic correction much smaller than the three-dimensional bulk GaAs result.

In order to understand the discrepancy between experiment and theory, Das Sarma improved the model calculation by including the effects of screening of the electron—optical-phonon interaction by the quasi-two-dimensional electrons and the form of the electron subband wave function. It is shown that these effects reduce the effective interaction between electrons and the LO bulk phonons appreciably, indicating that the calculations are in the right direction. Although his result is somewhat in agreement with experimental observations, the interaction of electrons with the interface phonons which is quite important[7,8] and cannot be negligible was not taken into account in his model.

As a result of the interest produced recently by the cyclotron-resonance studies of polarons in quasi-two-dimensional systems, we reexamine here some aspects which we understand can help to clarify the interface-polaron problem. In our work the electron not only couples to the bulk LO phonons but also interacts with interface optical phonons. We then show that the polaronic-mass-correction result is in excellent agreement with the experimental observations.

Let us consider the $z=0$ plane to be the interface between two semi-infinite media, GaAs (medium 1) and $Ga_{1-x}Al_xAs$ (medium 2) with the electrons occupying the $z>0$ GaAs half-space. In this case the electrons coupling to the interface phonons as well as to the bulk longitudinal optical phonons of GaAs can be described by the Fröhlich Hamiltonian[9] for the polaron problem as

$$H=H_0+H_I+H_B\ , \tag{1}$$

where

$$H_0=\frac{P^2}{2m}+\frac{p_z^2}{2m}+V(z)+\sum_j\sum_{\mathbf{Q}}\hbar\omega_j a^\dagger_{\mathbf{Q}j}a_{\mathbf{Q}j}+\sum_{\mathbf{q}}\hbar\omega_{L1}b^\dagger_{\mathbf{q}}b_{\mathbf{q}}\ , \tag{1a}$$

$$H_I=\sum_j\sum_{\mathbf{Q}}\Gamma_j(\mathbf{Q})e^{i\mathbf{Q}\cdot\mathbf{R}}e^{-Qz}(a^\dagger_{\mathbf{Q}j}+a_{\mathbf{Q}j})\ , \tag{1b}$$

$$H_B=\sum_{\mathbf{q}}D(\mathbf{q})e^{i\mathbf{Q}\cdot\mathbf{R}}\sin(Qz)(b^\dagger_{\mathbf{q}}+b_{\mathbf{q}})\ . \tag{1c}$$

The electron position and momentum operators are $\mathbf{r}=(\mathbf{R},z)$ and $\mathbf{p}=(\mathbf{P},p_z)$, respectively. $a^\dagger_{\mathbf{Q}j}$ creates the jth phonon eigenmode of the interface of wave vector $\mathbf{Q}$ and frequency ω_j. $b^\dagger_{\mathbf{q}}$ creates the longitudinal phonon modes of GaAs with wave vector $\mathbf{q}$ and frequency ω_{L1}. The interface eigenfrequencies ω_j are determined by $\epsilon_1(\omega_j)=-\epsilon_2(\omega_j)$ and the LO phonons of medium 1, ω_{L1}, by $\epsilon_1(\omega_{L1})=0$, where $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ are the frequency-dependent lattice dielectric functions of the two materials 1 and 2, respectively. $\Gamma_j(\mathbf{Q})$ and $D(\mathbf{q})$ are the Fourier coefficients for the interaction of the electron with the interface phonon modes and with the bulk phonon mode of the GaAs.[10,11] The potential $V(z)$ confining the electrons within the inversion layer is taken in the Hartree approximation,

$$V(z)=\frac{4\pi e^2}{\epsilon_{01}}\int_0^z dz'\int_0^{z'} dz''N(z'')+\frac{4\pi e^2}{\epsilon_{01}}N_d z\ , \quad (2)$$

where ϵ_{01} is the static dielectric constant of GaAs, $N(z)$ is the electron density distribution and N_d is the concentration of fixed charged in the depletion layer.

Using the Lee, Low, and Pines[12] variational procedure, we choose for the ground state of this coupled electron-phonon system a wave function $|\psi\rangle$ that is the product of an electron wave function and a coherent phonon state. As a consequence, this polaron state is not an eigenstate of the total parallel momentum operator $\mathbf{P}_T$,

$$\mathbf{P}_T=\mathbf{P}+\sum_j\sum_{\mathbf{Q}}\hbar\mathbf{Q}a_{\mathbf{Q}j}^{\dagger}a_{\mathbf{Q}j}+\sum_{\mathbf{q}}\hbar\mathbf{Q}b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}}\ . \quad (3)$$

Then, the minimization of the energy should be performed by constraining the total parallel momentum $\mathbf{P}_T$ by

$$\delta(\langle\psi|(H-\boldsymbol{\mu}\cdot\mathbf{P}_T)|\psi\rangle)=0\ , \quad (4)$$

where $\boldsymbol{\mu}$, the Lagrange multiplier, is introduced in order to keep the expected value of the total momentum a constant.

The method of calculation[13,14] consists of subjecting the Hamiltonian $H'=H-\boldsymbol{\mu}\cdot\mathbf{P}_T$ to a canonical transformation S which removes the electron coordinates $\mathbf{R}$,

$$S=\exp\left[-i\sum_j\sum_{\mathbf{Q}}\mathbf{Q}\cdot\mathbf{R}a_{\mathbf{Q}j}^{\dagger}a_{\mathbf{Q}j}\right]\exp\left[-i\sum_{\mathbf{q}}\mathbf{Q}\cdot\mathbf{R}b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}}\right]\ . \quad (5)$$

Next, the expectation value of the resulting Hamiltonian is evaluated by taking the wave function of the system to be

$$|\psi\rangle=e^{i\mathbf{Q}\cdot\mathbf{R}}\phi(z)U|0\rangle\ , \quad (6)$$

where $|0\rangle$ represents the state with no phonons, i.e., the vacuum state and U is the second canonical transformation,

$$U=\exp\left[\sum_j\sum_{\mathbf{Q}}(f_{\mathbf{Q}j}a_{\mathbf{Q}j}^{\dagger}-f_{\mathbf{Q}j}^{*}a_{\mathbf{Q}j})\right]\times\exp\left[\sum_{\mathbf{q}}g_{\mathbf{q}}e^{iqz}-g_{\mathbf{q}}^{*}e^{-iqz}b_{\mathbf{q}}\right] \quad (7)$$

with $f_{\mathbf{Q}j}$ and $g_{\mathbf{q}}$ to be determined variationally. For the electron perpendicular wave function $\phi(z)$ we use a variational approximation first proposed by Fang and Howard[15] for Si inversion layers. The trial wave function for the first subband of this system is then

$$\phi(z)=\begin{cases}(b^3/2)^{1/2}z\exp(-bz/2), & z>0\\ 0, & z<0\ ,\end{cases} \quad (8)$$

where b is the variational parameter given by

$$b^3=48\pi Ne^2/\epsilon_{01}\hbar^2\ ,$$

$N=N_d+(\frac{11}{32})N_s$. For a GaAs heterostructure in the usual experimental situation, $N\cong 10^{11}$ cm^{-2}, we get $b=2.5\times10^6$ cm^{-1}.

Minimization of the energy with respect to $f_{\mathbf{Q}j}$ and $g_{\mathbf{q}}$ and up to second order in the velocity $\boldsymbol{\mu}$, we obtain for the polaronic energy shift ΔE_p

$$\Delta E_p=\sum_j\Delta E_I^j+\Delta E_B\ , \quad (9)$$

$$\Delta E_I^j=-\alpha_j\hbar\omega_j\int_0^\infty dx\frac{\beta_j^6}{(1+x^2)(\beta_j+x)^6[\epsilon_{2D}(x)]^2}\ , \quad (9a)$$

$$\Delta E_B=-\frac{\alpha\hbar\omega_{L1}}{4}\int_0^\infty dz\frac{1}{[\epsilon_{2D}(x)]^2(1+x^2)}\times\left\{1+\frac{\gamma^3}{(\gamma+2x)^3}\times\left[\frac{3x}{2\gamma}\left[\frac{3}{2}+\frac{x}{\gamma}\right]-1\right]\right\}\ , \quad (9b)$$

where ΔE_I^j and ΔE_B are the contributions to the energy from the jth mode of the interface phonon and bulk phonon, respectively. The parameters β_j and γ are given by $\beta_j=b(\hbar/2m\omega_j)^{1/2}$ and $\gamma=b(\hbar/2m\omega_{L1})^{1/2}$. $\epsilon_{2D}(x)$ is the dielectric function of the quasi-two-dimensional electron gas. α_j and α are the electron—interface-phonon and electron—bulk-phonon coupling constants,[9]

$$\alpha_j=\frac{e^2}{\hbar\omega_j^3}\frac{(2m\omega_j/\hbar)^{1/2}}{\frac{\Theta_1(\omega_j)}{\omega_{p1}^2}[\epsilon_1(\omega_j)-1]^2+\frac{\Theta_2(\omega_j)}{\omega_{p2}^2}[\epsilon_2(\omega_j)-1]^2}\ , \quad (10)$$

with

$$\Theta_n(\omega_j)=\frac{1}{\left[1+\frac{\epsilon_{0n}}{3\epsilon_{\infty n}}\frac{(\epsilon_{\infty n}-1)(\epsilon_{\infty n}+2)}{(\epsilon_{0n}-\epsilon_{\infty n})\omega_{Ln}^2}(\omega_{0n}^2-\omega_j^2)\right]^2}\ , \quad (10a)$$

where

$$\omega_{0n}^2=\omega_{Ln}^2-2\frac{(\omega_{Ln}^2-\omega_{Tn}^2)}{(\epsilon_{\infty n}+2)} \quad (10b)$$

and

$$\omega_{pn}^2=\frac{9\epsilon_{\infty n}(\omega_{Ln}^2-\omega_{Tn}^2)}{(\epsilon_{\infty n}+2)^2}\ . \quad (10c)$$

ϵ_{0n} and $\epsilon_{\infty n}$ are the static and optical dielectric constants, ω_{Ln} and ω_{Tn} are the longitudinal and transverse optical phonon frequencies, and ω_{pn} is the ion plasma frequency of the material n ($n=1,2$).

For the polaronic mass correction of the electron in the heterojunction we obtain,

$$\Delta m_p = \sum_j \Delta m_j^j + \Delta m_B \; , \tag{11}$$

$$\Delta m_j^j = 2\alpha_j \beta_j^6 m \int_0^\infty dx \frac{x^2}{(\beta_j + x)^6 (1+x^2)^3 [\epsilon_{2D}(x)]^2} \; , \tag{11a}$$

$$\Delta m_B = \alpha \frac{m}{3} \int_0^\infty dx \frac{x^2}{[\epsilon_{2D}(x)]^2 (1+x^2)^3} \times \left\{ 1 + \frac{\gamma^3}{(\gamma+2x)^3} \left[\frac{3x}{2\gamma} \left[\frac{3}{2} + \frac{x}{\gamma} \right] - 1 \right] \right\} . \tag{11b}$$

It is interesting to note that we recover here the purely two-dimensional unscreened results for the energy and mass corrections if we take $\beta_j, \gamma \rightarrow \infty$ and $\epsilon_{2D}(x) = 1$ in Eqs. (9) and (11). In these limits we get

$$\Delta E_p = -\frac{\pi}{2} \sum_j \alpha_j \hbar\omega_j \text{ and } \Delta m_p = \frac{\pi}{8} m \sum_j \alpha_j \; .$$

In order to obtain the polaronic energy and mass correction as a function of the electron density we have numerically evaluated the integrals in Eqs. (9) and (11). In these calculations the screening effects have been taken into account through the random-phase-approximation (RPA) formalism.[16] The relevant physical parameters used in the calculations for the GaAs-$Ga_{1-x}Al_xAs$ heterostructure were for GaAs, $\hbar\omega_{L1} = 36.2$ meV, $\hbar\omega_{T1} = 33.3$ meV, $\epsilon_{\infty 1} = 10.9$, $\epsilon_{01} = 12.9$; for AlAs, $\hbar\omega_{L2} = 49.8$ meV, $\hbar\omega_{T2} = 45.1$ meV, $\epsilon_{\infty 2} = 12.0$, $\epsilon_{02} = 14.6$. The frequencies of the two interface modes are given by $\hbar\omega_- = 34.4$ meV and $\hbar\omega_+ = 47.8$ meV. The mode ω_- is a mixture of the $L1$ and $T1$ phonon modes of the GaAs and the mode ω_+ is a mixture of $L2$ and $T2$ phonon modes of AlAs.

The results we have obtained for the polaron binding energy and mass correction are plotted in Figs. 1 and 2, respectively, as a function of the electron density. In these figures we show separately the contributions of the two interface phonon modes and the bulk longitudinal phonon mode. We also show for comparison, recent theoretical results[17] where the quasi-two-dimensional nature of the electron gas is taken into account but the lattice properties is assumed to be the same as in the GaAs bulk case.

The results for Figs. 1 and 2 allow interesting conclusions. Firstly, the screening and the subband-wave-function effects play a decisive role in reducing appreciably the effective polaronic correction in GaAs heterostructure. These two effects are competitive. By increasing the electron density, the screening increases and the spatial extension of the wave function becomes shorter. In one sense the polaronic effect decreases and in the other it increases. For instance the inclusion of the wave-function width corresponding to the experimental situation ($N = 4 \times 10^{11}$ cm^{-2}), reduces the polaronic-effective-mass correction from $0.046m$ as it is for the purely unscreened two-dimensional case, to $0.0069m$. By including further the screening effects the correction becomes indeed smaller given $\Delta m_p = 0.0048m$ which is in excellent

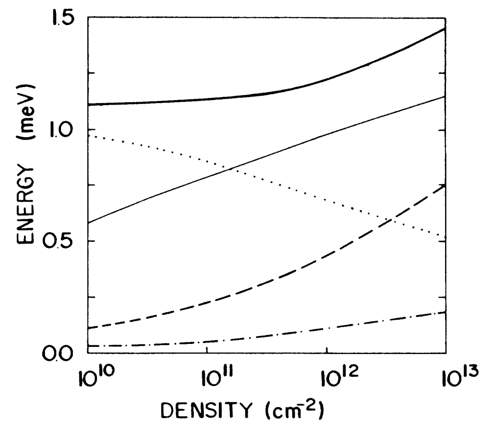

FIG. 1. Polaron binding energy in the GaAs-$Ga_{1-x}Al_xAs$ heterostructure as a function of the electron density. The dashed and dashed-dot lines correspond to the contributions of the ω_+ and ω_- interface phonon modes, respectively. The dotted line is the contribution of the L-bulk longitudinal phonon. The thick solid line is the present result corresponding to the contributions of the three phonon modes. For comparison we show the results obtained with the lattice properties assumed to be the same as in the GaAs bulk case (thin solid line) (Ref. 17).

agreement with the experimental observations. As we can see from Fig. 2 for carrier density smaller than 10^{12} cm^{-2} the electron couples mainly to the bulk longitudinal phonon mode. However the contribution of the interface phonon modes to the polaronic mass correction is of the order of 25% and obviously cannot be negligible. We also observe from Fig. 2 that the interface-phonon contributions become more important than the bulk-phonon contribution with the increasing of the electronic density of the GaAs heterostructure.

In conclusion, we have investigated the nature of the electron-phonon interaction in quasi-two-dimensional electron gas in GaAs-$Ga_{1-x}Al_xAs$ heterostructures and

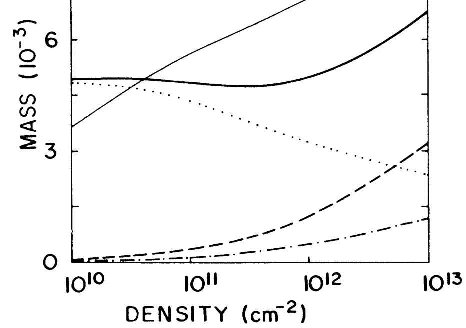

FIG. 2. Polaronic mass correction in the GaAs-GaAlAs heterostructure vs the electron density. The curves are described as in the Fig. 1.

its effects on the polaronic energy and mass corrections. The influence of electron subband wave function and screening were incorporated in the calculations as suggested by experimental investigations in this system. In contrast to previous works in the literature where the phonon modes were assumed to be the same as the bulk GaAs case, we found that the interface phonon modes give significant contribution to the polaronic energy and effective-mass corrections. The result we have obtained for the polaronic mass correction when the effects of electronic wave function width, screening, electron-interface, and electron-bulk phonons interaction are taken into account is in excellent agreement with the experimental observations.

[1]G. Lindemann, W. Seidenbusch, R. Lassing, J. Edlinger, and E. Gornik, Physica **117&118B**, 649 (1983).
[2]M. Horst, U. Merkt, and J. P. Kotthaus, Phys. Rev. Lett. **50**, 754 (1983).
[3]Z. Schlesinger, J. C. M. Hwang, and S. J. Allen, Phys. Rev. Lett. **50**, 2098 (1983).
[4]S. Das Sarma, Phys. Rev. B **27**, 2590 (1983); Surf. Sci. **142**, 341 (1984).
[5]R. Lassing and W. Zawadzki, Surf. Sci. **142**, 388 (1984).
[6]D. M. Larsen, Phys. Rev. B **29**, 3710 (1984).
[7]R. J. Nicholas, L. C. Brunel, S. Huant, K. Karrai, J. C. Portal, M. A. Brummell, M. Razeghi, K. Y. Cheng, and A. Y. Cho, Phys. Rev. Lett. **55**, 883 (1985).
[8]Ph. Lambin, J. P. Vigneron, A. A. Lucas, P. A. Thiry, M. Liehr, J. J. Pireaux, R. Caudano, and T. J. Kuech, Phys. Rev. Lett. **56**, 1842 (1986).
[9]H. Fröhlich, Proc. R. Soc. London **215**, 291 (1952).
[10]L. Wendler, Phys. Status Solidi B **129**, 513 (1985).
[11]M. H. Degani and O. Hipólito (unpublished).
[12]T. D. Lee, F. Low, and D. Pines, Phys. Rev. **90**, 297 (1953).
[13]E. L. de Bodas and O. Hipólito, Phys. Rev. B **27**, 6110 (1983).
[14]E. Evans and D. L. Mills, Phys. Rev. B **8**, 4004 (1973).
[15]F. F. Fang and W. E. Howard, Phys. Rev. Lett. **16**, 797 (1966).
[16]T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).
[17]S. Das Sarma and B. A. Mason, Phys. Rev. B **31**, 5536 (1985).