Interface optical phonons near perfectly conducting boundaries and their coupling to electrons

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The interface optical phonons are described for a GaAs/AlAs system enclosed within metal (or superconductor) boundaries. The requirement that the electrostatic potential associated with these modes vanishes at these boundaries alters the dispersion of the interface modes, especially that of the antisymmetric vibrations. The interaction of electrons with these modes is also considered, and a reduction in the rates is obtained, in particular, when the AlAs width is less than the GaAs width. As such, it is demonstrated that tampering with the long-range Coulomb fields of the optical phonons by external means, here by the proximity of perfectly conducting interfaces, leads to a weakening of the Frohlich interaction by effectively imposing a lower bound on the in-plane wave vector which arises in the coupling function. This lower bound is equal to the reciprocal of the AlAs width. In the special case of a metal/GaAs/metal device, the carriers do not couple to interface modes.

I. INTRODUCTION

Interest in the interface optical modes of the GaAs/AlAs system has recently been quite intense as they dominate the intrasubband scattering rate for electrons confined to thin quantum wells, especially the AlAs-like mode. On the experimental side they were first observed by Sood *et al.*[1] and their importance in intrasubband electron energy relaxation was demonstrated by the time-resolved Raman measurements of Tsen *et al.*[2] On the theoretical side their role in energy relaxation has been discussed by Mori and Ando,[3] Al-Dossary, Babiker, and Constantinou,[4] Rucker, Molinari, and Lugli,[5] among others. In Refs. 3 and 4 the dielectric continuum (DC) model was employed, although the coupling with electrons was taken to be $(e/m^*)\mathbf{A}\cdot\mathbf{p}$ in Ref. 4 where $\mathbf{A}$ is the vector potential and $\mathbf{p}$ the electron's momentum, rather than the $e\Phi$ coupling (Φ the electrostatic potential) used in Ref. 3 and elsewhere. The question of gauge choice has been discussed recently[6–8] with the main conclusion being that the two approaches yield identical rates.[8]

Microscopic calculations for thin wells, such as the 11 parameter rigid-ion model of Ren, Chu, and Chang[9] clearly show an intermixing of confined and interface modes. This conclusion has also been obtained by the work of Gerecke and Bechstedt[10] and by macroscopic models.[7,11–13] In fact the anisotropy of LO1 was recently demonstrated by the micro-Raman data of Miles and Scamarcio.[14] As for the electron-phonon interactions, investigations[15,16] in which an incomplete set of modes was considered, in particular the lack of polar interface modes, led to an incorrect prediction of a reduction in the electron-polar phonon interaction strength with reduced well width due simply to the quantization of the confinement wave vector in these systems. Sum rules have been demonstrated which show that the total rate is insensitive to the model used, provided a complete set of modes is considered and the total rate lies in between that given by bulk GaAs and AlAs phonons.[5] This is due to the important contribution made by the interface modes in these structures at small well widths, since their Frohlich coupling is proportional to $q_x^{-1/2}$ (where q_x is the in-plane wave vector which in a continuum approach has no lower bound). This state of affairs is unfortunate from the point of view of engineering the phonon properties in order to reduce the interaction with polar optical phonons which dominate energy relaxation at high temperatures and fields.[7]

In this paper an investigation of the properties of interface polar optical modes near perfectly conducting interfaces is considered, the rationale being that modifying the long-range electric fields of these excitations may modify the Frohlich interaction and hence result in a reduction in the interaction strength. Stroscio *et al.*[17] have recently considered a GaAs quantum wire with metal interfaces. The severity of the resulting boundary conditions ($\Phi=0$), in effect cuts out the scattering by interface modes and hence a reduction in the total scattering rate is predicted. In this paper the properties of interface modes near to semiconductor/metal interfaces is considered in two dimensions as here the growth technology is now quite advanced.[18]

The paper is organized as follows. In Sec. II the dispersion relation for these interface phonons is obtained and numerically evaluated. Section III deals with the quantization of the modes and their coupling to electrons whilst Sec. IV briefly discusses the other optical vibrations of this system, and finally Sec. V provides some conclusions.

II. INTERFACE POLAR MODE DISPERSION NEAR PERFECTLY CONDUCTING INTERFACES

In this section we derive the dispersion relation for the interface polar optical modes of the composite system depicted in Fig. 1 which also illustrates the coordinate system employed. A GaAs quantum well centered at $z=0$ of width d_1, which is symmetrically surrounded by AlAs of thickness d_2. This system is surrounded by a perfect

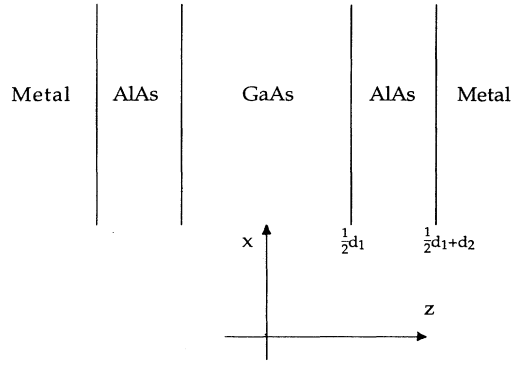

FIG. 1. The geometry of the metal/AlAs/GaAs/AlAs/metal structure.

conductor; all in-plane electric field components are assumed to vanish at the AlAs/metal interfaces. In fact, a superconductor may also be employed, and such a structure illustrated in Fig. 1 with the metal replaced by a superconductor was recently investigated by Waung and Feng[19] in the context of resonant Cooper pair tunneling. Two-dimensional low-temperature transport has recently been of interest in semiconductor-superconductor systems.[20] The paper concentrates on the interface modes which are localized at the GaAs/AlAs interfaces as these are the only interface modes that have long-range polar fields associated with them, and as such are the ones of interest in the discussion of the polar interaction. Other interface optical modes are also allowed which are localized at the semiconductor/metal interfaces and these excitations are nonpolar in character since they oscillate at the TO frequency of the semiconductor in order to satisfy the boundary conditions. Confined optical modes are also allowed and a discussion of these confined modes and the interface modes which are localized at the semiconductor/metal interfaces is deferred until Sec. IV.

The GaAs and AlAs layers are assumed to be adequately described by their bulk dielectric functions given by

$$\varepsilon_i=\varepsilon_{\infty i}\left[\frac{\omega_{Li}^2-\omega^2}{\omega_{Ti}^2-\omega^2}\right],\quad i=1,2\ , \tag{1}$$

where 1 (2) denotes GaAs (AlAs), $\varepsilon_{\infty i}$ is the high-frequency dielectric constant and $\omega_{Li\,(Ti)}$ are the zone-center LO (TO) frequencies of material i. The numerical value of these parameters are tabulated in the review article by Adachi.[21]

The symmetry of the system allows the modes to be split up into a set of symmetric and antisymmetric vibrations where the symmetry refers to that of the potential of the mode under reflection through $z=0$. It is straightforward to show that the potentials associated with the interface modes which satisfy Laplace's equation (retardation effects are ignored here), and vanish at the metallic (or superconducting) interfaces are given by

$$\Phi_{0j}=\begin{cases} A_j h_j(z), & |z|\le d_1/2\ , \\ B_j\{f\exp[q_x z]-\exp[-q_x z]\}, & \frac{1}{2}d_1\le z\le d_2+\frac{1}{2}d_1\ , \\ g_j B_j\{f\exp[-q_x z]-\exp[q_x z]\}, & -d_2-\frac{1}{2}d_1\le z\le -\frac{1}{2}d_1\ , \end{cases} \tag{2}$$

$$h_j(z)=\begin{cases}\cosh(q_x z), & j=s\ , \\ \sinh(q_x z), & j=a\ , \end{cases} \tag{3}$$

$$g_j=\begin{cases}1, & j=s \\ -1, & j=a\ , \end{cases} \tag{4}$$

where s (a) stands for symmetric (antisymmetric). A_j and B_j are amplitudes to be determined in the following section from the dispersion relation and quantization. The factor f is given by

$$f=\exp[-q_x(d_1+2d_2)] \tag{5}$$

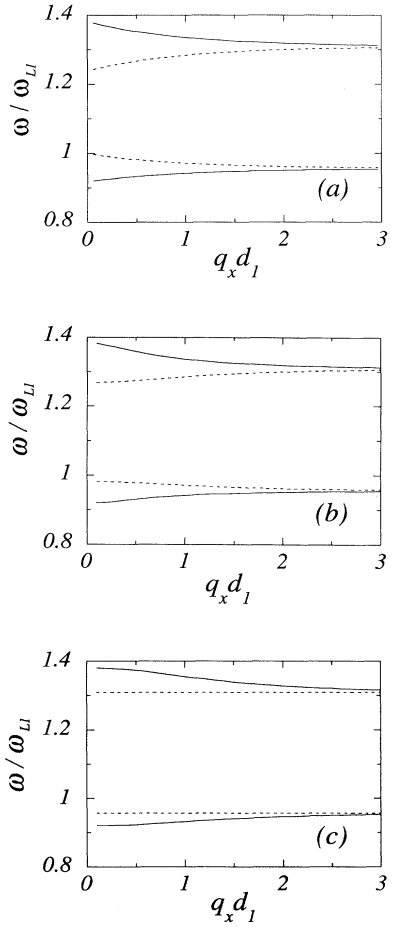

FIG. 2. The interface optical-phonon dispersion curves for (a) $d_2=\infty$ (no metallic interfaces), (b) $d_2/d_1=2$, and (c) $d_2/d_1=0.5$. In the above the full curves correspond to the symmetric modes and the dashed curves to the antisymmetric modes.

and arises from the vanishing of the potential at the AlAs/metal boundary, and q_x is the in-plane wave vector of the mode. Equations (2)–(5) define the z dependency of the electrostatic potential its in-plane dependence is $\exp(iq_x x)$ by symmetry.

It is now straightforward to apply the usual electrostatic boundary conditions at the boundary $z=d_1/2$, namely, continuity of the potential and the z component of the electric displacement field. The solvability condition leads to the following dispersion relations for the symmetric and antisymmetric interface modes:

$$\varepsilon_1 \tanh(q_x d_1/2)+\varepsilon_2 \coth(q_x d_2)=0 \quad \text{(symmetric)} , \tag{6}$$

$$\varepsilon_1 \coth(q_x d_1/2)+\varepsilon_2 \coth(q_x d_2)=0 \quad \text{(antisymmetric)} . \tag{7}$$

The dispersion relations for a single quantum well (e.g., Refs. 3 and 4) in the absence of metal boundaries ($d_2 \to \infty$), follows simply from the above and these familiar modes are illustrated in Fig. 2(a). Two pairs of branches, one set within the GaAs reststrahl band the other within the AlAs reststrahl band are allowed. Figure 2(b) shows the interface optical mode dispersion in the vicinity of metal interface ($d_2/d_1=2$). It is seen that the modes are now distorted, especially the antisymmetric vibrations. This is more drastically illustrated in Fig. 2(c) where $d_2/d_1=0.5$. The antisymmetric modes are now practically dispersionless. Furthermore they originate at a frequency within the reststrahl bands of GaAs and AlAs, in contrast to Fig. 2(a) where they emerge at ω_{L1} and ω_{T2}, respectively. For vanishing d_2/d_1, the modes in the AlAs reststrahl band both oscillate at ω_{L2} as here the only field of interest is that normal to the layers in the AlAs (the in-plane electric field is negligible, as are all electric field components in the GaAs layer), hence the oscillation at ω_{L2}. On the other hand, the modes in the GaAs region vibrate at ω_{T1} in this limit. These GaAs surface optical vibrations survive in the metal/GaAs/metal system, and since no Frohlich potential is involved the carriers may only couple to the confined LO vibrations of the GaAs leading to a marked reduction in the interaction strength (see Sec. IV).

III. QUANTIZATION AND ELECTRON-INTERFACE MODE INTERACTION

In this section the interaction Hamiltonian is obtained for the coupling of these modes to electrons. Mori and Ando[3] have presented a detailed account of the interaction of electrons with the various vibrational modes associated with a double heterojunction. Here we derive the interaction Hamiltonian for the modes described in the preceding section.

The starting point for the determination of the mode amplitudes is the field Hamiltonian given by[22]

$$\hat{H}_f=\frac{1}{2}\varepsilon_0 \sum_{\omega_j} \int \left[\frac{\partial[\omega\varepsilon]}{\partial\omega} \right]_{\omega=\omega_j} \hat{\mathbf{E}}_j^2 d^3\mathbf{r} , \tag{8}$$

where ε_0 is the permittivity of free space and ε is the frequency-dependent dielectric function. The above Hamiltonian contains both the mechanical and electrical contribution to the mode energy, and has been used to describe longitudinal modes in the bulk[23] and interface modes in layered systems.[4,8] The sum is over all the allowed modes, both symmetric and antisymmetric.

The operator corresponding to the potential $\hat{\Phi}_j$ is now expressed in second quantized notation, viz.,

$$\hat{\Phi}_j=\int \{\Phi_{0j} a_j(\mathbf{q}_x)\exp(i\mathbf{q}_x\cdot\mathbf{x})+\text{H.c.}\} d^2\mathbf{q}_x . \tag{9}$$

In the above the boson operators $a_j(\mathbf{q}_x)$ and $a_j^\dagger(\mathbf{q}_x)$ satisfy the usual commutator relations. The electric field operator is given by

$$\hat{\mathbf{E}}_j=-\nabla\hat{\Phi}_j . \tag{10}$$

Substitution of (10) into (8) and rewriting in canonical form, viz.,

$$\hat{H}_f=\frac{1}{2}\sum_{\omega_j} \int \hbar\omega_j [a_j^\dagger(\mathbf{q}_x)a_j(\mathbf{q}_x)+\text{H.c.}] d^2\mathbf{q}_x , \tag{11}$$

yields, after some algebra, the following expression for Φ_{0j}:

$$\Phi_{0j}=C(q_x)\begin{cases} \dfrac{h_j(z)}{h_j(d_1/2)}, & |z|\le d_1/2 , \\ -\alpha\{f\exp[q_x(z+d_1/2)]-\exp[-q_x(z-d_1/2)]\}, & \frac{1}{2}d_1 \le z \le d_2+\frac{1}{2}d_1 , \\ -g_j\alpha\{f\exp[-q_x(z-d_1/2)]-\exp[q_x(z+d_1/2)]\}, & -d_2-\frac{1}{2}d_1 \le z \le -\frac{1}{2}d_1 . \end{cases} \tag{12}$$

In the above α is given by

$$\alpha=\frac{\exp(q_x d_2)}{2\sinh(q_x d_2)} \tag{13}$$

and the coupling function $C(q_x)$ is

$$C(q_x)=\left\{ \frac{\hbar\varepsilon_1 \tanh(q_x d_2)}{2(2\pi)^2\varepsilon_0 q_x \Xi} \right\}^{1/2} \tag{14}$$

with Ξ expressible in the following concise manner:

$$\Xi=\varepsilon_1\frac{\partial\varepsilon_2}{\partial\omega}-\varepsilon_2\frac{\partial\varepsilon_1}{\partial\omega} . \tag{15}$$

In the limit $d_2 \to \infty$, Eq. (12) reduces, with ε_1 and ε_2 given by Eq. (1), to the results quoted by Mori and Ando.[3] It is worth commenting here that in deriving the quantized potential given by Eqs. (12)–(15), ε_1 and ε_2 are

unspecified and as such represent a generalization of the Mori and Ando results, although in all that follows the phonon response is employed. One could envisage further applications where the dielectric response is more complex, such as that for coupled phonon-plasmon excitations.

We are now in a position to discuss the electron-interface mode interaction in the vicinity of the metallic interfaces. It is noted that for small q_x (or d_2) the coupling function does not explicitly depend on the in-plane wave vector. In contrast, in the absence of a metallic boundary the coupling function varies as $q_x^{-1/2}$ and as such, one expects the interaction strength to weaken if the metal interfaces are close to the quantum well or q_x is small. In particular for small d_2 it *vanishes*. The introduction of ideal metallic interfaces is seen to modify the Frohlich interaction. If an "effective" in-plane wave vector is defined, q_x^{eff} $[=q_x\coth(q_x d_2)]$, then the coupling function [Eq. (14)] has the same mathematical form as in the absence of the conductor *except* that there is a lower bound on this effective in-plane wave vector ($q_x^{\text{eff}} \geq d_2^{-1}$).

The interaction of the modes with electrons is now considered in more detail. We assume that only emission processes are allowed, and consider only intrasubband scattering events (i.e., thin quantum wells). From symmetry, only the symmetric modes contribute. The electron wave function is taken to be that for the lowest subband of an infinite well within the effective-mass approximation. This wave function is well known and not repeated here for brevity. The interaction Hamiltonian is given by

$$\hat{H}_{\text{int}} = -e\hat{\Phi}_s \tag{16}$$

and the scattering rate Γ is determined from the golden rule

$$\Gamma(k_x^i) = \frac{2\pi}{\hbar}\int d^2\mathbf{q}_x \int d^2\mathbf{k}_x^f |\langle f|\hat{H}_{\text{int}}|i\rangle|^2 \times \delta(E_i - E_f - \hbar\omega_s)\ . \tag{17}$$

In Eq. (17), k_x denotes the electron's in-plane wave vector and i (f) the initial (final) state of the system. The integration involved in determining the rate needs to be evaluated numerically. Figure 3 illustrates the scattering rate as a function of the ratio d_2/d_1 for the interaction with the symmetric interface polar optical phonons for a well width of 40 Å and an in-plane electron energy of twice the GaAs LO phonon energy. The scaling rate Γ_0 ($\approx 8.7\times 10^{12}\ \text{s}^{-1}$ for GaAs) is given by

$$\Gamma_0 = \frac{e^2}{4\pi\varepsilon_0\hbar}\left[\frac{1}{\varepsilon_{\infty 1}} - \frac{1}{\varepsilon_{s1}}\right]\left[\frac{2m_1^*\omega_{L1}}{\hbar}\right]^{1/2}, \tag{18}$$

where m_1^* is the electronic effective mass, and ε_{s1} the static dielectric constant of GaAs. For large d_2, both rates are asymptotic to the rates in the absence of perfectly conducting interfaces as indeed they should be, while a noticeable reduction in the rates arise, especially for $d_2 < 2d_1$ and is due, primarily to the behavior of $C(q_x)$ discussed previously. Note that in both cases the rates vanish as $d_2 \to 0$. The horizontal dashed line is the scattering rate for the interaction with the GaAs LO modes calculated via the slab model[3,5,7] for comparison.

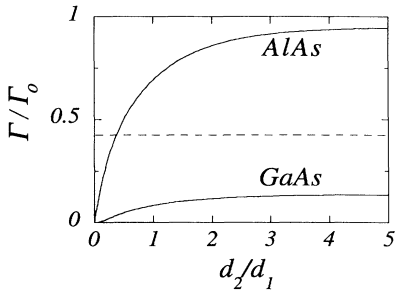

FIG. 3. The intrasubband scattering rate with $d_1 = 40$ Å and initial in-plane electron energy of $2\hbar\omega_{L1}$ for scattering by AlAs-like and GaAs-like interface polar optical phonons as a function of d_2. In the limit $d_2 \to \infty$ the asymptotic values are 0.95 and 0.14, respectively. The horizontal dashed line is the scattering rate via emission of GaAs slab modes for $d_1 = 40$ Å as a comparison.

IV. OTHER OPTICAL EXCITATIONS

The structure depicted in Fig. 1 allows for a variety of excitations which the electrons may further couple to. The most important of these are the confined polar modes in the GaAs and AlAs layers which vibrate at the respective LO frequencies, and are totally confined to either the GaAs or AlAs layer (the confined TO vibrations which also occur do not couple to electrons via the Frohlich interaction). As the wave-function penetration in the AlAs layer is ignored here, the interaction with the AlAs confined modes is identically zero.[3] What is more important is the interaction of electrons with the GaAs confined LO modes. In the limit of zero bulk dispersion, and only in this limit, these confined modes are not effected by the metallic boundaries and are best described, in a continuum approach either by the reformulated slab vibrations of Huang and Zhu[24] or by the simple dielectric continuum model (slab modes). That this is so was recently demonstrated by Rucker, Molinari, and Lugli.[5] What is of particular interest here is that for small well widths their interaction with electrons is *weaker* than that due to interface modes[2] and tends to zero for vanishing well width due to the quantization of the wave vector in the z direction.

It has been known for a long time that the interface between a polar semiconductor and a metal can support a rich spectrum of surface excitations both in the vicinity of the reststrahl of the semiconductor and near the plasma frequency (ω_p) of the metal[25,26] (the modes near the plasma frequency are not included here as their energy is large at the electron in-plane wave vectors of interest, typically a few eV). In particular in the unretarded regime and for a perfect conductor ($\omega_p \to \infty$) the interface modes which oscillate in the semiconductor must vibrate at the TO frequency of the semiconductor. To see this it is sufficient to consider a single interface between a polar semiconductor described by ε_2 and a metal described by a simple plasma response

$$\varepsilon_m = 1 - \frac{\omega_p^2}{\omega^2} . \quad (19)$$

Unretarded surface modes occur when the following condition is satisfied[27]

$$\varepsilon_2 = -\varepsilon_m \quad (20)$$

and for a perfect conductor ($\omega_p \to \infty$) the mode that survives is that at ω_{T2}. This interface mode has a nonvanishing ionic displacement field at the boundary which decays into the semiconductor. Two such modes exist in the structure depicted in Fig. 1 (one for each interface). Their ionic displacement fields are confined solely to the AlAs layers and are finite at the semiconductor/metal interface. They do not couple to electrons via the Frohlich mechanism (since $\omega = \omega_{T2}$) and this lack of interaction is important for the main conclusion of this work, namely, that the presence of the metal surfaces leads to a reduction in the electron-phonon scattering strength. These two modes together with the four polar interface modes considered in the main part of the paper, and the confined LO and TO modes of the GaAs and AlAs layers form a complete set of optical phonon vibrations. This completeness is required in order to obtain reliable scattering rates.[3,5,7]

V. CONCLUSIONS

In this paper, the interface modes which are associated with long-range polar fields were considered in the vicinity of perfectly conducting interfaces. It was demonstrated that the dispersion of the modes is effected, more especially that of the antisymmetric vibrations. More importantly, it was shown that the Frohlich interaction can be modified by the presence of the conducting interfaces, and in particular is weakened when these interfaces are close to the quantum well. It is interesting to note that tampering with the long-range polar fields of these optical modes by external means, in this case the proximity of a perfect conductor, leads to the possibility of weakening their coupling to electrons, by introducing a lower bound ($=d_2^{-1}$) for the "effective" in-plane wave vector which arises in the coupling function. In particular, in the special case of a metal/GaAs/metal device, the electrons do not scatter with the interface modes via the Frohlich mechanism, leading to the reduction in the overall interaction strength. The goal of reducing the interaction of electrons with polar modes has obvious advantages in improving device performance, and further investigations with this in mind are currently underway.

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