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Electron-phonon interaction in quasi-two-dimensional systems

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We present a calculation of the electron–LO-phonon scattering rate in quasi-two-dimensional systems, based on a fully microscopic description of the phonon spectra. The results obtained for a GaAs/AlAs quantum-well structure indicate the great importance of interface phonons and allow us to solve a long-standing controversy on the validity of simplified macroscopic models for describing the relevant vibrations.

Room-temperature mobilities of high-speed heterostructure devices as well as relaxation rates of photoexcited carriers in quantum wells (QW's) and superlattices (SL's) are mainly controlled by the carrier interactions with phonons. The study of such processes, nowadays directly accessible via ultrafast spectroscopy, constitutes, therefore, the key aspect to the understanding of charge transport in low-dimensional systems. In spite of the large amount of experimental and theoretical information existing on the vibrational properties of semiconductor superlattices,[1] a long-standing controversy is still open on the effect of the reduced dimensionality on the electron-phonon (*e*-ph) interaction and its implications for carrier transport.[2] The discussion concerns specifically the correct description of the phonon modes which are relevant to the electronic scattering, and points out the little exchange that has occurred so far between researchers dealing with lattice dynamical calculations and light-scattering measurements of phonon spectra on the one side, and researchers involved in the study of *e*-ph interaction and transport experiments and simulations on the other side.

Drastically different results concerning the rate of the electronic transitions in QW's and SL's have been obtained depending on the specific model adopted for the optical phonons.[3–13] In one case (the so-called "guided-modes model"),[4,8] very low intrasubband rates are obtained, suggesting that the reduced cooling rates detected experimentally in time-resolved optical measurements[2,14,15] are a direct consequence of the intrinsically reduced coupling to two-dimensional (2D) phonons. In the other ("slab model"),[3,5–7,9–13] an opposite phonon symmetry is found, which leads to higher intrasubband rates, requiring additional mechanisms (such as nonequilibrium phonons[7,9]) to describe the experimental data. In the present paper, we calculate the scattering rates using as an input phonon frequencies and displacements from a microscopic approach based on first-principles interatomic force constants.[16] The results allow us to solve the controversy, ruling out the first interpretation, and show that both interface (IF) and confined phonons play a crucial role in the coupling to carriers.

The status of the controversy mentioned above is summarized in Fig. 1. The slab model [Fig. 1(a)], which applies purely electrostatic boundary conditions at the interfaces, gives to sets of modes in the GaAs-like frequency range: (i) confined modes, whose displacements, represented by sine or cosine functions, have antinodes at the boundaries, where the potential vanishes; (ii) IF modes, whose potential and frequency strongly depend on the in-plane wave vector $\mathbf{q}_\parallel$. For large values of $q_\parallel$ the potentials are localized at the interfaces, while at small values they

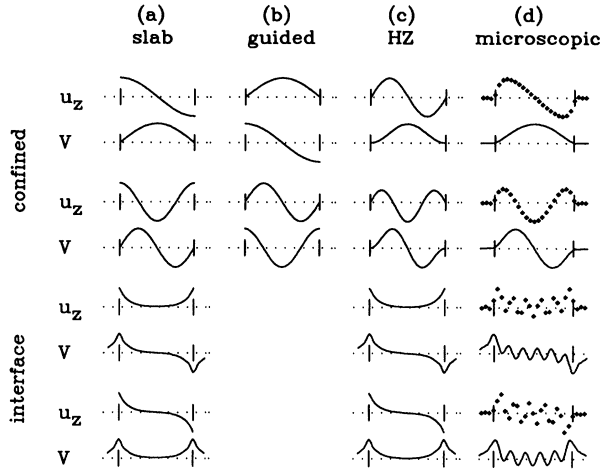

FIG. 1. z component of the atomic displacements (u_z) and the corresponding potentials (V) for GaAs-like optical modes in a (001)-oriented 56-Å QW surrounded by two AlAs layers. The QW interfaces are marked by vertical bars. The two confined modes of highest frequency and the two interface modes are displayed from top to bottom in order of decreasing frequency. (a), (b), and (c) are from the macroscopic models; (d) is the result of the microscopic calculation, with diamonds indicating the atomic displacements of anions. The plots are for $q_z=0$ and $q_\parallel=0.15$ Å^{-1} (one of the largest values of $q_\parallel$ significant for the coupling).

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extend much further. The guided modes model[8] [Fig. 1(b)], on the contrary, imposes phonon confinement by requiring vanishing displacements at the interfaces. Accordingly, the phonon potential has antinodes at the boundaries. Such a model has been presented as a simplified version of the dispersive dielectric continuum approach derived by Babiker.[4] Clearly, since the atoms at the interfaces are forced to have zero displacement, no IF modes are allowed. Because of the opposite symmetry of equal order modes, the two models lead to a very different coupling to confined electrons.[12]

Part of the confusion that permeates the discussion on e-ph coupling in 2D systems originates from the fact that macroscopic models were adopted by researchers in the transport community because of their simple analytical expressions for the displacements. However, the choice of the appropriate macroscopic description to be used in the calculations was sometimes driven by an erroneous extrapolation of the results of Raman experiments rather than from the output of microscopic calculations that have become available in the meantime.[1,16,17] Indeed, from off-resonance Raman spectra, generally taken in the backscattering configuration from the (001) surface, it is possible to conclude[1,18] that the confined mode of lowest order (and highest frequency, ω_{LO1}) has a nodeless displacement pattern, approximately vanishing at the interfaces; the successive modes have an increasing number of nodes and similar behavior at interfaces. This however, does *not* imply that such ordering applies to the e-ph coupling. In fact, Raman spectra in that scattering configuration probe the lattice vibrations at $q_\parallel = 0$ and small values of q_z. A different situation is found at $q_z = 0$ and small or vanishing $q_\parallel$, a direct consequence of the anisotropy induced by macroscopic electric fields.[16,17] As illustrated in Fig. 2(a), when the direction of the vanishing wave vector varies from ⟨001⟩ to ⟨100⟩, ω_{LO1} shifts to a lower frequency and ω_{LO2} becomes the highest mode. Moreover, ω_{LO1} shows increasing localization at interfaces with increasing $q_\parallel$, and is therefore identified as an IF mode. A second IF mode in the GaAs-like range originates from the lowest-order confined TO mode.

It is important to realize that the wave vectors $\mathbf{q}$ of interest for the treatment of e-ph scattering in QW's have the largest component *parallel* to the interfaces; the range of relevant $\mathbf{q}_\parallel$'s is shown in Fig. 2(b). The phonon displacements and potentials from the microscopic calculation at finite $\mathbf{q}_\parallel$ are shown in Fig. 1(d): the highest frequency corresponds to a displacement of odd parity with respect to the center of the GaAs layer, followed by confined modes of alternate parity. Such occurrence had already been noted by Huang and Zhu (HZ).[19] Their picture [Fig. 1(c)] is actually partially modified by the microscopic results, which show a high degree of hybridization of the IF modes with odd-order confined modes, at least as far as the GaAs-like vibrations are concerned.[16] It turns out that for small $\mathbf{q}_\parallel$'s the best approximation is given by the HZ model, whereas for larger $\mathbf{q}_\parallel$'s [as the one of Fig. 1(d)] the slab model is more adequate. Indeed, the wrong boundary conditions used in this last model seem to affect only a few atomic planes close to the interfaces, where the electron wave functions are small anyway.

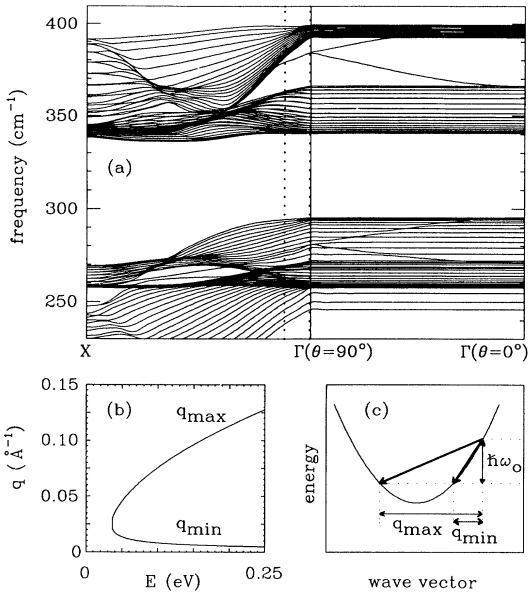

FIG. 2. (a) Phonon dispersion of a (001)-oriented $(GaAs)_{20}(AlAs)_{20}$ SL, along the in-plane (001) direction (left panel), and as a function of the θ angle between the direction of $\mathbf{q}$ and the growth direction, at $|\mathbf{q}| \to 0$ (right panel), calculated with the model of Ref. 16. The vertical-dotted lines mark the minimum and maximum $q_\parallel$'s for an intrasubband emission process [sketched in (c)] of a 0.25-eV electron. The E dependence of such limits is shown in (b).

We now move to the calculation of the scattering rates for Fröhlich-type polar electron LO-phonon interaction in a QW, based on the microscopic phonons.[20] For the electron wave function we use the solution of Schrödinger's equation within the effective-mass approximation.[9] Figures 3(a) and 3(b) show the room-temperature emission rates for the $1 \to 1$ and the $2 \to 1$ transitions (1 and 2 indicate the two lowest subbands), obtained for 56-Å wells with a barrier height of 1 eV. We note the following: (i) The first confined mode [topmost in Fig. 1(d)] contributes to about 28% of the total $1 \to 1$ intrasubband rate, while the third mode is already much weaker. The modes of opposite parity do not contribute. On the contrary, the second confined mode [second row in Fig. 1(d)] is the dominant one for the $2 \to 1$ intersubband transition. (ii) The IF GaAs-like modes (shown in Fig. 3 together with the remaining confined modes because of the above-mentioned hybridization) are important, carrying about 14% of the interaction. (iii) A very strong contribution to the scattering rate comes from the AlAs-like IF modes. The importance of such modes (for which almost no hybridization occurs) is explained by the fact that their potential extends far into the GaAs layer at the $q_\parallel$ of interest. The contribution of the remaining AlAs-like modes is negligible.

The resulting times for intrasubband and intersubband emission at room temperature are then 76 and 931 fs, respectively, confirming that the slow cooling rate detected experimentally cannot be associated to phonon confinement, and must therefore be related to hot-phonon

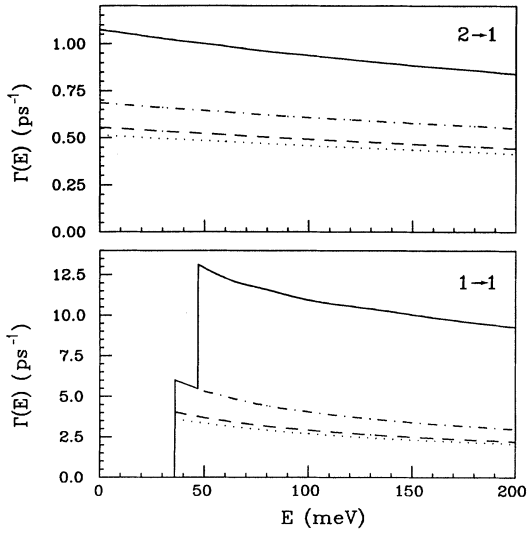

FIG. 3. Calculated total intrasubband and intersubband emission rates as a function of electron energy (solid lines), including all GaAs-like and AlAs-like modes. Dash-dotted lines show the contribution of all GaAs-like modes (including the interface ones). Dashed lines refer to the confined GaAs-like modes only, out of which the mode of lowest order (first for intrasubband and second for intersubband transitions) represents the largest contribution (dotted lines).

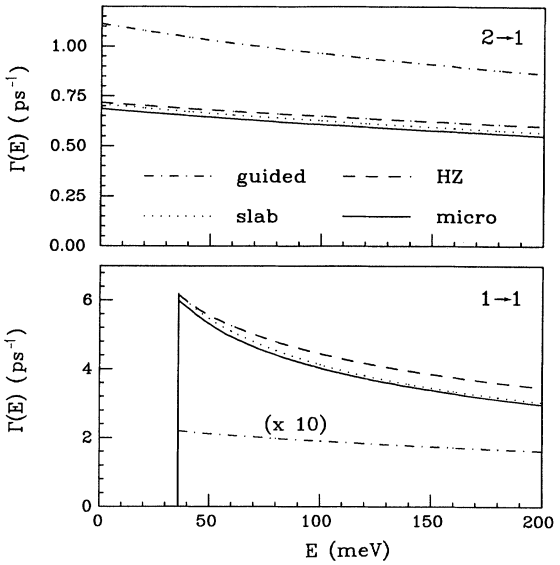

FIG. 4. Comparison of the scattering rates from our microscopic calculation with the results of macroscopic models. Only the contribution of GaAs-like modes is shown. The intrasubband rate of the guided model is multiplied by a factor of 10.

effects.[7,9] Full simulations based on our present results will be published elsewhere.[21]

In Fig. 4 we compare our results for GaAs-like modes with those obtained, for the same structure, from the models of Figs. 1(a)–1(c). The slab and HZ models (dotted and dashed lines, respectively) agree fairly well with the microscopic calculation (solid line), and are therefore adequate to describe the e-ph interaction. Such agreement can be understood from the fact that, although the microscopic displacements are not properly reproduced by the slab model at all $q_{\parallel}$'s, at the relevant values of $q_{\parallel}$ their deviations are limited to a small region near the interface. The predictions of the guided-modes model are instead completely inconsistent with ours. Finally, we point out that the use of bulk GaAs phonons turns out to be already an acceptable approximation for the total scattering rates.[21]

In conclusion, we have presented a calculation of the electron-LO phonon polar interaction in GaAs/AlAs systems, based on a fully microscopic approach for the phonon spectra. The results indicate that, while some of the macroscopic phonon models used so far lead to completely wrong predictions, a few of them are acceptable for the scattering rate calculations. Even the rough assumption of unmodified bulk modes may provide reasonable results. Instead, an accurate description of the phonons is necessary when one is interested in the contribution of individual modes, as, e.g., in time-resolved Raman spectroscopies.

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