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Electron-phonon scattering rates in quantum wires

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Electron-phonon scattering rates for quantum wires composed of one compound semiconductor material within another are calculated rigorously for arbitrary wire shapes within the dielectric continuum approach for the optical phonons and the effective-mass approximation for the electrons. No approximations are used for the boundary conditions satisfied by the phonons or by the electrons. Detailed results are given for the intrasubband and intersubband scattering rates as functions of the initial electron energy and of wire size for wires of rectangular cross section. An interesting maximum in the intersubband scattering rate as a function of wire size is found. We find that interface phonons give important contributions to the scattering rates, especially for small ($\lesssim 100$ Å) wire widths or high electron energies. We also give a quantitative appraisal of the rates obtained from simple separable approximations used previously for the phonons.

Semiconductor quantum wire structures currently are of considerable interest both because of the possibility of studying in them novel physical phenomena as well as for possible device applications such as quantum wire lasers. Electron-optical phonon scattering controls such phenomena as the cooling of optically excited carriers on the picosecond time scale as well as transport and optical properties at room temperature, and reliable values for these scattering rates in realistic structures are needed for numerical studies of their properties. The effect of confinement on the optical phonons has been a central focus of studies of electron-phonon scattering in these confined structures. In particular there has been considerable discussion concerning whether phonon confinement causes significant reduction of these scattering rates.

To date, however, a complete, rigorous treatment of electron-phonon scattering in quantum wires of general shape has not been given. Recent studies have been reported for wires having circular cross sections,[1] for which the equations for both the phonons and the electrons separate into simple one-dimensional problems. Wires of more general shapes, particularly those with rectangular cross sections, are of more interest experimentally. In addition, such shapes introduce qualitatively new features into the phonon properties, such as phonon localization in regions of high curvature.[2] To date, the effects of such features on electron-phonon scattering rates in these systems have not been addressed. In the present work we develop an approach which treats wires of arbitrary shapes, and we give detailed numerical results for wires having rectangular cross sections.

The principal difficulty in studying electron-phonon scattering in wires is that the equations of motion and boundary conditions for both the phonons and the electrons are not in general separable into one-dimensional problems. In previous work for rectangular wires[3] *ad hoc* approximations for the phonons have been used to separate the problem. In the present work we examine such approximations critically and find that they cause significant errors in the scattering rates.

The scattering rate for an electron from an initial state in subband α with wave vector k_i to a final state in subband β with wave vector $k_f = k_i - q$ accompanied by the emission of an optical phonon of wave vector q is calculated from Fermi's golden rule to be[4]

$$\Gamma_{\alpha k_i \to \beta k_f} = \frac{2e^2}{\hbar} \sum_{\nu} \{N[\omega_\nu(q)] + 1\} \left| \int d^2r\, \psi_\alpha(\mathbf{r}) \psi_\beta^*(\mathbf{r}) \phi_{\nu q}(\mathbf{r}) \right|^2 \mathrm{Im} \left[\frac{1}{\frac{\hbar^2 k_i^2}{2m} + \Delta_{\alpha\beta} - \frac{\hbar^2 k_f^2}{2m} - \hbar\omega_\nu(q)} \right], \qquad (1)$$

where $\psi_\alpha(\mathbf{r})$ are the electron wave functions, $\phi_{\nu q}(\mathbf{r})$ are the phonon potentials, $\hbar\omega_\nu$ are the (complex) phonon energies, $\Delta_{\alpha\beta}$ is the energy difference between the initial and final electron subbands, and m is the electron mass. The total phonon emission rate involves an integral of Eq. (1) over k_f (or equivalently over q). Here we consider the ground and first excited subbands of a GaAs wire embedded in AlAs. The index ν indicates the optical phonon modes of the wire system. These modes consist of the vibrations confined in the GaAs region ("confined" modes), those confined to the AlAs region ("excluded" modes), the interface (IF) modes involving predominantly motion of the GaAs atoms, and the IF modes involving predominantly the AlAs atoms. The wave vectors are scalars corresponding to motion along the wire, $\mathbf{r}$ is the position vector in the cross-sectional plane perpendicular to the wire axis, and $N(\omega) = [\exp(\hbar\omega/k_BT) - 1]^{-1}$.

We use an approach based on the macroscopic dielectric continuum treatment for the phonons.[5] It is particularly useful in studying electron-phonon scattering rates because it gives analytic results for the electron-phonon interactions and can be used to treat systems of widely varying size and shape. For semiconductor quantum wells this approach gives scattering rates which are in good agreement with those produced by lattice-dynamics calculations.[6,7] Lattice-dynamics studies for quantum wires[8–10] are limited to small ($\lesssim$15 Å) structures for computational reasons.

Recently we have developed a method to treat the IF phonons in quantum wire structures of general cross-sectional shape.[2] It involves the solution of Laplace's equation for the scalar potential $\phi(\mathbf{r})$ of the phonon with the boundary conditions that the tangential components of the electric field $\mathbf{E} = -\nabla\phi$ and the normal component of the displacement field $\mathbf{D} = \epsilon(\omega)\mathbf{E}$ are continuous at the interfaces. The frequency-dependent dielectric functions are given by $\epsilon_\alpha(\omega) = \epsilon_\infty(\omega_{\mathrm{LO},\alpha}^2 - \omega^2)/(\omega_{\mathrm{TO},\alpha}^2 - \omega^2)$, α=GaAs or AlAs.[11] This procedure yields a simple one-dimensional integral equation for the IF phonons. We solve the equation straightforwardly by discretizing it to give a matrix eigenvalue equation which we diagonalize by standard techniques. In the detailed calculations given here we add a small ($\approx$ 0.25%) imaginary part to the phonon frequencies to represent their finite phonon lifetimes due to anharmonicity.[12]

In the dielectric continuum approach the "confined" phonon modes are determined by requiring that their potentials vanish at the interfaces.[5] Recent lattice-dynamics calculations[6–10] for quantum wells and wires indicate that the phonon potentials satisfy this boundary condition and also that the phonon displacements go to zero within a few atomic layers of the interface. In order to study this effect we have calculated the scattering rates in two different ways, the first using the simple dielectric continuum model[5] for the confined phonons and the second using a complete orthogonalized set of phonon modes for which both the potentials and the displacements vanish at the interfaces.[13] We find that the additional requirement that the displacements go to zero at the interfaces has no effect on the scattering rates. We ascribe this to the fact that the confined mode scattering rates involve summations over a complete set of degenerate phonon modes.[15]

We obtain the electron wave functions in the effective-mass approximation with a finite potential barrier in the conduction band.[16] Schrödinger's equation does not separate for the nonelliptical wire cross sections treated here. We calculate $\psi_\alpha(\mathbf{r})$ by discretizing the wave equation in the plane perpendicular to the wire and iteratively solving the resulting matrix equation.[17]

The phonon emission rates for a 100 Å× 200 Å GaAs wire in AlAs at room temperature are shown in Fig. 1. The intersubband process involves the scattering of an electron from the excited subband to the ground subband, and the intrasubband process involves electronic

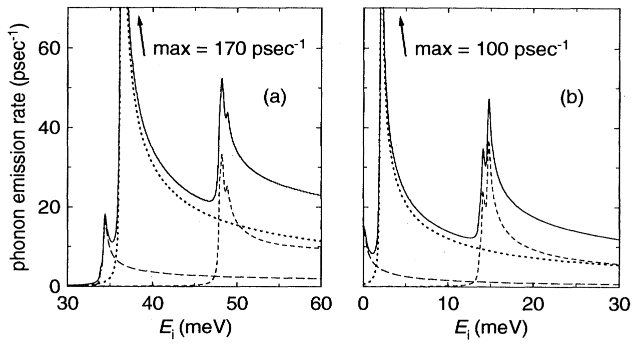

FIG. 1. (a) Intrasubband and (b) intersubband phonon emission rates as functions of initial energy E_i for rectangular quantum wires of cross section 100 Å × 200 Å. For intrasubband processes, E_i is measured from the bottom of the ground electronic subband, and for intersubband processes it is measured from the bottom of the first excited subband. For this wire width the energy splitting Δ_{10} between the two lowest subbands is 34.2 meV. The total rates are given by the solid lines. Contributions from the confined phonons, the AlAs-like IF phonons, and the GaAs-like IF phonons are, respectively, given by the dotted, the short-dashed, and the long-dashed lines.

scattering within the ground subband. The sharp features in the scattering rates arise from the divergent density of electronic states at the bottom of the ground subband. The two-peaked structure for the AlAs-like IF phonon contributions seen in Fig. 1 corresponds to different interface phonons. For wire widths smaller than that shown here, the intersubband spacing Δ_{10} exceeds the phonon energies, and these sharp features are not present in the intersubband rates. The largest contributions to the scattering rates are seen to come from the confined GaAs phonons and from the AlAs-like IF modes. For most electron energies and wire sizes, the rate of intrasubband scattering exceeds that of intersubband scattering because the functions in the electron-phonon matrix element in Eq. (1) contain less nodes for the former than for the latter.

We have pointed out earlier[2] that the IF phonon spectra of quantum wires depend on the wire shape. Modes tend to concentrate in regions of high curvature. In order to study this effect we have calculated scattering rates for rectangular wires with varying curvature in the corners. This curvature is characterized by the ratio a/r where a is the radius of curvature of the corner, and r is the length of the shorter side of the rectangle. The scattering rates are found to be insensitive to this ratio with variations of less than 1% for a/r between 0.2 and 10^{-4}. Thus, although the individual phonon modes depend sensitively on the shape of the wire the sum involved in the scattering rate does not.

In Fig. 2 the phonon emission rates are shown as functions of wire width r. The wire cross sections are rectangular with a length-to-width ratio of 2:1. For large r the confined GaAs modes dominate, and the intrasubband rate approaches that for scattering by bulk GaAs phonons. For small r the AlAs-like IF modes become important, and the intrasubband rate increases toward the

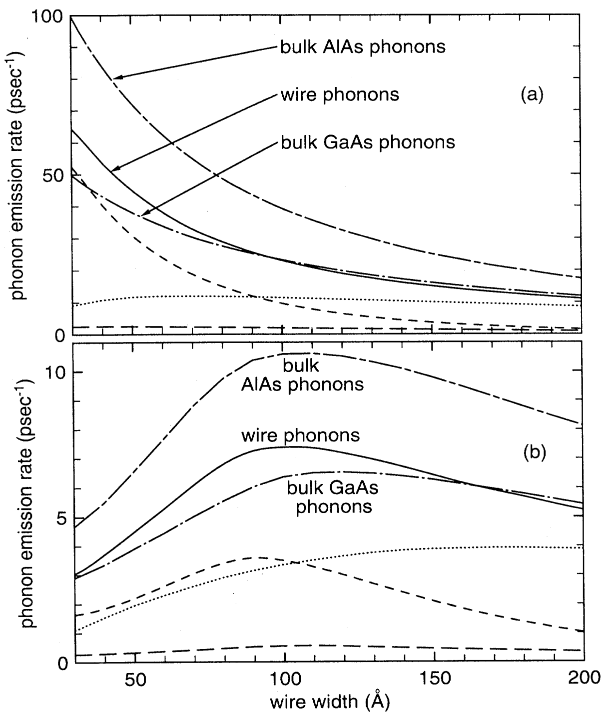

FIG. 2. (a) Intrasubband and (b) intersubband phonon emission rates as functions of the wire width r for wires of rectangular cross section $r \times 2r$. The initial electron energy is chosen to be 60 meV above the bottom of the initial subband (the ground subband for intrasubband processes and the first excited subband for intersubband processes). The total rates are given by the solid lines, and the rates from a model of bulk GaAs (AlAs) phonons are given by the dot-dashed (long-dashed–short-dashed) lines. Contributions from the confined phonons, the AlAs-like IF phonons, and the GaAs-like IF phonons are, respectively, given by the dotted, the short-dashed, and the long-dashed lines.

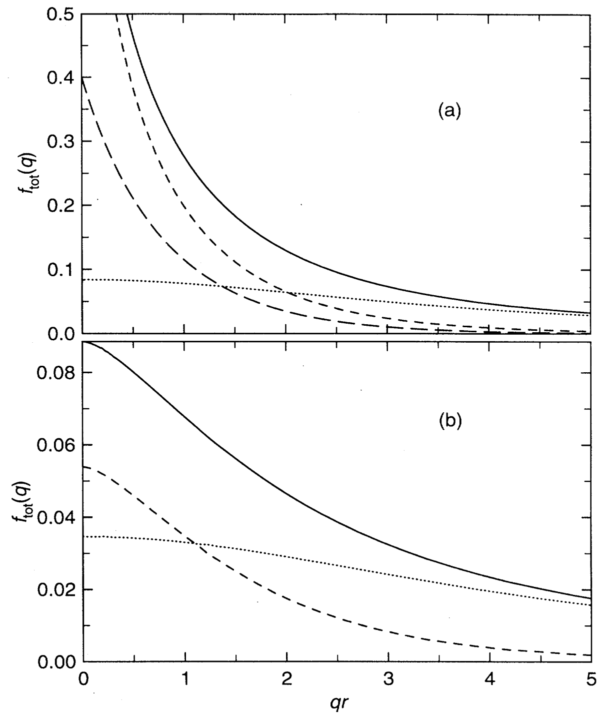

FIG. 3. $f_{\rm tot}(q)$ for (a) intrasubband and (b) intersubband scattering as functions of qr where r is the wire width. Contributions from the confined phonons and the IF phonons are given, respectively, by the dotted lines and the short-dashed lines, and the total by the solid lines. The long-dashed line in (a) gives the contribution from the IF phonons in the separable-phonon approximation of Ref. 3.

bulk AlAs value. The intersubband rate has an interesting maximum for $r \approx 100$ Å. This is the size for which the phonon energies are comparable to the intersubband spacing Δ_{10}.

In discussing the scattering rates it is useful to examine their q dependences, which are given by the quantity

$$f_\nu(q) = \frac{\left| \int d^2r\, \psi_\alpha(\mathbf{r}) \psi_\beta^*(\mathbf{r}) \phi_{\nu q}(\mathbf{r}) \right|^2}{\int d^2r' |(iq + \nabla)\phi_{\nu q}(\mathbf{r}')|^2}. \tag{2}$$

Here the denominator arises from the normalization of the phonon potentials. $f_\nu(q)$ gives the contribution of phonon mode ν at q to the scattering rates and are found to depend strongly on the reduced wave vector qr but only weakly on the wire width r. In Fig. 3 we give $f_{\rm tot}(q) \equiv \sum_\nu f_\nu(q)$ for intrasubband and intersubband scattering as functions of qr. The quantities shown in Fig. 3 are sums over all IF modes or all confined modes at each q.

For phonon emission the allowed wave-vector transfers are given by $q = \sqrt{2m}[\sqrt{E_i} \pm \sqrt{E_i + \Delta_{\alpha\beta} - \hbar\omega_\nu(q)}]/\hbar$, where $E_i \equiv \hbar^2 k_i^2/2m$. The scattering rates are given in terms of $f_\nu(q)$ evaluated at these q. The total rates for both intrasubband and intersubband scattering are larger at small qr than at large qr. For both intrasubband and intersubband rates the contributions from IF modes exceed those from the confined modes at small qr, and those from confined modes are larger at large qr. For intrasubband scattering the IF mode contribution to $f_{\rm tot}(q)$ diverges as $-\pi^{-1} \ln qr$ for small qr, and that for intersubband scattering goes to a constant. qr is small when either r is small or E_i is large. Thus the IF phonon contributions dominate for small wire width r or high energy E_i. For large r and small to moderate E_i, confined modes dominate the scattering rates.

For quantum wells the IF phonon contribution to $f_{\rm tot}(q)$ for intrasubband scattering diverges as q^{-1} for small q, which is faster than the logarithmic divergence for the case of a wire. Thus we expect that the approach of the intrasubband rate to that for bulk AlAs phonons at small size will be faster for wells than for wires. This is seen to be the case by comparing our results with those of Ref. 7. In the case of intersubband scattering when the splitting between the two subbands becomes comparable to the phonon energies the scattering rate involves small values of q, and thus the scattering rates are large. This accounts for the broad maximum of the intersubband rate for wire widths $r \approx 100$ Å in Fig. 2.

A widely used approximation for electron-phonon scattering in rectangular quantum wires involves making a separable approximation for the potential of the interface phonons.[3] In Fig. 3 we compare the results of this approximation with the present complete calculations. In the separable approximation, the IF mode contribution to $f_{\mathrm{tot}}(q)$ for intrasubband transitions goes to a constant for small qr rather than diverging as it should. This behavior results mainly from the poor representation of the potential for the totally symmetric IF mode. The ratio of the IF mode contribution to $f_{\mathrm{tot}}(q)$ in this approximation to that obtained in the present complete treatment varies from 0 at small qr to 0.5 at moderate values of qr. In addition, the separable approximation gives no contribution at all to the scattering rate between the first excited electronic state and the ground state. This is a result of the absence of IF modes which are symmetric along one axis of the rectangle and antisymmetric along the other in this approximation.[2,9] These modes are essential to give nonzero intersubband scattering. Thus this separable approximation has both qualitative and quantitative inadequacies in treating the electron-phonon scattering rates in semiconductor quantum wires.[18]

We have also investigated the effects on the scattering rates of using separable wave functions and boundary conditions for the electron wave functions. These effects are found to be small for all wire widths studied here (on the order of a few percent for $r = 100$ Å).

Here we have given a rigorous treatment of electron-phonon scattering rates in semiconductor quantum wires of general shape. The importance of the interface phonons to the scattering rates is seen, an interesting maximum of the intersubband rate as a function of wire width has been found, the approach of the scattering rate to that for bulk phonons has been studied as a function of wire size, and a quantitative assessment of reliability of using a separable approach to the IF phonons has been given. In this work we have demonstrated the importance of obtaining rigorous results for the contributions of both the interface phonons and also the confined phonons for a given wire geometry and of taking their sum to give the total scattering rate.

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