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FOR

SOLID-STATE DYNAMICS AND QUANTUM TRANSPORT IN NOVEL SEMICONDUCTOR NANOSTRUCTURES

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1. PROJECT SUMMARY

The objective of this research program is to study theoretically the underlying principles of solid-state dynamics and quantum mechanical transport of carriers in ultrasmall novel semiconductor devices. The areas of research to be investigated are: 1) theory of optical phonon modes in heterostructures and 2) quantum transport in solids with special emphasis on non-perturbative role of high-electric fields, many-body effects, and band-mixing in dynamical processes. These problems will be treated analytically through the development of macroscopic and microscopic physical models with an emphasis on quantum mechanical principles. Specific subjects discussed in this proposal include the effects of confined and interface phonon modes, two-electron quantum transport theory under hot-electron conditions, dielectric response function theory, and the effects of band-mixing in tunneling. The knowledge developed in this work will be of major importance in explaining the novel phenomena and fundamental questions relating to the breakdown of classical solid-state electronics as device dimensional scales are reduced to the submicron and ultra-submicron regime.

2. PROJECT DESCRIPTION

2.1 Introduction

Recent advances in semiconductor materials growth techniques, such as molecular beam epitaxy (MBE), metalorganic chemical vapor deposition (MOCVD), and atomic layer epitaxy (ALE), have made possible the fabrication of devices with one or more dimensions approaching the spacing between planes of atoms. These nanometer-scale techniques have also opened new possibilities for "band gap engineering" of novel semiconductor devices, including heterostructures with spatially modulated energy band gaps. By using the variability of the boundary conditions which can be imposed on the wavefunctions, electrical and optical responses in these structures can be tailored virtually at will. As fabrication technology has allowed such ultrasmall structures to be realized, many new and fundamental questions have emerged concerning the underlying physics of small dimensions with complex, quantum-scale boundary conditions in semiconductor devices. Important issues now under investigation include quantum mechanical phenomena such as size quantization, phase coherence, and highly nonequilibrium transport in which perturbative treatment or the assumption of linear response is not applicable (see, for example, Refs. 1-3). More than ever before, it is important that our ability to analyze these physical phenomena in ultrasmall devices keep in advance of the technological developments.

In 1990, the Office of Naval Research initiated sponsorship of a basic research program in the Department of Electrical and Computer Engineering at North Carolina State University. The general goal of this research program is to study theoretically solid-state dynamics and quantum mechanical transport of carriers in ultrasmall novel semiconductor devices. The emphasis is on the development of physical understanding of the novel phenomena through analytical approaches rather than numerical modeling. Our efforts have been devoted to investigating two important problems. The first one is the theory of optical phonon modes in heterostructures. The changes in longitudinal-optical (LO) phonon

frequencies, lifetime, and interaction with carriers as a result of reduced dimensionality are the main subjects in this part of research. Due to the advent of lattice mismatched strained-layer (i.e., pseudomorphic) structures, the effects of strain on LO-phonon modes have been investigated as well. The results will be of major importance to a wide variety of III-V semiconductor devices in which the scattering by LO-phonon modes is an important (at times, dominant) energy loss mechanism. The second topic is the quantum mechanical transport of charge carriers with specific emphasis on the role of electron-electron and electron-phonon interactions in the presence of high-electric fields, many-body effects, and band-mixing in dynamical processes. A novel formalism for treating Bloch electron dynamics and quantum transport in electric fields of arbitrary strength and time dependence has been studied in an attempt to include all quantum mechanical effects collectively in the lowest order in the scattering strength [1]. Specific interest in this inelastic scattering problem arises from issues and questions relevant to the role of high-electric fields in influencing transport, electron relaxation, noise generations as well as ionization processes in quantum wells, tunnel barriers, and superlattices [4]. At the same time, attempts are made to study the effects of quantum mechanical principles on carrier transport with more macroscopic approaches such as dielectric function theory.

Although less than three years old, this program has already resulted in twenty refereed publications in the literature, four additional manuscripts are currently in press, and five more have been submitted to major technical journals. Numerous invited talks and presentations have been and will be given at conferences and workshops throughout the United States and in other countries. A listing of these publications is given in APPENDIX A. In addition, this research program provides a perfect complement to other aspects of our research efforts in which numerical aspects of transport study are emphasized. Due to the complicated geometry and boundary conditions, a realistic answer for a realistic device structure is attainable only through numerical approaches. The accurate physical models and understanding developed in this research will facilitate the development of the numerical models better able to explain experimental observations and to predict new physical phenomena. Overall, this

research program supported by ONR has been efficient and productive. The quality of our program will continue to improve in the future. In this annual report, the progress and accomplishments made during the past contract period will be summarized.

The structure of the rest of this report is as follows: in Section 2.2, the research results of the past contract period are summarized; Section 2.3 provides the list of publications resulting from this research supported by ONR during the 1991 contract period; Section 3 contains background information describing project personnel; and the Appendices include a list of refereed publications supported by this research program since 1990 and the title page of each paper published during the 1991 contract period.

2.2 Summary of Research Results

This section provides the current status of our research efforts on the theory of electron-optical-phonon interactions and quantum mechanical transport in semiconductor nanostructures. The major accomplishments during the past contract period are:

- We have modeled the electron-interface-phonon interaction with a scalar potential and calculated the scattering strength in a short-period superlattice in an effort to alleviate controversies surrounding the nature of interface phonon interaction. The results have provided a criterion which, in conjunction with experiments, has been used to examine and, subsequently, to further demonstrate the validity of the dielectric continuum model;
- We have studied the effects of surface roughness (i.e., non-uniform thickness) on electron-optical-phonon scattering rates in a rectangular quantum wire and have estimated electron mobilities by applying an ensemble Monte Carlo method;
- We have investigated the electron-interface-phonon interaction in a double-barrier heterostructure to explore the possibility of achieving a simplified description for interaction Hamiltonians in

multi-heterointerface structures. It is found that when the dimensions of the structures are larger than approximately 30 Å, the Hamiltonians developed for a single quantum-well structure can, in general, be applied to multi-heterointerface structures with reasonable accuracy;

- We have demonstrated that optical phonon modes may be tailored through the judicious use of metal-semiconductor interfaces in such a way as to dramatically reduce unwanted emission of interface phonons;
- We have developed the dielectric response function which properly incorporates the finite particle lifetime in heavily-doped zincblende semiconductors at finite temperature and have demonstrated its importance in electron transport, especially, in p-type semiconductors; and
- We have derived the envelope functions for Bloch electron in the Wannier representation in the presence of Slater-Koster type impurities and have deduced the "transmission coefficient" for electron tunneling through impurities and "band-engineered" quantum barriers.

Each of these results is discussed in detail below.

Role of interface-phonon scattering in mesoscale structures

Since the early work of Fuchs and Kliewer [5], the effects of confinement on LO-phonon modes have been studied theoretically by a number of researchers (including ourselves). There have been indications that interactions by interface modes can be significant and may become the dominant energy loss mechanism in polar semiconductors with ultra-small dimensions. Therefore, an appropriate treatment of electron-interface-phonon scattering in quantized systems is essential for the understanding of electron transport in heterostructures. Recently, however, the role of interface phonons in electron transport has been questioned [6]. The predicted strong influence of electron-interface-phonon coupling is obtained by applying the dielectric continuum model with electrostatic boundary conditions. There is concern regarding the validity of using the electrostatic boundary conditions as well as with describ-

ing the interface modes in terms of a scalar potential.

In order to alleviate controversies surrounding this issue, we have modeled the electron-interface-phonon interaction with a scalar potential to calculate the ratio of electron-interface-phonon scattering to electron-confined-LO-phonon scattering in a short-period superlattice. The results provide a criterion which, in conjunction with experiments, can be used to examine the validity of the dielectric continuum model. The specific example considered in this study is a GaAs/AlAs short-period superlattice with the GaAs layer width of a and the AlAs layer width of b. The ratio of electron-interface-phonon scattering to electron-confined-LO-phonon scattering in this superlattice is calculated through the Fermi golden rule by taking the electronic wavefunction along the growth direction (i.e., the z-direction) as that given by Cho and Prucnal for the maximum edge of the first subband [7]. To obtain an order-of-magnitude estimate of the ratio of electron-interface-phonon scattering to electron-confined-LO-phonon scattering, we consider the ratio of principal factors, Y, in the integrands of the respective scattering rates. In this calculation, the contribution by the S– mode is neglected due to its relatively small contribution as compared with the S+ mode. In addition, we have included only the lowest order confined mode since it makes the dominant contribution among all of the confined modes for the electronic states under consideration. Figure 1 shows the ratio, Y, plotted as a function of X (=qa where q is the phonon momentum parallel to the heterointerface) for a superlattice with b=a and b=3a/2. For $X \leq \pi$, the ratio Y is larger than unity. A principal factor contributing to the rapid increase in Y as shown in Fig. 1 for small values of qa is the exponential increase in the strength of the interface-phonon mode near the heterojunction. In agreement with our results, a surge in the strength of the S+ mode with decreasing well-width, a, is observed in the recent low-temperature Raman experiment by Tsen et al. [8], which appears to indicate the dominance of the S+ interface-phonon mode over the confined LO-phonon modes. In addition, electron mobilities measured by Zhu in short-period superlattices show a degradation as the well-width is reduced to a very small dimension, which can be attributed to an increasing interface-phonon scattering as well [9]. Therefore, we expect that electron-interface-phonon

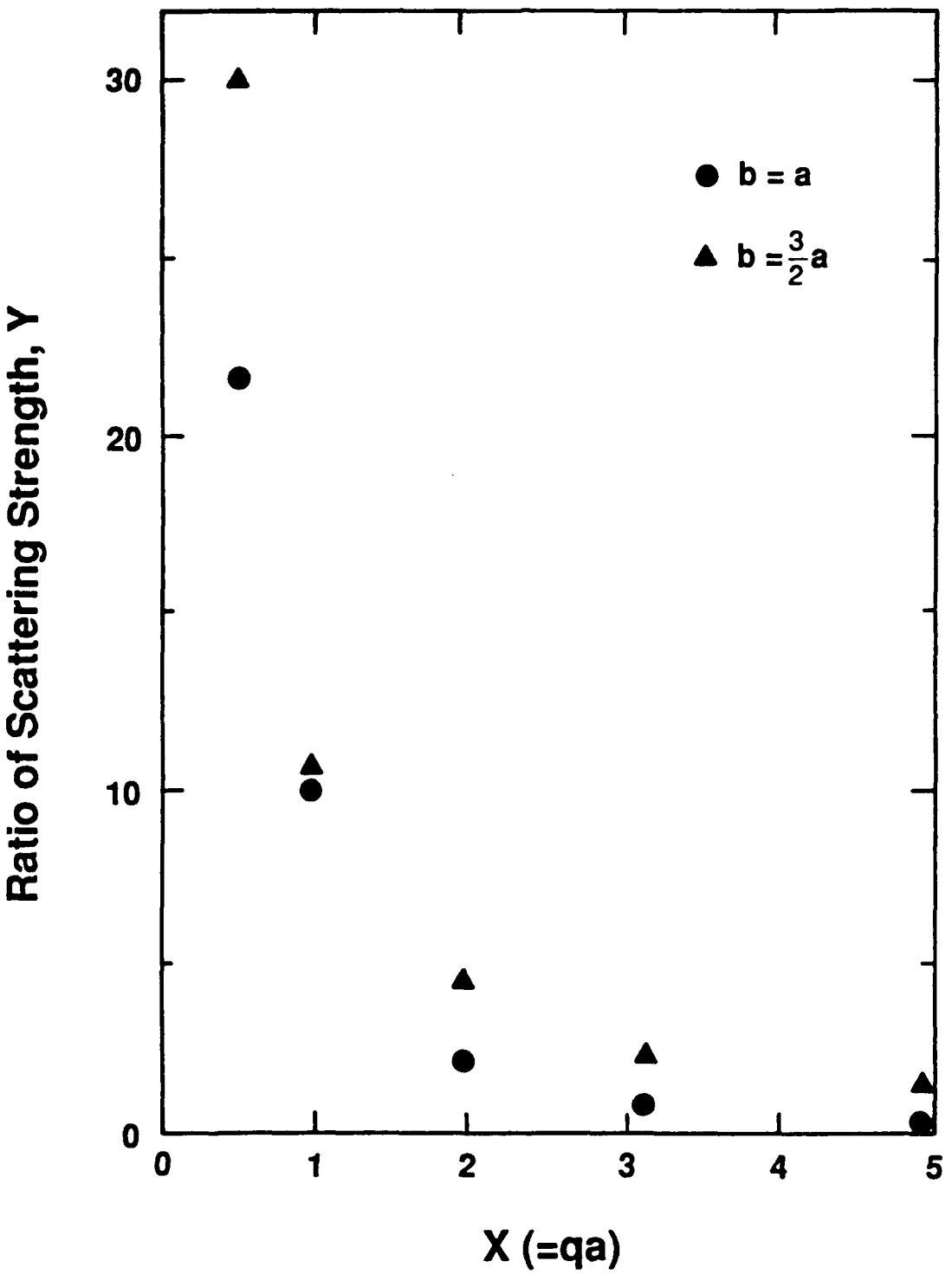
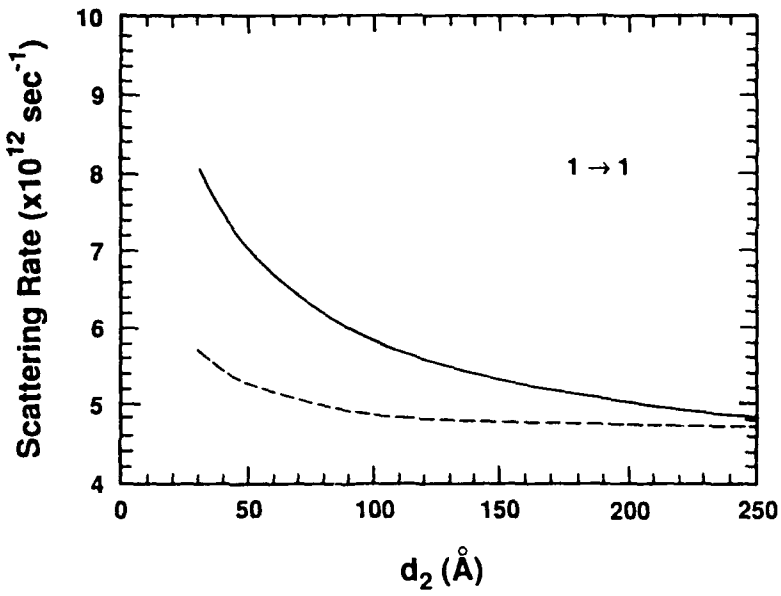


Figure 1. Approximate ratio of electron-interface-phonon (S+ mode) scattering to electron-confined-LO-phonon (m=1 lowest order mode) scattering in a GaAs/AlAs short-period superlattice with the GaAs layer width of a and the AlAs layer width of b.

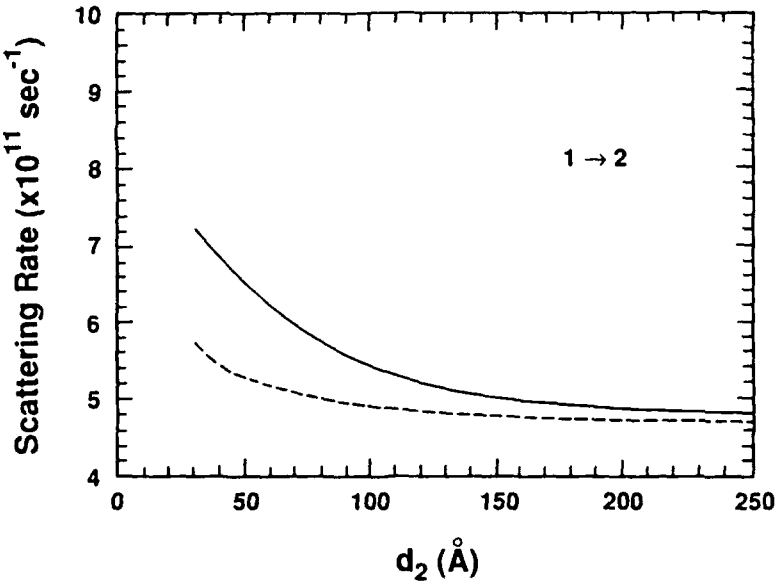
interaction can be described by the dielectric continuum model appropriately and should be included in the study of low-voltage (also, low-temperature in general) operation characteristic of mesoscale devices currently being considered by the electron device community. This point has been proved further by the recent development in detailed microscopic calculations of interface modes in polar semiconductors [10].

As discussed above, an appropriate treatment of the optical phonon modes in quantized systems is essential for the understanding of electron transport in heterostructures. However, most of the theoretical analyses have been confined to highly symmetric and/or simple structures such as single quantum wells or superlattices. Application of even a simple macroscopic model, not to mention the microscopic *ab initio* models, becomes highly complicated due to the coupling between adjacent interfaces when the structure has multiple heterointerfaces or is asymmetric. Thus, it is desirable to investigate the possibility of utilizing an approximate description of phonon modes and related interaction Hamiltonians, while retaining the quantized nature of phonon modes in multi-heterointerface structures. During the past contract period, we have studied the electron-optical-phonon interaction in a GaAs/AlAs double-barrier heterostructure to explore the possibility of achieving a simplified description such as discussed above. The double-barrier structure has been chosen as a specific example due to its structural similarity (with the added complexity of finite barrier width) to single quantum wells (i.e., infinite barrier width) for which quantized optical phonon modes are already well known. At the same time, this structure has played a prominent role in recent studies which demonstrated the existence and importance of interface-phonon modes (see, for example, Ref. 11). In our study, the interaction Hamiltonians were derived by applying the macroscopic dielectric continuum model (application of which is justifiable as discussed above) without any further approximations. Then, the resulting scattering rates were compared with those obtained by assuming the Hamiltonians appropriate for single quantum wells for which finite barrier widths are neglected. Since the dielectric continuum model approximates the confined LO modes as being completely confined to the respective layer and

not affected by or coupled to the adjacent layers, we have only considered the influence of finite barrier widths on the interface LO modes as well as their interactions with electrons. Figure 2 shows the electron scattering rates via interface-phonon emission as a function of barrier thickness, d_2, when the well width, d_1, is fixed to 60 Å. Each of these rates is evaluated at a value of $E_{||}$ which is chosen to be just large enough to permit a phonon emission so that there is an electronic transition from an initial state to a final state; i.e., for Fig. 2(a), $E_{||}$ is fixed at 37 meV while, for Fig. 2(b), it is 37 meV plus the energy separation between the first and second subbands. As expected, the two rates merge smoothly with increasing d_2. By the time d_2 is approximately equal to d_1 (i.e., 60 Å), the difference is only about 20 %. This reduces to roughly 10 % with $d_2 = 2d_1$ (=120 Å). In the other limit, the difference magnifies rapidly as d_2 shrinks below 30 Å. Thus, the results in Fig. 2 suggest that when $d_2 \gtrsim 30$ Å, our simplified description using Hamiltonians for single quantum wells can be applied with good accuracy in place of the more complicated expressions derived for each double-barrier structure. When the well width is reduced from the 60 Å used in Fig. 2, it is expected that there will be some effects on the coupling between the interface-phonon modes in the barrier region. Our calculation shows that when d_1 is reduced to 30 Å, only a minor change is observed in the phonon modes in the barrier region. At the same time, the electronic wavefunctions are rather well confined in the well region with this thickness range. Hence, when the thicknesses of both the barrier and well regions are larger than 30 Å (roughly), it is expected that the electron-interface-phonon scattering rates can be well approximated by the Hamiltonians originally developed for single quantum-well structures. This finding can be applied to multi-heterointerface structures in general as well as to the double-barrier structures investigated in this study. Application of the simplified Hamiltonians to calculate the phonon-assisted tunneling current in a double-barrier resonant tunneling structure resulted in remarkably good agreements with experimental data [11], which provides further justification for the dielectric continuum model.



(a)



(b)

Figure 2. Electron scattering rates by interface-phonon emission as a function of barrier thickness, d_2, when the well width, d_1, is 60 Å in a GaAs/AlAs double-barrier heterostructure at 300 K. The data in (a) describe the intra-subband scattering rates of the lowest resonant subband in the GaAs quantum well (i.e., $1 \rightarrow 1$), and those in (b) show the inter-subband scattering rates from the lowest to the second lowest subband (i.e., $1 \rightarrow 2$). The electron energy $E_{||}$ is fixed at 37 meV for (a), while it is 37 meV plus the energy separation between the first and second subbands (ΔE_{12}) for (b). The solid line is obtained from the interaction Hamiltonians derived for the double-barrier structure, while the dashed line is estimated by the simplified Hamiltonians appropriate for single quantum-well structures.

The significance of interface phonon scattering with decreasing structural sizes, as demonstrated above, poses a serious problem in achieving nanoscale structures with greater complexity and higher speed. Last year, we have realized that elimination or dramatic reduction of this unwanted energy loss mechanism may be possible under a special set of boundary conditions. Based on the dielectric continuum model [5], it is predicted that at the semiconductor boundaries with an ideal metal, the optical phonon modes become evanescent and vanish unless they have even polarization vectors normal to the interface. Thus, the phonon modes may be tailored through the judicious use of metal-semiconductor interfaces in such a way as to drastically reduce the scattering rates by interface phonons. This may represent a major breakthrough for the future generation electronic devices. For further demonstration of this concept, more investigation is warranted which takes into account the full dependence of phonon suppression on the conductivity of the metal.

Electron-optical-phonon interaction in realistic quantum wires

The progress in semiconductor technology has provided the means to fabricate so-called quantum wires with quasi-one-dimensional (1D) structures. It has been suggested that quantum wires will exhibit carrier mobilities well above 10^6 $cm^2/V \cdot sec$, but these high values of the mobility have not yet been observed experimentally. The expected enhancement of the carrier mobility in quantum wires should stem from the restriction of momentum space to one dimension as well as the resulting reduction of final states for scattered electrons. This point, however, needs to be clarified since electron interactions with the dominant optical phonon modes are strongly modified by phonon confinement and localization as well.

During the 1990 contract period, we have reported the derivation of electron-optical-phonon interaction Hamiltonians in a rectangular quantum wire, in which the phonon confinement and localization (i.e., confined and interface modes) are considered by applying the dielectric continuum model [12]. In this study, an "ideal" structure is assume which means that the surface roughness of the

quantum wire is neglected (i.e., a constant thickness along the structure). Real quantum wires, however, always have variable thickness along the structure. Generally, electron beam or X-ray lithography on a quantum well surface, with subsequent reactive ion (beam) etching, is used for quantum wire fabrication. State-of-the-art technology allows the quantum well width to be controlled down to one monolayer. However, the etching results in quantum wires with thicknesses varying within several percent along the structure. Even the most sophisticated technologies fail to provide abrupt interfaces between the layers. Thus, it appears that all current and foreseeable future technologies for fabricating quantum wires do not assure the possibility to creating ideal structures with constant thickness. The variation of quantum wire thickness results in the variation of subband energies and, consequently, electron scattering is no longer energetically coherent in different parts of a quantum wire. This may significantly affect the unique features of ideal 1D systems (such as diverging density of states at the subband minimum) and alter the carrier transport properties in realistic situations.

As a generalization of our previous results, we have started an investigation on the accurate description of electron transport in real quantum wire structures. For simplicity, the real quantum wires are assumed to have a smooth, harmonic variation of thickness along the structure so that the characteristic length of the fluctuations is much greater than the de Broglie wavelength Λ_B. The variation amplitudes δL_y and δL_z have been chosen as a fraction ranging from 1 % to 10 % of the corresponding thicknesses L_y and L_z. We have considered three cases with different mutual phases of the variation of L_y and L_z: i.e., $L_z = L_{zo} + \delta L_z \cos(Kx)$, $L_z = L_{zo} + \delta L_z \sin(Kx)$, and $L_z = L_{zo} + \delta L_z \cos(2Kx)$ with $L_y = L_{yo} + \delta L_y \cos(Kx)$ in all three cases. The scattering rates λ by confined and interface optical phonon modes are calculated with a give L_y and L_z based on the 1D interaction Hamiltonians developed previously [12], and properly averaged over the quantum wire length L with varying thicknesses:

$$\lambda(E_o,L_{yo},L_{zo}) = \frac{1}{L}\int_0^L dx\ \lambda[E_x(x),L_y(x),L_z(x)] \quad , \tag{1}$$

where $E_x = E_o + \delta E(x)$, $E_o = E - \langle E_{jl}\rangle$ is the electron kinetic energy corresponding to a given total energy E and average subband position $\langle E_{jl}\rangle$, $\delta E(x)$ is the electron kinetic energy variation (opposite to the variation of subband position) due to the variation of thickness. It has been found that the results do not show significant differences between these models as long as it is in the limit of smooth fluctuations (i.e., $K\Lambda_B \ll 1$). A typical electron transition rate from the first subband to elsewhere due to emission of confined LO phonons is presented in Fig. 3 for ideal and real quantum wires. A GaAs quantum wire embedded in AlAs is assumed with the dimensions of L_y=150 Å and L_z=250 Å. The forward and backward scatterings are plotted as separate scattering mechanisms in order to reveal the polar character of electron-phonon interaction. The scattering rates by interface modes are not considered since they are more than an order of magnitude smaller than those by confined LO modes, as discussed in our previous report. For a reasonable 5 % variation in amplitude (i.e., $\delta L_y/L_{yo} = \delta L_z/L_{zo} = 0.05$), one can see in Fig. 3 that the scattering rates are considerably modified in real quantum wires compared to the ideal wire. It is interesting to note that the well-pronounced resonant nature of electron scattering in the form of multiple sharp peaks (which is one of the unique features in an ideal 1D system) is significantly broadened and reduced (for the first peak) or even completely disappeared (for the higher peaks). Similar curves with a different degree of broadening are obtained for other variation amplitudes. Even a variation in amplitude as small as 1 % leads to the disappearance of the divergence at the resonant energies and a dramatic smearing out of the peak-like structure on the curves discussed.

The calculated scattering rates for an ideal quantum wire have been included in the Monte Carlo program and electron transport has been simulated at various electric fields as well. The aim of these simulations is to reveal the role of electron intersubband scattering due to confined and interface pho-

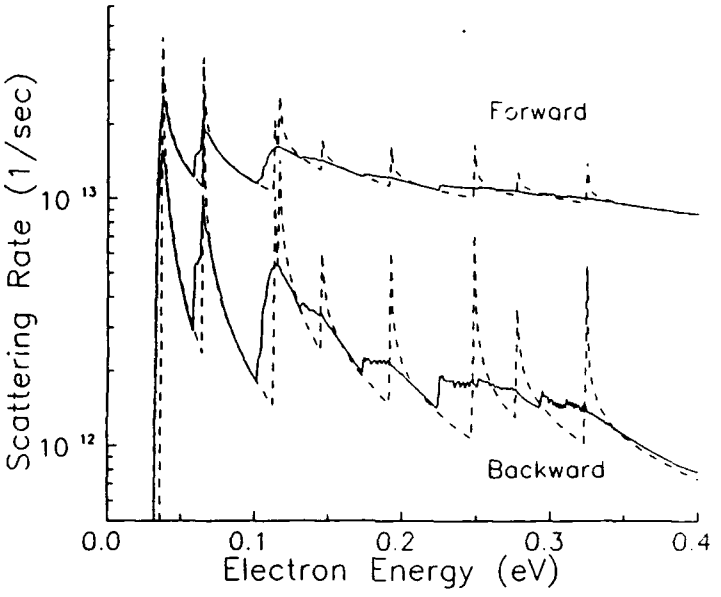


Figure 3. Electron scattering rate due to LO phonon emission in/from the first subband as a function of the electron kinetic energy. Dashed curves are for the ideal quantum wire; and solid curves for the real quantum wire with 5 % thickness variation along the structure. Upper curves represent forward electron scattering (wavevector direction does not change); and lower curves represent backward scattering (wavevector change its direction to opposite). A GaAs quantum wire embedded in AlAs is assumed with the dimensions of L_y=150 Å and L_z=250 Å at 300 K.

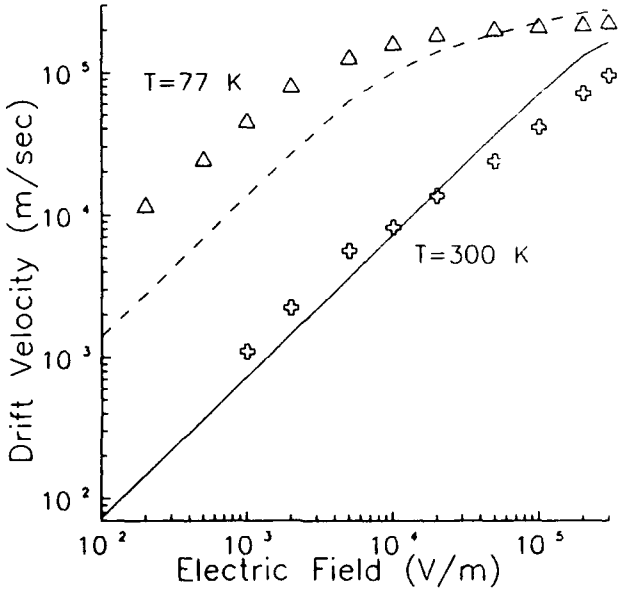


Figure 4. Electron drift velocity as a function of electric field. The data points represent the results obtained for the quantum wire and the curves are those for bulk GaAs. Upper dots and curves are at 77 K and the lower dots and curves are at 300 K.

nons in electron transport phenomena in quantum wires, and to examine the feasibility of the suggested high mobilities in quantum wire structures. Under the conditions of intensive intersubband scattering at 300 K, electrons do not exhibit the expected high mobilities, as one can see from Fig. 4 where velocity-field dependences for the quantum wire and bulk undoped GaAs are plotted for comparison. At this temperature, electron scattering by confined LO phonons determines electron low-field mobility. The role of acoustic and impurity scattering as well as scattering by interface phonons is negligible. Electron mobility enhancement in ideal quantum wires is seen in Fig. 4 at 77 K and low electric fields; in that case electrons do not undergo effective scattering in the "passive" region below the optical phonon energy. However, at 77 K the probability of absorption of optical phonons is of the same order as that of acoustic scattering and the electron mobility is controlled not only by the electron-optical-phonon scattering but also by the acoustic phonon scattering which is not considered in the present work. Therefore, we observe higher mobility than it should be. It must be noted that electron scattering by interface phonons does not influence considerably electron steady-state high-field transport. However, interface phonons which have energies different from those of confined LO phonons yield very fast energy dissipation and are essential to study the relaxation of the electron energy distribution function at low electric fields. In the case when interface phonon scattering is not considered, the injected electron distribution function exhibits sharp peaks at energies which are multiples of the confined LO phonon energy and does not relax to the equilibrium distribution function in the absence of an electric field.

Effects of finite particle lifetime on electron transport in heavily-doped semiconductors

During the past contract period, we have initiated a study on the dielectric response function theory to advance our understanding of many-body effects, such as plasmon-phonon coupling and dynamic screening, within the frame work of the random phase approximation (RPA) or the self-consistent field approach (SCF). It is well known that the dynamic response of a free electron gas is

described by the Lindhard dielectric function in the RPA or the SCF when the electron lifetime τ is infinite. The free electron gas formula is easily applicable to heavily-doped n-type semiconductors since they have a single conduction band with s-like symmetry. For p-type semiconductors, the situation is much more complicated because of the $p^{3/2}$-like symmetry of the valence bands. Recently, Yevic and Bardyszewski [13,14] evaluated the Lindhard dielectric function for a p-type semiconductor at finite temperature. These authors showed that the structure of the spectral density function is quite different from that for zero temperature. However, they still neglected the effects of the finite hole lifetime even for finite temperature. Although the Lindhard dielectric function inherently incorporates the effects of single particle excitation (Landau damping) including both intra- and interband transitions, it does not take into account the finiteness of particle lifetime due to the collision effects such as impurity scattering and phonon scattering. At finite temperature, these effects are very important since such scattering disturbs the collective motion of quasi-particles and therefore the dynamic response function will be affected significantly. As a result, electron transport in such environments will be influenced strongly as well. A detailed understanding of the behavior of electrons in heavily-doped semiconductors is increasingly important, especially for the design of high speed HBTs and HETs, since electron transport in the base region is one of the critical factors limiting the maximum switching speed of such devices.

By modifying an approach proposed by Mermin for free electron gas [15], we have developed the dielectric response function which properly incorporates the finite particle lifetime in heavily-doped zincblende semiconductors (denoted as the Lindhard-Mermin dielectric function hereinafter). The dielectric response function for a polar semiconductor comprises three terms which can be written as

$$\varepsilon(q,\omega) = \varepsilon_{\infty} + \varepsilon^{lat}(q,\omega) - \frac{4\pi e^2}{q^2} p(q,\omega) \quad . \tag{2}$$

The first term is the high frequency dielectric constant with vanishingly small free carrier density, which arises from the polarization of valence electrons due to virtual interband transitions. The second

term is the lattice dielectric function usually described by the well-known Lyddane-Sachs-Teller relationship:

$$\varepsilon^{latt}(q,\omega) = \varepsilon_\infty \frac{\omega_{LO}^2 - \omega_{TO}^2}{\omega_{TO}^2 - \omega^2} \quad . \tag{3}$$

Here, the spatial dispersion and damping of phonons due to multiple phonon processes are neglected to avoid unnecessary details. The third term in Eq. (2) is attributed to the contribution of the carrier polarization where $p(q,\omega)$ represents the polarization. When the lifetime of the carrier gas is infinite, the first and third terms give the well-known Lindhard dielectric function:

$$\varepsilon^{L}(q,\omega) = \varepsilon_\infty - \frac{4\pi e^2}{q^2} \sum_{n,l} \sum_{k} |F_{n,l}^{k,k+q}|^2 \left\{ \frac{f_n(k) - f_l(k+q)}{E_n(k) - E_l(k+q) - \hbar\omega} \right\} \quad , \tag{4}$$

where E_n and f_n are the particle energy and the Fermi distribution in the n-th band. The summation on n and l indices correspond to just n=l=c (i.e., the conduction band) for n-type semiconductors. For p-type semiconductors, the indices correspond to either the heavy hole (hh) or the light hole (lh) band. The overlap factor $|F_{n,l}^{k,k+q}|^2$ which is obtained from the lowest $\mathbf{k}\cdot\mathbf{p}$ terms is 1 for $n = l = c$; $1 - 3q^2\sin^2\theta/4|\mathbf{k}+\mathbf{q}|^2$ for $n = l = hh,lh$; and $3q^2\sin^2\theta/4|\mathbf{k}+\mathbf{q}|^2$ for $n,l = hh,lh$ with $n \neq l$. When the finite lifetime τ is considered, the third term in Eq. (2) is modified to give

$$\varepsilon^{LM}(q,\omega) = \varepsilon_\infty + \frac{(1+i/\omega\tau)[\varepsilon^{L}(q,\omega+i/\tau) - \varepsilon_\infty]}{1 + (i/\omega\tau)[\varepsilon^{L}(q,\omega+i/\tau) - \varepsilon_\infty]/[\varepsilon^{L}(q,0) - \varepsilon_\infty]} \quad . \tag{5}$$

The evaluation of the appropriate value of the relaxation time τ is quite complicated when considering the validity of relaxation time approximation. However, since τ is related to the conductivity, an approximate value can be estimated from experimental data for mobility. Once Eq. (5) is obtained, the total inelastic scattering (by coupled plasmon-phonon interactions) rate is given by

$$\Gamma_e(E) = \frac{e^2}{\pi\hbar^2} \left[\frac{2m_e}{E} \right]^{1/2} \int_0^\infty \frac{dq}{q} \int_{\hbar\omega_{min}}^{\hbar\omega_{max}} d(\hbar\omega)\, \mathrm{Im}\left[-\frac{1}{\varepsilon(q,\omega)} \right] (1 + n_\omega) \tag{6}$$

for an electron with energy E in the conduction band, where n_ω is the Bose function for the phonon distribution.

As a specific example, we have chosen p-type GaAs to demonstrate the significance of finite τ in the electron transport studies. The spectral density functions are obtained for three different values of $\hbar/\tau$ (0, 0.02 eV, and 0.05 eV) and a hole density of $p = 2\times10^{18}$ cm^{-3} at 300 K. For these conditions, the hole mobility is about 100 $cm^{-2}/V\cdot sec$, which corresponds to $\hbar/\tau$=0.023 eV. For small values of q ($\sim1\times10^5$ cm^{-1}), the plasmon damping is small when $\hbar/\tau$=0, as shown previously [13]. This is due to the smallness of the Landau damping. However, as expected, when the relaxation time is set to a finite value, the plasmon mode is heavily damped and broadened. For $\hbar/\tau$=0.05 eV, the plasmon feature almost completely disappears. We also noticed that the anti-screening effect is weakened and the phonon-like mode is also damped at a small q. As q becomes larger ($\geq1\times10^6$ cm^{-1}), collision effects (due to the finite hole lifetime) become less dominant and Landau damping dominates. Thus, for minority electron transport, the finite hole lifetime influences the long range interaction (i.e., small q) between an electron and a hole gas significantly, while the short range interaction is not affected appreciably. The effects of finite hole lifetime on the inelastic scattering rates of minority electrons calculated from Eq. (6) are shown in Fig. 5. The collision effects in the valence bands clearly enhance the transition rates of minority electrons. This result is attributed mainly to the larger value of the spectral density function at small q and ω due to the collision-induced broadening, as discussed above. Although, only the case of $p = 2\times10^{18}$ cm^{-3} at 300 K is reported here, the collision effects are important in most cases for heavily-doped semiconductors (in the n-type cases, the influence is generally smaller but still sizable). As the doping density increases, the Landau damping and collision effects (i.e., finite particle lifetime) both become larger at finite temperature. In this sense, the simple plasmon model, which has been used in some Monte Carlo simulations is highly questionable.

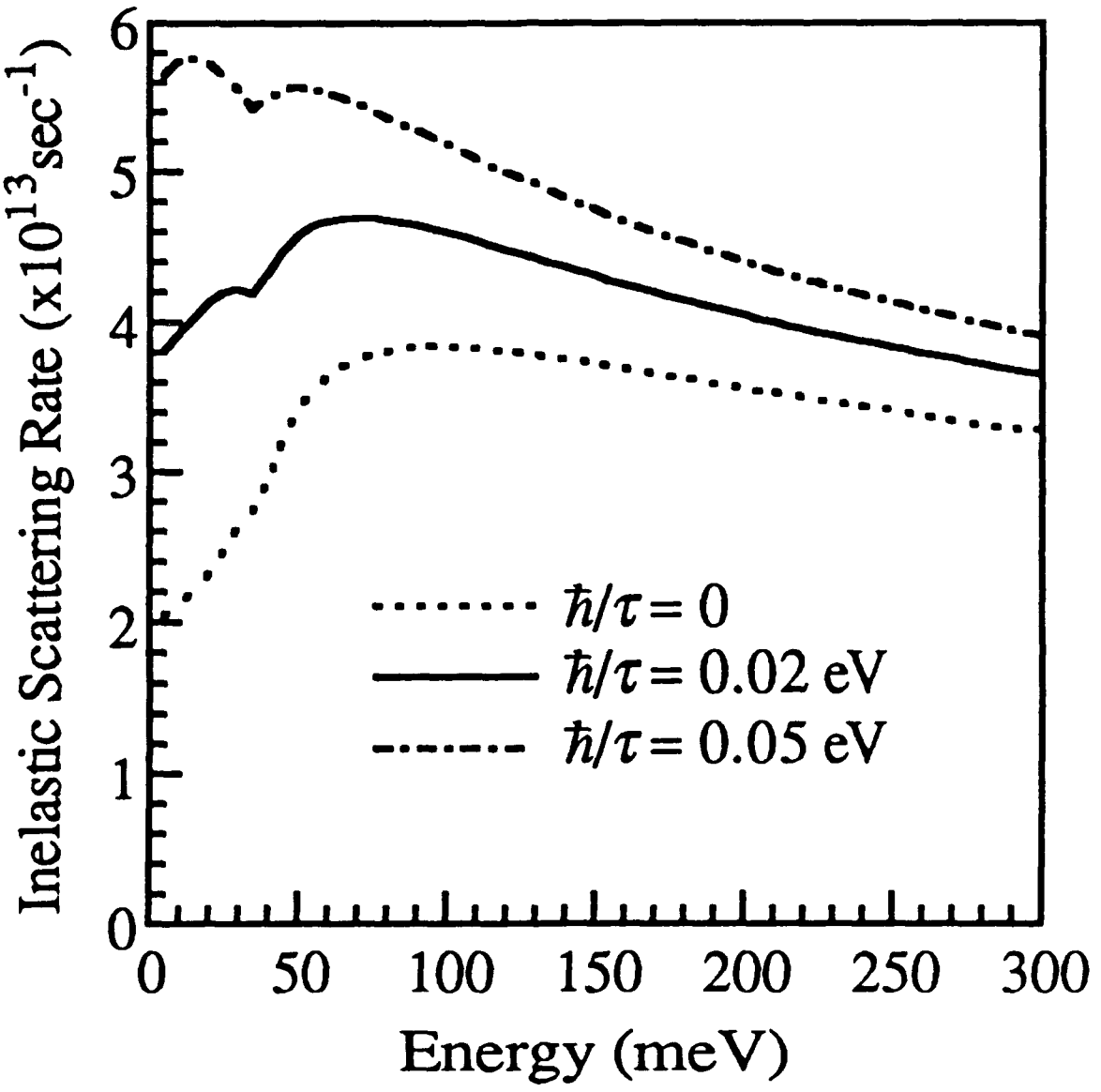


Figure 5. Inelastic scattering rates of minority electrons as a function of electron energy for $p = 2\times10^{18}$ cm^{-3} at 300 K. Note that the scattering rates are not zero even for E = 0 due to the thermal broadening.

Electric field assisted quantum transport in solids

When we deal with carrier transport in semiconductor devices with ultrasmall dimensions, it is necessary to study quantum effects of carriers in semiconductors subjected to rapidly varying, spatially inhomogeneous electric fields and non-steady state temporal conditions. At this scale, many new and interesting effects, which are currently treated as only high order corrections, will begin to dominate the device performance and the semi-classical Boltzmann equation approach becomes highly questionable.

A novel formalism for treating Bloch electron dynamics and quantum transport in inhomogeneous electric fields of arbitrary strength and time dependence was developed previously by Iafrate et al. [1,16]. In this formalism, the electric field is described through the use of vector potential. This choice of gauge leads to a natural set of basis functions for describing Bloch electron dynamics; in addition, a basis set of localized, electric field dependent Wannier functions is established and utilized to derive a quantum "Boltzmann equation" which includes explicit band-mixing transients such as effective mass dressing and Zener tunneling. In this localized Wannier representation, the differential equation for the envelope function $f_n(\mathbf{r},t)$ in the Wannier representation is given by

$$i\hbar\frac{\partial f_n(\mathbf{r},t)}{\partial t} = \varepsilon_n(-i\nabla-\frac{e}{\hbar c}\mathbf{A}_o)\, f_n(\mathbf{r},t) - e\mathbf{E}_o\cdot\sum_{n'} \mathbf{R}_{nn'}(-i\nabla-\frac{e}{\hbar c}\mathbf{A}_o)\, f_{n'}(\mathbf{r},t) \qquad (7)$$

$$+ \sum_{n'}\sum_{l'} eV_{nn'}(l',\mathbf{r})\, f_{n'}(l',t)\ ,$$

where $\varepsilon_n(\mathbf{K})$ is the n-th Bloch energy band with crystal momentum $\mathbf{K}$, $\mathbf{R}_{nn'}$ are the band-mixing terms terms due to the homogeneous electric field, $V_{nn'}$ are the matrix elements of the inhomogeneous potential with respect to the localized basis, and $\mathbf{A}_o$ is the vector potential due to the field of spatially homogeneous part. In this representation, the complete set of Wannier functions is used as basis functions. These functions have the desirable property of being localized which makes them most convenient for discussing a localized perturbation and the localized states arising from this perturbation.

As an application of the formalism, we have studied the solution to Eq. (7) for the case of a nearest neighbor tight-binding band at zero homogeneous field with Slater-Koster impurities as inhomogeneous fields. In this case, the time-independent envelope function $g_n(r)$ can be written as

$$g_n(r) = e^{iur} + \sum_{l}\sum_{l'} V_n(l',l)\, W_n(r,l)\, g_n(l') \,, \tag{8}$$

where $W_n(r,l)$ is the Green's function. The Green's function has been derived within the nearest neighbor tight-binding approximation. The impurity energy levels within the energy bandgap as well as the "transmission coefficients" for a Bloch electron tunneling through one and two Slater-Koster type impurities were obtained respectively. It is found that the transmission coefficient T is always less than one in the one impurity case. However, resonant tunneling occurs in the two Slater-Koster impurity case. The transmission coefficient for an electron to tunnel through two impurities with impurity strength V_o and V_1 is found to be

$$T = \sqrt{T^*T} = \frac{1}{1 + [2ab\sin(ul) - (a+b)\cos(ul)]^2 + (a-b)^2\sin^2(ul)} \,, \tag{9}$$

where a and b are band structure dependent parameters, u is the momentum of the electron, and l is the distance between two impurities. For the nearest neighbor tight-binding band, $\varepsilon_n(k)=\varepsilon_o+2\varepsilon_1\cos(ka)$; $a=V_o/[2\varepsilon_1\sin(u)]$; and $b=V_1/[2\varepsilon_1\sin(u)]$. For the impurities of identical strength,

$$T = \frac{1}{1 + 4[\frac{V_o}{2\varepsilon_1\sin(u)}]^2\,[\frac{V_o}{2\varepsilon_1\sin(u)}\sin(ul) - \cos(ul)]^2} \tag{10}$$

The resonant transmission (T=1) occurs when

$$\frac{V_o}{2\varepsilon_1\sin(u)}\sin(ul) - \cos(ul) = 0 \,. \tag{11}$$

Clearly at energies determined by Eq. (11), electrons resonantly tunnel through impurity-based double barriers.

By treating a different crystal (lattice-matched) as many impurities, we have examined the transport of electron through a double heterojunction structure (i.e., band-engineered quantum barrier or well) and a single heterojunction (i.e., infinite impurities) as well. The transmission coefficient T for an electron to tunnel through these heterostructures have been derived. For a double heterojunction structure (described as L+1 impurities),

$$\sqrt{T} = \frac{(1-c)e^{-iu'L} + (d-c)e^{-iu'L} - (1-d)e^{-iu'L}}{(1-c)^2e^{-iu'L} - (1-d)^2e^{-iu'L}} , \tag{12}$$

where c and d are determined by the momentum of electron u and u′ in the two different crystals, respectively. With some assumptions for the energy bands, the transmission coefficient T is simplified as

$$T = \frac{1}{1 + \frac{\sin^2[u'(L+1)]}{\sin^2(u')\sin^2(u)}[\cos(u') - \cos(u)]^2} = \frac{1}{1 + (\frac{V_o}{2\varepsilon_1})^2 \frac{\sin^2[u'(L+1)]}{\sin^2(u')\sin^2(u)}} . \tag{13}$$

It predicts the resonant tunneling when

$$\sin[u'(L+1)] = 0 \quad \Rightarrow \quad u' = \frac{m\pi}{L+1} , \tag{14}$$

where m is an integer.

This formalism has also been applied to quantum transport and Bloch oscillations in a homogeneous electric field. In the case where no inhomogeneity is present, it has been found that in a one-band model the homogeneous electric field leads to inherent localization of charge in periodic potential, and the energy forms a Stark ladder spectrum. This field-induced localization is explicitly revealed by the time evolution of the envelope function

$$f_n(l,t) = \sum_{l'} K(l-l',t-t')\, f_n(l',t') = \sum_{l'} e^{i\Phi(l-l',t)}\, J_{l-l'}(\xi)\, f_n(l',0) , \tag{15}$$

where the propagator $K(l-l',t-t')=e^{i\Phi(l-l',t)}J_{l-l'}(\xi)$, with $\xi=(W/\hbar\omega_B)\sin(\omega_B t/2)$ and the Bessel function

$J_{l-l'}(\xi)$, is a localized function for small ξ (or high electric field). Here, W is the band width and ω_B is the Bloch frequency. Equation (15) predicts localization of electron within a single lattice site when $W/\hbar\omega_B < 1$. In a three dimensional solid, in which the lattice spacing a is on the order of an Å and the band width W is on the order of an eV, the confinement of an electron in a lattice site requires a very high electric field strength ($\sim 10^7$ V/cm). On the other hand, in a superlattice with a period of ~100 Å and W in the range of 0.01-0.1 eV, the electronic motion could be restricted to a distance comparable to the superlattice period for moderately high electric fields ($\sim 10^5$ V/cm). Localization in a superlattice under such a field has been observed by Mendez et al. [17]. At such a high electric field, the possible path for electron to escape from the lattice site will be the transition to another band (or Zener tunneling).

2.3 Publications and Presentations

During the last year, this program has resulted in eleven refereed publications in the literature, four additional manuscripts are currently in press, and five more have been submitted to major technical journals. Eight presentations and invited talks have been given at conferences and workshops. The following paragraphs summarize the publications and presentations made under this program during the past contract period.

A. Refereed Publications

M. A. Stroscio, K. W. Kim, G. J. Iafrate, M. Dutta, and H. L. Grubin, "Reduction and Control of Inelastic Longitudinal-Optical Phonon Scattering in Nanoscale and Mesoscopic Device Structures," *Proceedings of the 1991 Int. Semiconductor Device Research Symp.*, pp. 87-91, 1991.

T. Kaneto, K. W. Kim, and M. A. Littlejohn, "Effects of Finite Hole Lifetime on Electron Transport in P-Type Zincblende Semiconductors," *Proceedings of the 1991 Int. Semiconductor Device Research Symp.*, pp. 235-238, 1991.

V. V. Mitin, R. Mickevicius, M. A. Stroscio, G. J. Iafrate, and K. W. Kim, "Electron Dynamics in Quantum Wires," *Proceedings of the 1991 Int. Semiconductor Device Research Symp.*, pp. 111-114, 1991.

M. A. Stroscio, G. J. Iafrate, K. W. Kim, M. A. Littlejohn, H. L. Grubin, V. V. Mitin, and R.

Mickevicius, "Role of Phonon Confinement in Nanoscale Systems," in *Nanostructures and Mesoscopic Systems*, edited by W. P. Kirk and M. A. Reed (Academic Press, San Diego, Calif., 1992), Chap. 8, pp. 379-386.

K. W. Kim, M. A. Littlejohn, M. A. Stroscio, and G. J. Iafrate, "Transition from LO-Phonon to SO-Phonon Scattering in Mesoscale Structures," *Semicond. Sci. Technol.* 7, B49 (1992).

R. Mickevicius, V. V. Mitin, K. W. Kim, and M. A. Stroscio, "Electron High-Field Transport in Multi-Subband Quantum Wire Structures," *Semicond. Sci. Technol.* 7, B299 (1992).

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M. A. Stroscio, K. W. Kim, G. J. Iafrate, M. Dutta, and H. L. Grubin, "Dramatic Reduction of the Longitudinal-Optical Phonon Emission Rate in Polar-Semiconductor Quantum Wires," *Phil. Mag. Lett.* 65, 173 (1992).

R. Mickevicius, V. V. Mitin, K. W. Kim, and M. A. Stroscio, "Electron Intersubband Scattering in Real Quantum Wires," *Superlatt. Microstruct.* 11, 277 (1992).

R. Mickevicius, V. V. Mitin, K. W. Kim, M. A. Stroscio, and G. J. Iafrate, "Electron Intersubband Scattering by Confined and Localized Phonons in Real Quantum Wires," *J. Phys.: Condens. Matter* 4, 4959 (1992).

K. W. Kim, A. R. Bhatt, M. A. Stroscio, P. J. Turley, and S. W. Teitsworth, "Effects of Interface Phonon Scattering in Multi-Heterointerface Structures," *J. Appl. Phys.* 72, 2282 (1992).

H. Qiang, F. H. Pollak, C. M. Sotomayor-Torres, W. Leitch, A. H. Kean, M. A. Stroscio, G. J. Iafrate, and K. W. Kim, "Size Dependence of the Electron-Optical Phonon Coupling in GaAs/$Ga_{0.7}Al_{0.3}As$ Single Quantum Wells," accepted for publication in *Appl. Phys. Lett.*

T. Kaneto, K. W. Kim, and M. A. Littlejohn, "Dielectric Response Functions of heavily-Doped Zinc-blende Semiconductors with Finite Particle Lifetime," accepted for publication in *J. Appl. Phys.*

M. A. Stroscio, K. W. Kim, G. J. Iafrate, M. Dutta, and H. L. Grubin, "Reduction of Inelastic Longitudinal-Optical Phonon Scattering in Narrow Polar-Semiconductor Quantum Wells," accepted for publication in *Proc. SPIE* 1675 (1992).

T. Kaneto, K. W. Kim, and M. A. Littlejohn, "Minority Carrier Transport in Heavily-Doped p-Type Semiconductors," submitted to *Phys. Rev. B.*

A. R. Bhatt, K. W. Kim, M. A. Stroscio, G. J. Iafrate, M. Dutta, H. L. Grubin, R. Haque, and X. T. Zhu, "Reduction of Interface Phonon Modes Using Metal-Semiconductor Heterostructures," submitted to *J. Appl. Phys.*

M. U. Erdogan, K. W. Kim, and M. A. Stroscio, "Effects of Band Mixing on Hole Tunneling Times in GaAs/AlAs Double-Barrier Heterostructures," submitted to *Appl. Phys. Lett.*

T. Kaneto, K. W. Kim, and M. A. Littlejohn, "A Comparison of Minority Electron Transport in $In_{0.53}Ga_{0.47}As$ and GaAs," submitted to *Appl. Phys. Lett.*

M. A. Stroscio, G. J. Iafrate, K. W. Kim, A. R. Bhatt, M. Dutta, and H. L. Grubin, "Reduction in Longitudinal-Optical Phonon Emission Rate in Polar-Semiconductor Quantum Wires and Quantum Wells," to be published in the Proceedings of the 7th Intl. Conf. on Phonon Scattering in Condensed Matter (August, 1992, Ithaca, New York).

J. He and G. J. Iafrate, "Multi-Band Theory of Zener Tunneling in Solids," submitted to *Phys. Rev. B.*

B. Conference Presentations

M. A. Stroscio, K. W. Kim, G. J. Iafrate, M. Dutta, and H. L. Grubin, "Reduction and Control of Inelastic Longitudinal-Optical Phonon Scattering in Nanoscale and Mesoscopic Device Structures (Invited)," presented at the 1991 Intl. Semiconductor Device Research Symp. (December, 1991, Charlottesville, Virginia).

T. Kaneto, K. W. Kim, and M. A. Littlejohn, "Effects of Finite Hole Lifetime on Electron Transport in P-Type Zincblende Semiconductors," presented at the 1991 Intl. Semiconductor Device Research Symp. (December, 1991, Charlottesville, Virginia).

V. V. Mitin, R. Mickevicius, M. A. Stroscio, G. J. Iafrate, and K. W. Kim, "Electron Dynamics in Quantum Wires (Invited)," presented at the 1991 Intl. Semiconductor Device Research Symp. (December, 1991, Charlottesville, Virginia).

K. W. Kim, A. Bhatt, H. Grubin, T. Zhu, M. Dutta, R. Haque, G. J. Iafrate, and M. A. Stroscio, "Reduction of Interface Phonon Scattering in Polar Mesoscopic Systems," presented at the March Meeting of the American Physical Society (March, 1992, Indianapolis, Indiana), *Bull. Am. Phys. Soc.* 37, 397 (1992).

M. A. Stroscio, K. W. Kim, G. J. Iafrate, M. Dutta, and H. L. Grubin, "Reduction of Inelastic Longitudinal-Optical Phonon Scattering in Narrow Polar-Semiconductor Quantum Wells," presented at the SPIE Symp. on Compound Semiconductor Physics and Devices (March, 1992, Somerset, New Jersey).

M. A. Stroscio, G. J. Iafrate, K. W. Kim, A. Bhatt, M. Dutta, and H. L. Grubin, "Reduction of Carrier-Interface-Phonon Scattering Near Metal-Semiconductor Interfaces for Phonon Frequencies Below the Plasmon Frequencies," presented at the 19th IEEE Intl. Conf. on Plasma Science (June, 1992, Tampa, Florida).

X. T. Zhu, H. Goronkin, G. Maracas, R. Droopad, M. Stroscio, G. Iafrate, K. Kim, and A. Bhatt, "Electron Mobility Enhancement by Confining Optical-Phonons in Ultrathin GaAs/AlAs Multiple Quantum Wells," presented at the 1992 Electronic Materials Conference (June, 1992, Cambridge, Mass.).

M. A. Stroscio, G. J. Iafrate, K. W. Kim, A. R. Bhatt, M. Dutta, and H. L. Grubin, "Reduction in Longitudinal-Optical Phonon Emission Rate in Polar-Semiconductor Quantum Wires and Quantum Wells," presented at the 7th Intl. Conf. on Phonon Scattering in Condensed Matter (August, 1992,

Ithaca, New York).

K. W. Kim, "Theory of Optical-Phonon Modes in Ultrasmall Electronic Devices (Invited)," to be presented at the Advanced Heterostructure Transistor Conference (November, 1992, Kona, Hawaii).

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3. PERSONNEL

Three faculty members; Dr. K. W. Kim, Dr. G. J. Iafrate, and Dr. M. A. Stroscio, in the Dept. of Electrical and Computer Eng. at North Carolina State Univ. (NCSU) are involved in this research effort. Dr. Kim serves as the principal investigator in charge of the day-to-day management and direction of the research program aspects. He joined the NCSU faculty in August 1988 after completing his Ph.D. degree at the Univ. of Illinois at Urbana-Champaign. He is experienced in the Monte Carlo method and other simulation techniques, and has a strong background in theoretical semiconductor physics. Currently, he is involved in various studies ranging from the hot electron effects in MOSFET's to quantum transport theory.

Dr. G. J. Iafrate has been engaged in teaching and research for over 20 years, and is currently Adjunct Professor of Electrical Engineering at NCSU and Director of U.S. Army Research Office. His main research interests include solid-state physics and electronics, especially the fundamental questions relating to the breakdown of classical solid-state electronics as device geometries approach the submicron and ultrasubmicron-size regime. Currently, he is involved in the development of a quantum transport formalism to elucidate tunnel-barrier and superlattice hot-electron transport phenomena. In addition, he is also examining the potential technical impact of high-temperature superconductivity on electronic applications. Dr. M. A. Stroscio has been associated with NCSU and with U.S. Army Research Office since 1985, most recently as Adjunct Professor of Electrical Engineering and as Senior Research Scientist, respectively. His main research area is quantum transport theory including path integral formalism and solid-state dynamics. He is currently engaged in the study of optical phonon modes in heterostructures, especially the effects of reduced dimensionality.

Dr. Iafrate and Dr. Stroscio are actively involved in the direction of a post-doctoral associate and a graduate student along with Dr. Kim. Due to the ties with the Army Research Office, the research activities by both Dr. Iafrate and Dr. Stroscio related to this proposal have been at no cost to the Office of Naval Research.

APPENDIX A: List of Refereed Publications on This Program Since 1990

1. K. W. Kim, M. A. Stroscio, and J. C. Hall, "Frequencies of confined longitudinal-optical phonon modes in GaAs/GaP short-period strained-layer superlattices," *J. Appl. Phys.* 67, 6179 (1990).
2. M. A. Stroscio, K. W. Kim, and J. C. Hall, "Variation in frequencies of confined longitudinal-optical phonon modes due to changes in the effective force constants near heterojunction interfaces," *Superlatt. Microstruct.* 7, 115 (1990).
3. M. A. Stroscio, K. W. Kim, M. A. Littlejohn, and H. Chuang, "Polarization Eigenvectors of Surface-Optical-Phonon Modes in a Rectangular Quantum Wire," *Phys. Rev. B* 42, 1488 (1990).
4. K. W. Kim and M. A. Stroscio, "Electron-Optical-Phonon Interaction in Binary/Ternary Hetero-structures," *J. Appl. Phys.* 68, 6289 (1990).
5. K. W. Kim, M. A. Stroscio, and J. C. Hall, "Frequencies of Confined Longitudinal-Optical Phonon Modes in Short-Period Strained Semiconductor Superlattices," *Proc. SPIE* 1336, 43 (1990).
6. M. A. Stroscio, K. W. Kim, and M. A. Littlejohn, "Theory of Optical-Phonon Interactions in a Rectangular Quantum Wire," *Proc. SPIE* 1362, 566 (1990).
7. M. A. Stroscio, K. W. Kim, and S. Rudin, "Boundary Conditions for Electron-LO-Phonon Interaction in Polar Semiconductor Quantum Wires," *Superlatt. Microstruct.* 10, 55 (1991).
8. K. W. Kim, M. A. Stroscio, A. Bhatt, R. Mickevicius, and V. V. Mitin, "Electron-Optical-Phonon Scattering Rates in a Rectangular Semiconductor Quantum Wire," *J. Appl. Phys.* 70, 319 (1991).
9. M. A. Stroscio, G. J. Iafrate, K. W. Kim, M. A. Littlejohn, H. Goronkin, and G. Maracas, "Transition from Longitudinal-Optical Phonon Scattering to Surface-Optical Phonon Scattering in Polar Semiconductor Superlattices," *Appl. Phys. Lett.* 59, 1093 (1991).
10. M. A. Stroscio, K. W. Kim, G. J. Iafrate, M. Dutta, and H. L. Grubin, "Reduction and Control of Inelastic Longitudinal-Optical Phonon Scattering in Nanoscale and Mesoscopic Device Structures," *Proceedings of the 1991 Intl. Semiconductor Device Research Symp.*, pp. 87-91, 1991.
11. T. Kaneto, K. W. Kim, and M. A. Littlejohn, "Effects of Finite Hole Lifetime on Electron Transport in P-Type Zincblende Semiconductors," *Proceedings of the 1991 Intl. Semiconductor Device Research Symp.*, pp. 235-238, 1991.
12. V. V. Mitin, R. Mickevicius, M. A. Stroscio, G. J. Iafrate, and K. W. Kim, "Electron Dynamics in Quantum Wires," *Proceedings of the 1991 Intl. Semiconductor Device Research Symp.*, pp. 111-114, 1991.
13. M. A. Stroscio, G. J. Iafrate, K. W. Kim, M. A. Littlejohn, H. L. Grubin, V. V. Mitin, and R. Mickevicius, "Role of Phonon Confinement in Nanoscale Systems," in *Nanostructures and Mesoscopic Systems*, edited by W. P. Kirk and M. A. Reed (Academic Press, San Diego, Calif., 1992), Chap. 8, pp. 379-386.
14. K. W. Kim, M. A. Littlejohn, M. A. Stroscio, and G. J. Iafrate, "Transition from LO-Phonon to SO-Phonon Scattering in Mesoscale Structures," *Semicond. Sci. Technol.* 7, B49 (1992).
15. R. Mickevicius, V. V. Mitin, K. W. Kim, and M. A. Stroscio, "Electron High-Field Transport in Multi-Subband Quantum Wire Structures," *Semicond. Sci. Technol.* 7, B299 (1992).

16. S. Das Sarma, V. B. Campos, M. A. Stroscio, and K. W. Kim, "Confined Phonon Modes and Hot Electron Energy Relaxation in Semiconductor Microstructures," *Semicond. Sci. Technol.* 7, B60 (1992).

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19. R. Mickevicius, V. V. Mitin, K. W. Kim, M. A. Stroscio, and G. J. Iafrate, "Electron Intersubband Scattering by Confined and Localized Phonons in Real Quantum Wires," accepted for publication in *J. Phys.: Condens. Matter* 4, 4959 (1992).

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23. M. A. Stroscio, K. W. Kim, G. J. Iafrate, M. Dutta, and H. L. Grubin, "Reduction of Inelastic Longitudinal-Optical Phonon Scattering in Narrow Polar-Semiconductor Quantum Wells," accepted for publication in *Proc. SPIE* 1675 (1992).

24. T. Kaneto, K. W. Kim, and M. A. Littlejohn, "Minority Carrier Transport in Heavily-Doped p-Type Semiconductors," submitted to *Phys. Rev. B.*

25. A. R. Bhatt, K. W. Kim, M. A. Stroscio, G. J. Iafrate, M. Dutta, H. L. Grubin, R. Haque, and X. T. Zhu, "Reduction of Interface Phonon Modes Using Metal-Semiconductor Heterostructures," submitted to *J. Appl. Phys.*

26. M. U. Erdogan, K. W. Kim, and M. A. Stroscio, "Effects of Band Mixing on Hole Tunneling Times in GaAs/AlAs Double-Barrier Heterostructures," submitted to *Appl. Phys. Lett.*

27. T. Kaneto, K. W. Kim, and M. A. Littlejohn, "A Comparison of Minority Electron Transport in $In_{0.53}Ga_{0.47}As$ and GaAs," submitted to *Appl. Phys. Lett.*

28. M. A. Stroscio, G. J. Iafrate, K. W. Kim, A. R. Bhatt, M. Dutta, and H. L. Grubin, "Reduction in Longitudinal-Optical Phonon Emission Rate in Polar-Semiconductor Quantum Wires and Quantum Wells," to be published in the Proceedings of the 7th Intl. Conf. on Phonon Scattering in Condensed Matter (August, 1992, Ithaca, New York).

29. J. He and G. J. Iafrate, "Multi-Band Theory of Zener Tunneling in Solids," submitted to *Phys. Rev. B.*

APPENDIX B: Reprints of Publications

This appendix contains the title page of each paper published in the refereed literature which were supported by the ONR project during the 1991 contract period. Copies of these papers have been sent to the program manager under separate cover. A list of these papers is included below.

1) M. A. Stroscio, K. W. Kim, G. J. Iafrate, M. Dutta, and H. L. Grubin, "Reduction and Control of Inelastic Longitudinal-Optical Phonon Scattering in Nanoscale and Mesoscopic Device Structures," *Proceedings of the 1991 Int. Semiconductor Device Research Symp.*, pp. 87-91, 1991.

2) T. Kaneto, K. W. Kim, and M. A. Littlejohn, "Effects of Finite Hole Lifetime on Electron Transport in P-Type Zincblende Semiconductors," *Proceedings of the 1991 Int. Semiconductor Device Research Symp.*, pp. 235-238, 1991.

3) V. V. Mitin, R. Mickevicius, M. A. Stroscio, G. J. Iafrate, and K. W. Kim, "Electron Dynamics in Quantum Wires," *Proceedings of the 1991 Int. Semiconductor Device Research Symp.*, pp. 111-114, 1991.

4) M. A. Stroscio, G. J. Iafrate, K. W. Kim, M. A. Littlejohn, H. L. Grubin, V. V. Mitin, and R. Mickevicius, "Role of Phonon Confinement in Nanoscale Systems," in *Nanostructures and Mesoscopic Systems*, edited by W. P. Kirk and M. A. Reed (Academic Press, San Diego, Calif., 1992), Chap. 8, pp. 379-386.

5) K. W. Kim, M. A. Littlejohn, M. A. Stroscio, and G. J. Iafrate, "Transition from LO-Phonon to SO-Phonon Scattering in Mesoscale Structures," *Semicond. Sci. Technol.* 7, B49 (1992).

6) R. Mickevicius, V. V. Mitin, K. W. Kim, and M. A. Stroscio, "Electron High-Field Transport in Multi-Subband Quantum Wire Structures," *Semicond. Sci. Technol.* 7, B299 (1992).

7) S. Das Sarma, V. B. Campos, M. A. Stroscio, and K. W. Kim, "Confined Phonon Modes and Hot Electron Energy Relaxation in Semiconductor Microstructures," *Semicond. Sci. Technol.* 7, B60 (1992).

8) M. A. Stroscio, K. W. Kim, G. J. Iafrate, M. Dutta, and H. L. Grubin, "Dramatic Reduction of the Longitudinal-Optical Phonon Emission Rate in Polar-Semiconductor Quantum Wires," *Phil. Mag. Lett* 65, 173 (1992).

9) R. Mickevicius, V. V. Mitin, K. W. Kim, and M. A. Stroscio, "Electron Intersubband Scattering in Real Quantum Wires," *Superlatt. Microstruct.* 11, 277 (1992).

10) R. Mickevicius, V. V. Mitin, K. W. Kim, M. A. Stroscio, and G. J. Iafrate, "Electron Intersubband Scattering by Confined and Localized Phonons in Real Quantum Wires," accepted for publication in *J. Phys.: Condens. Matter* 4, 4959 (1992).

11) K. W. Kim, A. R. Bhatt, M. A. Stroscio, P. J. Turley, and S. W. Teitsworth, "Effects of Interface Phonon Scattering in Multi-Heterointerface Structures," *J. Appl. Phys.* 72, 2282 (1992).

Proceedings of the 1991 International Semiconductor Device Research Symposium
(Charlottesville, VA, 1991)

Reduction and Control of Inelastic Longitudinal-Optical Phonon Scattering in Nanoscale and Mesoscopic Device Structures

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Novel quantum-effect polar-semiconductor devices underlie technologies portending dramatic enhancements in the capability to process information orders-of-magnitude faster than is possible currently. In many of these quantum-effect devices, charges are transported in quantum-well and quasi-one-dimensional quantum wires which must support the transport of charges at high mobilities. However, it has recently been demonstrated that longitudinal-optical (LO) phonons established at quantum-wire interfaces lead to dramatic enhancements in mobility-degrading carrier-phonon interactions. In novel mesoscopic de Broglie wave devices, LO phonons are confined in structures with complex geometries which frequently incorporate metal-semiconductor interfaces. This paper outlines the theory of confined and interface LO phonons in mesoscopic devices and demonstrates that phonon modes may be tailored through the judicious use of metal-semiconductor interfaces in such a way as to dramatically reduce unwanted emission of interface LO phonons.

Modern techniques for making semiconductor structures with dimensional features controlled on the nanometer scale have been essential in leading to fundamental discoveries as well as in stimulating concepts for future information processing systems based on the exploitation of quantum effects occurring in such structures [1-3]. As originally proposed by Sakaki [4], the predicted high mobilities of quasi-one-dimensional wire-like regions of semiconducting material underlie

Proceedings of the 1991 International Semiconductor Device Research Symposium
(Charlottesville, VA, 1991)

Effects of finite hole lifetime on electron transport in p-type zincblende semiconductors

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Abstract

The dielectric response function in the valence bands of a zincblende semiconductor has been evaluated in the random phase approximation (RPA) incorporating the finite lifetime of holes at finite temperature. Scattering rates of minority electrons have been calculated in the Born approximation. Our results show that the collective motion of holes (plasmons) is heavily damped due to the finite lifetime of holes. Scattering rates of minority electrons are increased due to these effects.

1. Introduction

An understanding of the behavior of electrons in highly doped semiconductors is increasing in its importance, especially for the design of high speed HBT's and HET's, since electron transport in the base region is one of the critical factors limiting the maximum switching speed of such devices. It is well known that the dynamic response of a free electron gas is described by the Lindhard dielectric function in the RPA for the electron lifetime $\tau = +\infty$ [1]. The free electron gas formula is easily applicable to heavily doped n-type semiconductors since they have a single conduction band with s-like symmetry. For p-type semiconductors, the situation is much more complicated because of the p3/2-like symmetry of the valence bands. Recently, D. Yevic et al. evaluated the Lindhard dielectric function for a p-type semiconductor at finite temperature. These authors showed that the structure of the spectral density function is quite different from that for zero temperature. The scattering rates of minority electrons were also calculated [2, 3]. However, they still neglected the effects of the finite hole lifetime even for finite temperature. Although the Lindhard dielectric function inherently incorporates the effects of single particle excitation (Landau damping) including both intra- and interband transitions, it does not take into account the finiteness of particle lifetime due to the collision effects such as impurity scattering and phonon scattering. At finite temperature, these effects are very important since such scattering disturbs the collective motion of quasi-particles and therefore the dynamic response function will be affected significantly. The purpose of this paper is to demonstrate the effects of the finite hole lifetime on the dynamic response of a hole gas, as well as the effects on the lifetime of minority electrons in p-type semiconductors.

2. Theory

From the fluctuation-dissipation theorem, the total inelastic scattering rate for an electron with energy E in the conduction band is given by

$$\Gamma_d(E) = \frac{e^2}{\pi\hbar^2}\left(\frac{2m_e}{E}\right)^{1/2}\int_0^{\infty}\frac{dq}{q}\int_{\hbar\omega_{min}}^{\hbar\omega_{max}} d(\hbar\omega)\,\mathrm{Im}\left[-\frac{1}{\varepsilon(q,\omega)}\right](1+n_\omega) \qquad (1)$$

Proceedings of the 1991 International Semiconductor Device Research Symposium
(Charlottesville, VA, 1991)

ELECTRON DYNAMICS IN QUANTUM WIRES

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We present a review of our recent results on electron dynamics in high and low electric fields in multisubband quasi-one-dimensional quantum wire (QWI) structures.

First we derive expressions for the rates of electron intra- and intersubband scattering by surface optical (SO) and confined longitudinal optical (LO) phonons in QWIs. Numerical results are obtained for a GaAs QWI embedded in AlAs [1,2]. There are two branches of SO phonons one being related to GaAs and another to AlAs. Their frequencies are considerably different and both differ from the LO phonon frequency. It is demonstrated that electron intrasubband scattering is mainly due to LO phonons whereas electron intersubband transitions under certain conditions are strongly influenced by SO phonons. These conditions occur when the intersubband energy separation in QWIs coincide with the SO phonon energy (so called resonant condition). In this case the rate of intersubband electron scattering assisted by SO phonons tends to infinity for any electron energy. The rate of electron-LO-phonon scattering in a QWI does not depend crucially on the intersubband energy separation. Note that only "forward" electron scattering can be in the resonance. The "backward" scattering rate depends weakly upon resonant conditions. High intersubband scattering rates under resonant conditions must yield fast electron redistribution between subbands in resonance. However, there is no momentum relaxation due to "forward" resonant intersubband electron scattering. Therefore, resonant intersubband scattering should not affect electron transport unless the subbands in resonance

THE ROLE OF LONGITUDINAL-OPTICAL PHONONS IN NANOSCALE STRUCTURES

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As device dimensions in nanoscale structures and mesoscopic systems are reduced, the characteristics and interactions of dimensionally-confined longitudinal-optical (LO) phonons deviate substantially from those of bulk polar semiconductors. This account emphasizes LO-phonon effects arising in three separate systems: Short-period AlAs-GaAs superlattices; rectangular GaAs quantum wires embedded in AlAs; and metal-semiconductor interfaces such as those in de Broglie wave quantum-interference devices.

I. INTRODUCTION

In nanoscale and mesoscopic systems, the effects of confinement on carriers have been studied extensively. However, to properly model carrier energy loss in nanoscale and mesoscopic systems, it is essential that calculations of carrier scattering by longitudinal-optical phonons take into account the fact that confinement also changes the strength and spatial properties of longitudinal-

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Transition from LO-phonon to SO-phonon scattering in mesoscale structures

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Abstract. Macroscopic dielectric continuum models of optical-phonon modes predict enhancements in the magnitudes of the surface-optical (SO) modes in double-barrier heterostructures as the heterojunction-to-heterojunction separation is reduced. In this paper, the ratio of electron scattering by the SO-phonon modes to that by the (electrostatic) confined longitudinal-optical- (LO-) phonon modes is calculated for a GaAs/AlAs short-period superlattice based on the assumption that electron–SO-phonon scattering may be described by a scalar potential. The scaling of the ratio of electron–SO-phonon scattering to electron–LO-phonon scattering as a function of the superlattice period provides a sensitive test of the appropriateness of the scalar-potential model. The effect of phonon confinement on electron–optical-phonon scattering rates is presented for rectangular quantum wires as well. A major conclusion of these new results is that it is essential to model phonon confinement properly in predicting carrier transport properties in mesoscale structures.

Interactions between carriers and longitudinal-optical (LO) phonon modes in heterostructures are strongly affected by the changes in the Fröhlich Hamiltonian caused by phonon confinement and localization, as well as by the changes in the electronic wave function due to the confining potential. The presence of heterointerfaces gives rise to the confinement of optical phonons in each layer (i.e., confined modes) and the localization in the vicinity of interfaces (i.e., interface modes or surface-optical (SO) modes). There have been suggestions that interactions by the interface modes can be significant and that the scattering rate due to the confined modes can be considerably reduced in some structures compared to the bulk LO-phonon scattering rate [1–3]. Therefore, an appropriate treatment of the optical-phonon modes in quantized systems is essential for the understanding of electron transport in heterostructures. Recently, both macroscopic and microscopic approaches to electron–optical-phonon interactions in heterostructures [1–11] have been applied in theoretical treatments. Enhanced electron–SO-phonon scattering in polar semiconductors with confining dimensions less than about 50 Å has been indicated recently [12, 13] on the basis of scalar-potential modes. The appropriateness of using a scalar potential to model the electron–SO-phonon interaction has been questioned [14]. In this paper, we model the electron–SO-phonon interaction with a scalar potential to calculate the ratio of electron–SO-phonon scattering to electron–confined-LO-phonon scattering in a short-period GaAs/AlAs superlattice; the results scale inversely with the superlattice quantum-well dimension in qualitative agreement with recent experiments [15]. Such comparisons provide convincing evidence that the SO modes present in these experiments contain an active LO component. This scalar-potential description is also applied to calculate the electron–optical-phonon scattering rates in GaAs rectangular quantum wires.

The GaAs/AlAs short-period superlattice considered in this study has the GaAs layer width a and the AlAs layer width b. The ratio of electron–SO-phonon scattering to electron–LO-phonon scattering in this superlattice is calculated through the Fermi golden rule by treating the electron–LO-phonon and electron–SO-phonon interaction Hamiltonians [4, 6] as perturbation Hamiltonians and by taking the electronic wavefunction along the growth direction (i.e., the z-direction) as that given by Cho and Prucnal for the maximum edge of the first subband [16]. To obtain an order-of-magnitude estimate of the ratio of electron–SO-phonon scattering to electron–LO-phonon scattering in the GaAs/AlAs superlattice, we consider the ratio of principal factors, Y, in the integrands of the respective scattering rates. In this calculation, the contribution by the S− mode is neglected due to its relatively small contribution as compared with the S+ mode [6]. Figure 1 shows the ratio, Y, plotted as a function of X ($=qa$ where q is the phonon momentum parallel to the heterointerface) for a GaAs/AlAs short-period superlattice with $b = a$ and

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Electron high-field transport in multisubband quantum wire structures

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Abstract. The Monte Carlo simulation of electron transport in multisubband quasi-one-dimensional GaAs/AlAs quantum wires (QWIS) are presented. The electron intrasubband and intersubband scattering by surface-optical and confined longitudinal-optical phonons in QWIS has been included in the program. It is demonstrated that at room temperature the electron drift velocity in the QWI is suppressed by electron intersubband scattering and does not exceed the bulk material values. The energy dependence of the total scattering rate in ideal QWIS exhibits multiple sharp peaks related to intersubband transitions. The scattering rates in the real QWIS with variable thicknesses are calculated as well. The results show that even small variation in thickness leads to a significant broadening of the very first peaks and complete washing-out of the peak-like structure at higher energies.

1. Introduction

During the years following Sakaki's work [1], a number of papers on quantum wires (QWIS) appeared, dealing mainly with theoretical analyses of quantization, scattering mechanisms and linear transport in low electric fields (see e.g., [2] and papers in [3]). Most of the previous studies on nonlinear electron transport in QWIS have been limited to the case of scattering by bulk three-dimensional (3D) phonon modes [4]. However, experiments clearly demonstrate the importance of surface-optical (SO) modes [5] and phonon confinement [6] in QWIS. Moreover, most theoretical studies on QWIS deal with ideal 1D systems characterized by fixed subband energy positions. However, all current and foreseeable future technologies of fabricating QWIS do not assure the possibility to create ideal structures with constant thickness [7–10]. The variation of QWI thickness results in the variation of subband energy positions. Consequently, electron scattering is no longer energetically coherent in different parts of a QWI and this should lead to the broadening or even complete washing-out of the resonant peaks [8–10].

In the present paper we consider nonlinear (hot) electron transport in a rectangular GaAs QWI embedded in AlAs. Both the phonon confinement and multisubband structure are taken into account. We consider electron scattering in an ideal QWI with a constant thickness along the wire as well as in a real QWI with variable thickness. The Monte Carlo simulations are performed for the ideal QWI.

2. Scattering rates

The model of the QWI and the scattering rates is discussed in detail in [10, 11]. We consider ideal QWIS with constant thickness and real QWIS with a smooth variation of thickness along the structure so that the characteristic length of the fluctuations is much greater than the de Broglie wavelength Λ_B. Numerical calculations of the scattering rates have been performed for the GaAs QWI of dimensions $L_y = 150$ and $L_z = 250$ Å embedded in AlAs. We have considered 9 subbands. The scattering rates in real QWIS have been calculated assuming a thickness varying with the harmonic law. The variation amplitudes δL_y and δL_z have been chosen from 0.01 to 0.1 fraction of the corresponding thicknesses L_y and L_z. We have considered three cases with different mutual phases of the variation of L_y and L_z: $L_z = L_{z0} + \delta L_z \cos(Kx)$, $L_z = L_{z0} + \delta L_z \sin(Kx)$ and $L_z = L_{z0} + \delta L_z \cos(2Kx)$ with $L_y = L_{y0} + \delta L_y \cos(Kx)$ in all cases. It has been found that the results do not show significant difference between these models as long as we are in the limit of smooth fluctuations $K\Lambda_B \ll 1$. The calculated energy dependences of the total electron transition rate from the

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Confined phonon modes and hot-electron energy relaxation in semiconductor microstructures

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Abstract. The role of confined phonon modes in determining the energy relaxation of hot electrons in low-dimensional semiconductor microstructures is discussed within a dielectric continuum model for the LO phonon confinement and a long wavelength Fröhlich model for the electron–phonon interaction. Numerical results are provided for the hot-electron relaxation rate as a function of electron temperature and density for GaAs quantum wells and quantum wires by taking into account emission of slab phonon modes. Comparison with existing experimental results shows some evidence for slab phonon emission in *inter-subband* electronic relaxation in reasonably narrow quantum wells. It is argued that most experiments can be interpreted in terms of an electron–bulk phonon interaction model (i.e. by taking into account the effect of confinement only on the electrons and assuming the phonons to be the usual bulk three-dimensional phonons) because a number of important physical processes, such as screening, the hot phonon effect, phonon self-energy correction etc, make it difficult to distinguish quantitatively between various models for phonon confinement, except perhaps in the narrowest (<50 Å) wells and wires. Detailed numerical results for the calculated intra-subband relaxation rate in GaAs quantum wires are provided within the slab phonon and the electron temperature model, including the effects of dynamical screening, quantum degeneracy and non-equilibrium hot phonons.

1. Introduction

A large number of theoretical papers have recently appeared [1–21] on the subject of interaction between free electrons and optical phonons in *confined* low-dimensional semiconductor structures such as semiconductor heterostructures, quantum wells, superlattices and quantum wires. While it is well established [1] that the effect of quantum confinement on the electronic degrees of freedom must be included in any reasonable theoretical model of electron–phonon interactions in these microstructures, the recent emphasis in the literature has been on the inclusion of confinement effects on the phonon modes of the structures and the consequent modification of the Frölich Hamiltonian describing the electron–phonon interaction in the system. Because Fröhlich interaction plays an important quantitative role in determining many aspects of the electronic properties (e.g. electron mobility, hot-electron relaxation, inelastic mean free path, polaron effective mass) of microstructures, the possible influence of confined phonon modes in semiconductor microstructures is of some interest. The purpose of this paper is to discuss the quantitative role of confined phonon modes from the perspective of one particular class of phenomena, namely, the hot-electron energy relaxation process in quantum wells and wires. Our main concern in this article is the role of confined phonon modes in the energy relaxation of hot electrons in GaAs microstructures with the particular emphasis on qualitative and quantitative understanding of recent experimental results [22–30].

The most unambiguous evidence for the existence of confined phonon modes in microstructures comes from Raman scattering experiments [22–24] in thin GaAs–AlAs superlattices where confinement effects on both the acoustic phonons [22] and optical phonons [23, 24] have directly been observed for layer thicknesses typically below 50 Å. Unfortunately, such Raman measurements cannot tell us much about the role of confined phonon modes in determining various electronic properties. In addition, the Raman measurements (and this limitation applies also to all of the 'so-called' first principles or microscopic lattice-dynamical calculations) are necessarily on superlattices whereas the electronic experiments

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Dramatic reduction in the longitudinal-optical phonon emission rate in polar-semiconductor quantum wires

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ABSTRACT

Novel quantum-effect polar-semiconductor structures underlie technologies portending dramatic enhancements in the capability to process information orders of magnitude faster than is possible currently. In many embodiments of these quantum-effect structures, charges are transported in quasi-one-dimensional quantum wires which must support the transport of charges at high mobilities. However, it has recently been demonstrated that the longitudinal-optical (LO) phonons established at quantum-wire interfaces lead to dramatic enhancements in carrier–phonon interactions and concomitant degradation in carrier mobility. This letter demonstrates that phonon modes may be tailored through the judicious use of metal–semiconductor interfaces in such a way as to dramatically reduce unwanted emission of interface LO phonons and, consequently, to lead to the achievement of high quantum-wire mobility.

Modern fabrication techniques for making semiconductor structures with nanometre-scale dimensional features have been essential in leading to fundamental discoveries (Esaki 1974, Stein, von Klitzing and Weimann 1983) as well as in stimulating concepts for future information-processing systems based on the exploitation of quantum effects occurring in such structures (Capasso and Datta 1990). As originally proposed by Sakaki (1980), the predicted high mobilities of quasi-one-dimensional wire-like regions of a semiconducting material underlie many proposed quantum-wire system concepts (Luryi and Capasso 1985, Sakaki 1989) and have resulted in pioneering efforts leading to the actual fabrication of quantum wires (Watt, Sotomayor Torres, Arnot and Beaumont 1990). Furthermore, quantum-wire structures have been essential to seminal studies underlying quantum-wire laser concepts (Tsuchiya *et al.* 1989) and quantum-coupled electronic systems (Reed *et al.* 1988). Recently, however, theoretical studies of the interaction between longitudinal-optical (LO) phonons and carriers in a polar-semiconductor quantum wire (Stroscio 1989) have revealed the presence of discrete LO phonon modes similar to those identified for polar-semiconductor quantum wells (Kliewer and Fuchs 1966, Licari and Evrard 1977, Mori and Ando 1989, Kim and Stroscio 1990). As for the case of quantum wells, interface LO phonons are established at the semiconductor–semiconductor boundaries of quantum wires (Kim *et al.* 1991). In addition, it has been shown that, for carrier

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ELECTRON INTERSUBBAND SCATTERING IN REAL QUANTUM WIRES

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(Received 19 May 1991)

The rates of electron intra- and intersubband scattering by surface optical (SO) and confined longitudinal optical (LO) phonons in quasi-one-dimensional GaAs/AlAs quantum wires (QWIs) are calculated. It is shown that electron-SO-phonon intersubband scattering can be resonant, so that the scattering rate tends to infinity when intersubband energy separation approaches SO phonon energy. The energy dependence of the total scattering rate in ideal QWIs exhibits multiple sharp peaks related to intersubband transitions. The scattering rates in the real QWIs with variable thickness are calculated. The results show that even small variation in thickness leads to the significant broadening of the very first peaks and complete washing-out of the peak-like structure at higher energies. Monte Carlo simulations of electron transport in the QWI have been performed. It is demonstrated that electron drift velocity in the QWI is considerably suppressed by electron intersubband scattering and is considerably lower than the bulk material values. The role of SO phonons in electron energy dissipation is discussed.

I. Introduction

Despite rapidly growing number of publications on quantum wires (QWIs), the theoretical investigations are limited either to the case of extreme quantum limit (EQL) wherein only one subband is considered [1,2] or (and) to the case of scattering by bulk three-dimensional (3-D) phonon modes [3]. However, it is difficult to meet these limitations because electrons can populate upper subbands at higher temperatures or in the hot-electron regime [4] and experiments evidently demonstrate importance of surface-optical (SO) modes [5] and phonon confinement [6] in QWIs. Moreover, most theoretical studies on QWIs deal with ideal 1-D systems characterized by fixed subband energetic positions. The unique feature of ideal QWI is the well-pronounced resonant nature of electron scattering as a result of multiple sharp peaks (diverging to infinity) on energy dependence of the total electron scattering rate. However, all current and foreseeable future technologies of fabricating QWIs do not assure the possibility to create ideal structures with constant thickness [4,7]. The variation of QWI thickness results in the variation of subband energetic position. Consequently, electron scattering is no longer energetically coherent in different parts of a QWI and this should lead to the broadening or even complete washing-out of the resonant peaks [8,9].

The aim of the present paper is to investigate both the phonon confinement and multi-subband structure in a rectangular QWI of polar semiconductor embedded in another polar semiconductor. We consider an ideal QWI with thickness constant along the wire (Section II) and a real QWI with variable thickness (Section III). In Section IV some preliminary results of Monte Carlo simulation are discussed.

II. Ideal QWI

The 1-D electron energy in a rectangular QWI is of well-known form

$$E(q_x,j,l) = E_x(q_x) + E_{jl},$$

$$E_x(q_x) = \frac{\hbar^2 q_x^2}{2m^*},$$

$$E_{jl} = \frac{\hbar^2}{2m^*}\left[\left(\frac{\pi j}{L_y}\right)^2 + \left(\frac{\pi l}{L_z}\right)^2\right], \qquad (1)$$

where E_x is the electron kinetic energy, q_x being the electron wave-number in x-direction, and E_{jl} is the subband $\{j,l\}$ energetic position with respect to the bulk ground level. It is seen from Eq.(1) that subband energetic positions depend on the structure thickness L_y and L_z. In this Section we will consider an ideal QWI with constant thickness along the wire, so that E_{jl} is independent of x.

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Electron intersubband scattering by confined and localized phonons in real quantum wires

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Abstract. The present study deals with electron intersubband scattering in real quantum wire structures. Both the multi-subband structure and confined phonon modes are considered together. The rates of scattering by confined longitudinal-optical (LO) phonons and by surface-optical (SO) phonons are calculated taking into account all possible LO phonon modes as well as all possible electron intersubband transitions. The estimations of transition rates for GaAs/AlAs QWIs have shown that intrasubband electron scattering and most intersubband transitions are due primarily to scattering by confined LO phonons, but in resonant intersubband transitions the contribution of SO phonons may be dominant when the phonon energy is close to the intersubband energy separation. Moreover, electron–SO-phonon scattering might play an important part in low-temperature electron transport because the GaAs-like SO mode is shifted towards lower frequencies compared with that of LO phonons. The energy dependence of the total scattering rate in an ideal quantum wire exhibits multiple sharp peaks related to each intersubband transition. These peaks originate from the resonant nature of the density of states in ideal one-dimensional systems. It is demonstrated that in real quantum wires with variable thickness the resonant peaks broaden or even disappear due to variation of subband energies.

1. Introduction

The progress in semiconductor technology has provided the means to fabricate the so-called quantum wires (QWIs) with quasi-one-dimensional (1D) structures. It has been suggested that QWIs will exhibit carrier mobilities well above 10^6 cm^2 V^{-1} s^{-1} [1], but these high values of the mobility have not yet been observed experimentally. The expected enhancement of the carrier mobility in QWIs should stem from the restriction of momentum space to one dimension as well as the resulting reduction of final states for scattered electrons. This point, however, needs to be clarified. Despite the rapidly growing number of publications on QWIs, the theoretical investigations of electron transport controlled by optical phonon scattering are limited either to the case of the extreme quantum limit (EQL) wherein only one subband is considered [2–4] and/or to the case of scattering by bulk three-dimensional (3D) phonon modes [5–7]. However, due to technological limitations the confinement of electrons is relatively weak and electrons can populate upper subbands at higher temperatures or in the hot-electron

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Effects of interface phonon scattering in multiheterointerface structures

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In this paper, the commonly used but idealistic formulation of quantized optical-phonon modes for a heterostructure system with only two heterojunctions (i.e., single quantum-well structures) is extended to the more realistic case of multiheterointerface structures. By applying the macroscopic dielectric continuum approach, dispersion relations and interaction Hamiltonians for interface-phonon modes are derived for a double-barrier structure and scattering rates based on these results are used to determine the range of practical validity of the idealistic model using interaction Hamiltonians appropriate for single quantum wells with infinite barrier widths. It is found that when the dimensions of the structures are larger than approximately 30 Å, this simplified description can be applied to multiheterointerface structures in general with reasonable accuracy.

I. INTRODUCTION

It is well known that electron interactions with longitudinal-optical (LO) phonon modes in heterostructures are strongly affected by the changes in the Fröhlich Hamiltonian caused by phonon confinement and localization, as well as by the changes in the electronic wave function due to the confining potential. The presence of heterointerfaces gives rise to the confinement of optical phonons in each layer (i.e., confined modes) and the localization in the vicinity of interfaces (i.e., interface modes). There have been suggestions that carrier interactions with the interface modes can be significant and that the scattering rate due to the confined modes can be considerably reduced in some structures compared to the bulk LO-phonon scattering rate.[1-5] Therefore, an appropriate treatment of the optical-phonon modes in quantized systems is essential for the understanding of electron transport in heterostructures. Recently, both macroscopic[1-10] and microscopic[11,12] approaches of electron-optical-phonon interactions in heterostructures have been applied in theoretical treatments. Detailed microscopic calculations of optical-phonon modes in polar semiconductors indicate that the dielectric continuum model provides an accurate formalism for modeling electron-optical-phonon interactions.[12] However, most of these theoretical analyses have been confined to highly symmetric and/or simple structures such as single quantum wells or superlattices. Application of even a simple macroscopic model, not to mention the microscopic *ab initio* models, becomes highly complicated due to the coupling between adjacent interfaces when the structure has multiple heterointerfaces or is asymmetric. There are many such structures in which a rather accurate description of the electron-optical-phonon interaction (such as the role of interface phonons) is of prime concern.[13-18] Thus, it is desirable to investigate the possibility of utilizing an approximate description of phonon modes and related interaction Hamiltonians, while retaining the quantized nature of phonon modes in the multiheterointerface structures.

In this paper, we report a detailed study of the electron-optical-phonon interaction in a double-barrier heterostructure to explore the possibility of achieving a simplified description such as discussed above. The double-barrier structure has been chosen as a specific example due to its structural similarity (with an added complexity of finite barrier width) to single quantum wells (i.e., infinite barrier width) for which quantized optical-phonon modes are already well known, and its prominence in recent studies which demonstrated the existence and importance of interface-phonon modes.[13-16] In this study, the interaction Hamiltonians are derived by applying the macroscopic dielectric continuum model[4-10] without any further approximations. The resulting scattering rates are compared with those obtained by assuming the Hamiltonians appropriate for single quantum wells for which finite barrier widths are

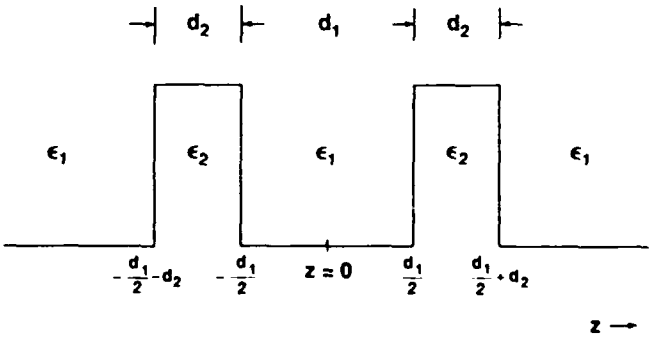

FIG. 1. Schematic drawing of the double-barrier heterostructure discussed in this study. The z axis is chosen as the growth direction of the lattice.

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