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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 are: 1) theory of phonon modes in reduced dimensions, 2) effects of band structure on electronic and optical properties of heterostructures, and 3) quantum transport in solids with special emphasis on non-perturbative role of high-electric fields and many-body effects in dynamical processes. The treatment of these problems is mainly analytical through the development of macroscopic and microscopic physical models with an emphasis on quantum mechanical principles. At the same time, numerical approaches has also been utilized for realistic solutions with accuracy. Specific subjects discussed in this report include the effects of confinement and localization on optical phonon modes, band mixing in tunneling, Bloch electron quantum transport theory under hot-electron conditions, and dielectric response function theory. 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 occurring at ultrasmall scales proceeds technological developments and leads the way to future advances.

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. However, numerical evaluation has also been employed for realistic solutions with accuracy. Our efforts have been devoted to investigating three important problems. The first one is the

theory of 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. Recently, the scope of this research effort has been expanded to investigate the effects of acoustic phonon confinement on the piezoelectric scattering and deformation potential scattering. The results will be of major importance to a wide variety of nanoscale semiconductor devices in which the scattering by quantized phonon modes plays a significant (at times, dominant) role in determining the electronic and optoelectronic properties. The second topic is the quantum mechanical transport of charge carriers with specific emphasis on the effects of electron-electron and electron-phonon interactions in the presence of high-electric fields and many-body effects 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 generation as well as ionization processes in quantum wells, tunnel barriers, superlattices, and quantum wires. At the same time, attempts are made to study the effects of quantum mechanical principles on carrier transport with macroscopic approaches such as dielectric function theory. As the third topic, we have recently begun to emphasize the effects of band structure which are critical to understanding electronic and optoelectronic properties of heterostructures. Detailed knowledge of band structure in the presence of heterointerfaces, such as mixing and evanescent states, is essential for the characteristic response of a mesoscopic system which is beyond the realm of the conventional effective mass approximation. The main subjects of interest in this topic include the effects of band mixing in tunneling and phonon-assisted transitions.

Although only three years old, this program has already resulted in thirty refereed publications in the literature, three additional manuscripts are currently in press, and one more has been submitted to a major technical journal. 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 modeling aspects of transport study are emphasized. Due to the complicated geometry and boundary conditions, a realistic model for a realistic device structure is attainable only through numerical approaches. The accurate physical models and understanding developed in this research facilitates 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 1992-93 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 1992-93 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, the effects of band mixing, and quantum mechanical transport in semiconductor nanostructures. The major accomplishments during the past contract period are:

- We have demonstrated quantitatively that significant reductions in LO-phonon scattering strengths may be achieved for metal-semiconductor structures not only with ideal metals but also with non-ideal metals of realistic conductivities and Thomas-Fermi screening lengths. Based on an approximate treatment of the dielectric continuum model, our results show that the assumption of "perfect" metal with infinite conductivity at the metal-semiconductor interface affects the optical phonon modes only slightly and, thus, is not critical to the dramatic reduction of interface phonon scattering rates. This finding could potentially lead to the development of a virtually scattering-free environment for electrons;
- We have developed a simple microscopic model of optical phonons in dimensionally confined structures based on the valence shell model. For this simplified model which circumvents performing a complicated ab initio calculation of the force constants at the interface, it is demonstrated that the resulting dispersion relation and scattering rates for electron-optical-phonon interactions in quantum well structures agree very well with those obtained from detailed ab initio studies. Our model provides an accurate but simpler alternative to the complicated ab initio treatments;
- We have calculated the tunneling time of holes in GaAs/AlAs double-barrier heterostructures within the envelope function approximation including band-mixing effects. The results show clearly that mixing plays a very important role in hole tunneling. In particular, our study suggests that the conventional effective mass models (without band mixing) can significantly overestimate the heavy hole tunneling time and, thus, are not suitable for the estimation of the hole tun-

neling time. When the mixing effect is included, the hole tunneling times are comparable to those for electrons contrary to the conventional perception;

- We have developed a novel multi-band theory of Bloch electron dynamics in homogeneous electric fields of arbitrary strength and time-dependence. Through the use of Wigner-Weisskopf approximation for multi-band coupling, a generalized Zener tunneling time is derived in terms of the applied electric field and the relevant band parameters; and
- We have formulated a new approach for the calculation of minority carrier mobility based on a dielectric function formalism (for accurate treatment of many body effects) and an appropriate transport theory (which goes beyond the relaxation time approximation). Our results on minority electron mobilities for heavily-doped p-type GaAs and Si show excellent agreement with available experimental data for a wide range of hole concentrations, thus, demonstrating the accuracy of our model.

Each of these results is discussed in detail below.

Reduction of interface-phonon scattering in metal-semiconductor structures

In recent years it has become clear that carrier interactions with LO phonon modes in heterostructures are strongly affected by the changes in the Fröhlich Hamiltonian caused by phonon confinement and localization. Of special importance to the field of nanoscale device physics is the realization that carrier-LO-phonon scattering in narrow quantum wells may be dominated by the interaction between carriers and interface LO phonons established near heterojunctions. Indeed, for typical phonon wavevectors of $0.02 \text{ \AA}^{-1}$, our previous efforts in this research program have demonstrated that carrier scattering by interface LO phonons may dominate over that by confined LO phonons in multiple quantum well structures for well widths of about $100 \text{ \AA}$ or less. In numerous nanoscale structures and devices, the trends to greater complexity and higher speed lead to the simultaneous requirements for reduced structural dimensions and minimal inelastic scattering. The enhancement of inelastic carrier-

interface-phonon scattering with decreasing structural size is contrary to the desired trend for a wide class of nanoscale structures.

During the 1991-92 contract period, we have reported an observation based on a simple analysis that phonon modes may be tailored through the judicious use of metal-semiconductor interfaces in such a way as to reduce unwanted inelastic scattering due to interface LO phonons. This qualitative model for interface LO phonons at heterojunctions between semiconductors and ideal metals has been extended through an approximate mathematical treatment to the case of metals with finite conductivity and finite, frequency-dependent Thomas-Fermi screening lengths. To illustrate this concept, variations of a basic GaAs/AlAs single quantum well have been considered with one or both of the AlAs semiconductor (S) barrier layers substituted by an epitaxially grown metal (M) layer; i.e., AlAs/GaAs/AlAs (SSS), metal/GaAs/AlAs (MSS), and metal/GaAs/metal (MSM) structures.

As well known from the previous analyses, the SSS structure has four possible interface modes, two symmetric and two antisymmetric. They all contribute towards increasing the scattering rate for the carriers. Our results show that the use of an ideal metal in place of one of the outer AlAs layers plus half of the GaAs layer adjacent to AlAs layer (i.e., MSS), blocks symmetric modes. Using ideal metal on both sides of the GaAs layer (i.e., MSM) will block both symmetric and antisymmetric modes. This eliminates interface phonon scattering completely. For the case of non-ideal metals, the dispersion relations using non-ideal metals in place of ideal metals do not give as sharply defined curves as for the case of ideal metals; this is understandable since the field associated with the phonon does exist in the non-ideal metal region beyond the very small dimensional scale of several Thomas-Fermi screening lengths. However, our study demonstrates that the relative amplitudes of the optical-phonon modes in the MSS structure are changed very little by replacing the ideal metal with a non-ideal metal having realistic Thomas-Fermi screening lengths in the range of 1 to 10 Å. Thus it is concluded that the previous assumption of a "perfect" metal with infinite conductivity at the metal-

semiconductor interface is not critical to the dramatic reduction of interface phonon scattering rates. This conclusion takes on added significance in light of recent theoretical [4] and experimental [5] findings that the strength of the carrier-interface-phonon interaction scales approximately inversely with the thickness of the confining region.

In many polar semiconductors, the presence of a metal-semiconductor interface will lead to the depletion of carriers from the semiconductor near the metal-semiconductor heterojunction. However, for some metal-semiconductor combinations such as Al-InAs an accumulation is created in the polar semiconductor due to the presence of an As antisite defect in the conduction band on InAs; accordingly, charge depletion effects do not arise as a result of using metal-semiconductor interfaces to reduce carrier-interface-phonon scattering. For the cases where depletion does occur and the majority carriers are depleted near the metal-semiconductor interface, it will be possible, in general, to maintain minority carriers in the semiconductor. Furthermore, modulation doping or other forms of tailored doping such as interface doping may provide the means to achieve the desired level of carriers in the semiconductor. Particularly, the use of modulation doping is suited to the case of a device structure with two heterojunctions having a semiconductor layer with metal at one interface and another semiconductor at the second interface.

Microscopic model for optical phonon modes in nanoscale structures

In spite of the success of dielectric continuum model, recent progress in both microscopic [6,7] and macroscopic [8] approaches for optical phonons in polar semiconductor heterostructures makes it clear that the microscopic methods will be invaluable in understanding both optical phonon dispersion relations and amplitudes in ultrasmall geometries where there is significant mixing of confined and interface modes. This point is illustrated straightforwardly for the case of a nanoscale rectangular quantum wire. Considering the fact that the e^{-1} decay length is $50 \text{ \AA}$ for a typical phonon wavevector of $0.02 \text{ \AA}^{-1}$, the interface modes of one quantum wire surface (e.g., the $z=0$ plane) can easily couple

with the confined modes of an adjacent surface (e.g., the $y=0$ plane) when quantum wires have such characteristic dimensions. It is therefore essential to model the mixing of optical phonon modes in a formalism which properly accounts for the anisotropic nature of polar semiconductors with the zinc-blende lattice structure. Macroscopic models can be expanded to incorporate complex descriptions of the phonon mode coupling [8]. However, such approaches assume an isotropic polar semiconductor medium and, thus, are inadequate for state-of-the-art nanoscale structures with dimensions of a few lattice constants, in which characteristics are inherently dependent on the crystal direction.

A fully microscopic ab initio theory of optical phonon dynamics has been developed and applied very recently by the European group of Molinari et al. [6]. Though such a model provides the most accurate analysis of the structure, it has not been used extensively. This can be attributed to the fact that the ab initio microscopic analysis involves very arduous and time consuming first principle calculations of lattice dynamics rather than employing adjustable parameters. Precise ab initio calculation of force constants at the interface may not be essential for most of the heterostructures except those involving extremely thin layers. It is well known that even a simple linear-chain model with nearest-neighbor force constants can predict the zone center LO phonon frequencies in a superlattice with a reasonable accuracy except in the cases where layers are single monolayer thick. Thus, the development of a simple but yet accurate microscopic model has been called for to study the effects of reduced dimensionality on phonon characteristics and the related optoelectronic and electronic processes in nanoscale semiconductor devices and structures beyond the range of validity of macroscopic treatments. The research effort on this subject has been scarce in the United States. During the past contract period, we have formulated a simplified microscopic model which facilitates the accurate modeling of confined and interface phonons without ab initio calculations of force constants. The valence shell model developed by Kunc and Nielson for bulk [9] has been generalized to the case of superlattice structures. The calculated phonon dispersion and atomic displacements have been used to derive the interaction Hamiltonian and the electron-optical-phonon scattering rates in quantum well

heterostructures. A brief description of our model is as given below.

In a shell model, three types of interactions are included: the core-to-core (R), shell-to-core (T), and shell-to-shell (S) interactions. Then the equation of motion can be found using the following matrix equations:

$$\omega^2 M \vec{u} = (R - ZBZ) \vec{u} + (T - ZBY) \vec{w} , \quad (1)$$

and

$$0 = (T^+ - YBZ) \vec{u} + (\Delta - YBY) \vec{w} , \quad (2)$$

where M, Z, Y, B and Δ are matrices of masses, ionic charges, shell charges, the real part of Coulomb interaction, and the effective shell-shell interaction, respectively, as specified in Ref. 9. Here, $\vec{u}$ and $\vec{w}$ stand for the core and relative shell displacement, respectively. The dynamical matrices shown in Eqs. (1) and (2) reduce to an eigen value problem,

$$[C(\vec{q}) - \omega^2 I] \vec{e} = 0 \quad (3)$$

with

$$C(\vec{q}) = M^{-1/2} [(R - ZBZ) - (T - ZBY)(\Delta - YBY)^{-1}(T^+ - YBZ)] M^{-1/2} . \quad (4)$$

In a bulk zincblende structure, this equation results in 6 eigen values ω_v and 6 eigen vectors $\vec{e}_v$ for a given phonon wavevector $\vec{q}$. The corresponding phonon dispersion relations and displacements are obtained directly from the expressions given above. The results are essentially the same as those calculated in a simple linear-chain model with nearest-neighbor force constants. The long-range Coulomb interaction turns out to be less important because its force range is effectively reduced and its effect is only to slightly modify the nearest-neighbor and next nearest-neighbor force constants. The parameters (or force constants) for three types of interactions (R, S, and T) can be obtained by fitting to the experimental bulk phonon characteristics in each material. All the other required parameters can be found in the literature (Ref. 9 and the references therein). Extension of this approach to a superlattice is rather

straightforward. In a superlattice grown in the (001) direction, the bulk symmetry along the x-y plane is maintained, while the translational period in the z direction needs to be modified. We define a new superlattice unit cell L along the z direction which consists of n unit cells of both materials and a new superlattice wavevector q_z . Hence, along the z direction all summations need to be performed over all unit cells of the superlattice cell instead of a single unit cell as in bulk. Interactions up to the second nearest neighbors are taken into account. The bulk parameters are used in each layer except at the heterointerfaces where the interpolated force constants are adopted [10], thus, circumventing a complicated ab initio calculation of the force constants at the interface. The resulting dynamic matrices provides all of the superlattice eigen frequencies and eigen vectors for phonon modes. These solutions for the phonon dispersion relation and the atomic displacement can be used subsequently to construct the polar electron-optical-phonon interaction Hamiltonian in heterostructures. In a single quantum well, the envelope of the scalar potential can be written as

$$\phi(z) = \sum_{n,v,q_{\parallel}} U^v e_n^* \left[\frac{iq_{\parallel} u_{nz}^v(q_{\parallel})}{|q_{\parallel}|} - u_{nz}^v(q_{\parallel}) \text{sgn}(z - z_n) \right] e^{-(q_{\parallel}|z - z_n|)} \quad (5)$$

with

$$U^v = \frac{1}{2\Omega_{\parallel}\epsilon_{\infty}} \left[\frac{\hbar}{2N_0\omega_v(q_{\parallel})} \right]^{1/2}, \quad (6)$$

where e_n^* is effective charge (2.07|e| for GaAs and 2.17|e| for AlAs), n ranges all the N_0 lattice points in the normalization volume, and $\Omega_{\parallel}$ is the area of the two-dimensional unit cell. The Hamiltonian for polar interaction is given by $-e\phi$ and the appropriate scattering rates can be obtained easily based on the Fermi golden rule.

We have applied this microscopic model to GaAs/AlAs heterostructures and compared with the results from the ab initio calculation of Molinari et al. [6]. Figure 1 shows the phonon dispersion relation for a (001) oriented (GaAs)₂₀/(AlAs)₂₀ superlattice along the in-plane (100) direction and also as a

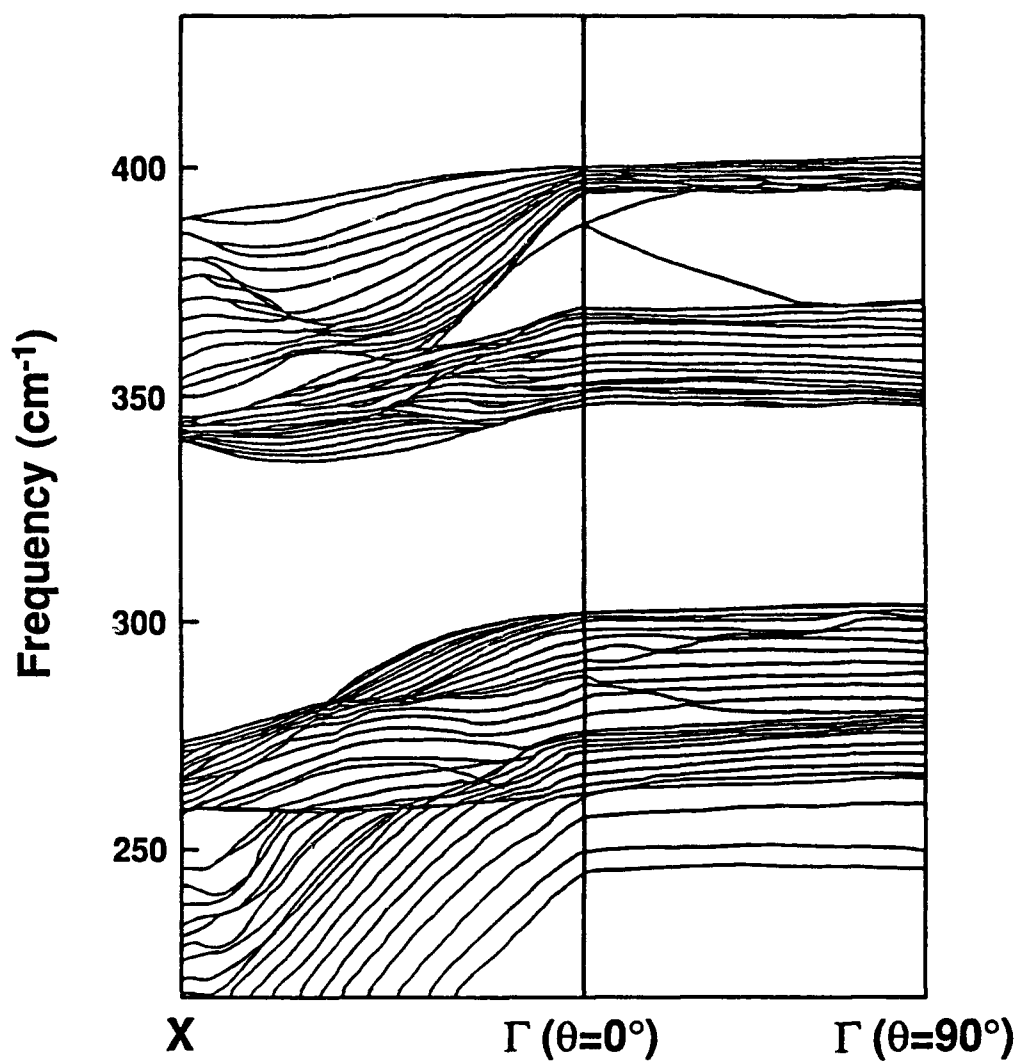


Figure 1. Phonon dispersion relation of a (001)-oriented $(\text{GaAs})_{20}/(\text{AlAs})_{20}$ superlattice along the in-plane direction and as a function of angle θ between the direction of wavevector $\vec{q}$ and the in-plane direction for vanishingly small q .

function of angle θ between the direction of wavevector $\vec{q}$ and the in-plane direction for vanishingly small q ; θ ranges from 0 to $\pi/2$. Two clearly defined GaAs-like and AlAs-like frequency ranges are apparent in Fig. 1. Along with LO and transverse-optical (TO) modes, it should be noted that the two "AlAs-like" principal modes and two "GaAs-like" principal modes take the limit of the well known "interface modes" of the dielectric continuum model over a portion of the domain of Fig. 1. Another feature of interest is the anti-crossing of the modes in the right-hand panel (i.e., angular dependence). Compared to the results from the *ab initio* approach [6], it is clear that our simple microscopic model can describe detailed characteristics of phonon dynamics accurately at dimensional scales of current interest. As the layer thickness decreases, however, the accuracy of our model may suffer due to the assumptions made for the interface force constants. As an indication for validity of our model, the LO phonon frequencies have been calculated for the $(\text{GaAs})_m/(\text{AlAs})_n$ superlattices with $m=n$ ranging from 1 to 4. In this comparison, our results match well with the observed LO phonon frequencies [11] for $m=n \geq 2$ (within 3 cm^{-1}). For the monolayer case, the agreement between the experimental data and our microscopic model is not as good, but it is considerably better than those calculated by using the simple linear chain model [11]. To study this case accurately, one will have to employ first principle calculations using *ab initio* calculations at the heterostructure interface. Nevertheless, our model should provide excellent results for the great majority of device applications since layer thicknesses generally exceed one monolayer.

Figure 2 shows the calculation of the scattering rates for the polar electron-optical-phonon interaction based on our method. A GaAs/AlAs single quantum well structure with a 20-monolayer GaAs well is considered for the $1 \rightarrow 1$ (intrasubband) and $2 \rightarrow 1$ (intersubband) transitions by phonon emission at 300 K. Electronic envelope functions are obtained from the solutions of the Schrödinger equation within the effective mass approximation. For purposes of comparison, Fig. 2 also depicts the corresponding rates as obtained using the *ab initio* calculation [6] and the dielectric continuum model. It is observed in our calculation that for intrasubband scattering, the lowest order and highest

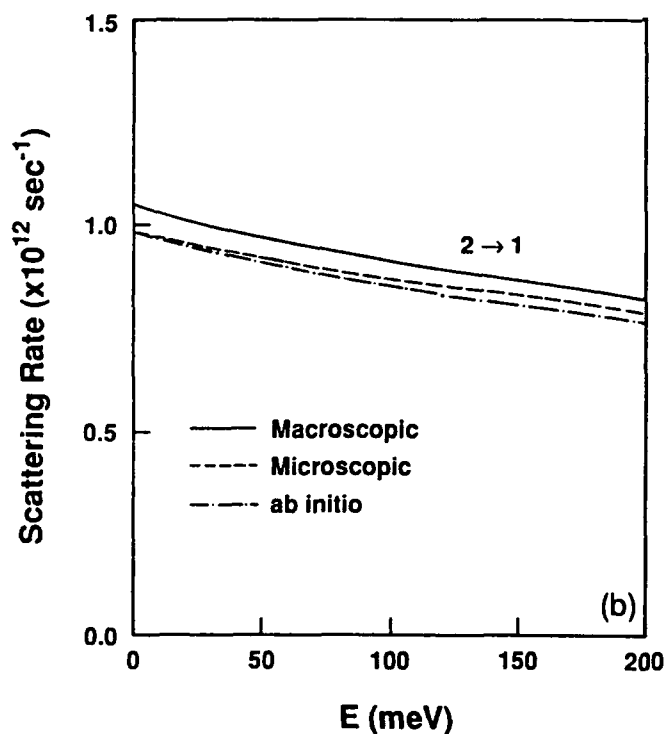
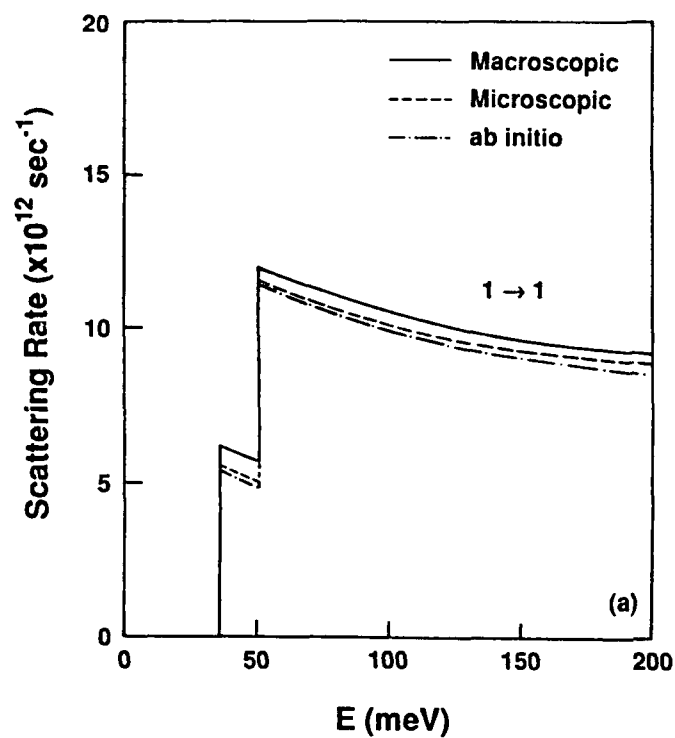


Figure 2. Scattering rates by electron-optical-phonon interaction as a function of electron energy in a GaAs/AlAs single quantum well with a 20-monolayer GaAs well at 300 K. The results in (a) present the intrasubband transition rates of the lowest subband ($1 \rightarrow 1$), while the data in (b) show the intersubband transition rates from the second lowest to the lowest subband ($2 \rightarrow 1$). The results obtained from the dielectric continuum model and the ab initio treatment [6] are also plotted for comparison.

frequency, ω_{LO1} , confined mode is the dominant mode and will dominate over all higher order modes; similarly, for the case of intersubband scattering, ω_{LO2} is the mode which provides the maximum contribution to the scattering strength. Interface modes also provide sizable contributions. These observations and the scattering rates predicted by our microscopic model are in excellent agreement with the results from the ab initio calculation. It is also interesting to note from the figure that the macroscopic model overestimates the scattering rate only slightly in this structure (i.e., 20-monolayer quantum well), as compared to our model. To examine the accuracy of the dielectric continuum model in ultrasmall structures, we have studied the $1 \rightarrow 1$ and $2 \rightarrow 1$ scattering rates as a function of quantum well width in Fig. 3. Surprisingly, the macroscopic approach is in excellent agreement with the microscopic treatment for well widths as small as 25 Å. As the width of the well is reduced further beyond the range of validity of continuum approximations, the agreement suffers slightly, but still it is well within the acceptable range.

From these results, it is shown that our model provides an excellent approximation to the fully microscopic model based on ab initio calculations of lattice dynamics over a wide range of dimensional parameters. The simple and efficient nature of the new microscopic model makes it ideal with a good accuracy to study the effects of reduced dimensionality on phonon characteristics and the related optoelectronic and electronic processes in dimensionally-confined compound semiconductor devices and structures beyond the range of validity of macroscopic treatments. For the calculation of electron-optical-phonon scattering rates, the macroscopic dielectric continuum model predicts rates in good agreement with those of the microscopic models.

Effects of band mixing on hole tunneling times

Recently, we have begun to study the effects of band structure on electronic and optoelectronic properties of heterostructures. Detailed knowledge of band structure in the presence of heterointerfaces, such as mixing and evanescent states, is essential for the characteristic response of a mesoscopic

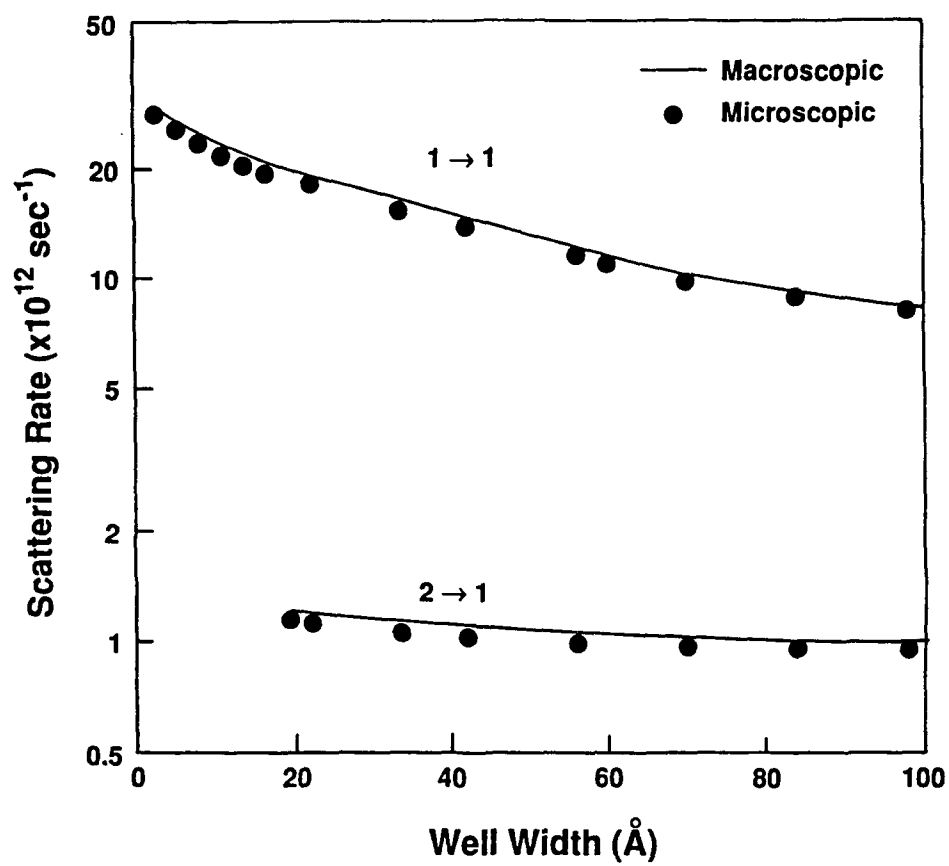


Figure 3. $1 \rightarrow 1$ and $2 \rightarrow 1$ scattering rates as a function of quantum well width at 300 K. The electron energy is fixed at 50 meV.

system which is beyond the realm of the conventional effective mass approximation. As the first topic in this research area, we have concentrated on the effects of band mixing on hole tunneling in double-barrier heterostructures. The double-barrier structures, which were first proposed by Tsu and Esaki [12], are potentially useful as ultrahigh speed devices. The tunneling time of carriers is important because the ultimate device response is directly related to it. Up to now, most of the attention in tunneling devices has been paid to electrons due to their expected fast response compared to holes. However, it is important to understand the tunneling time of holes in opto-electronic devices such as coupled quantum well modulators, where both electrons and holes are involved in the operation and the device speed is limited by the transfer time of the slowest carrier. At the same time, hole tunneling is a physically interesting subject due to the degeneracy at the top of the valence band and the resulting complicated band structure, which gives rise to band mixing and tunneling through different channels originating from heavy hole (hh) and light hole (lh) states.

Theoretically, it is generally assumed that transmission properties for non-zero $k_{\parallel}$ (the carrier momentum component in the plane of layers) are the same as for $k_{\parallel}$ equal to zero. Unlike the case for electrons, however, the tunneling time estimated for holes from conventional independent effective mass models do not agree with the experimental results. While the simple theories predict much longer tunneling time due to the large effective mass of heavy holes, experiments show that tunneling times for holes are comparable to those of electrons [13]. This discrepancy may be explained by using a more realistic band structure which considers band mixing effects for holes. The assumption of $k_{\parallel}=0$ is not appropriate due to strong mixing of hh and lh states in the presence of sizable non-zero $k_{\parallel}$ due to finite temperature (on the order of lattice thermal energy $k_B T$) and the degeneracy of the hole gas.

To obtain a realistic band structure in a double-barrier resonant tunneling structure, we have used a $\vec{k} \cdot \vec{p}$ method. By solving the 4×4 Luttinger-Kohn Hamiltonian in the envelope-function approach, the eigen functions are calculated in each region for a given $k_{\parallel}$ and E . After taking a linear combination of

the bulk solutions, continuity and current conserving boundary conditions are applied. For $k_y=0$, the Hamiltonian is diagonal and, as a result, there is no mixing between the light holes and heavy holes. When k_y is not equal to zero, however, the Hamiltonian is no longer diagonal, and interactions occur between the hh and lh bands as mentioned above. Thus, the $\vec{k} \cdot \vec{p}$ method used in this study takes into account the mixing between hole states. Our model also includes the difference in Luttinger-Kohn parameters of the well and barrier materials. For simplicity, the spin-orbit split-off band and inelastic effects are neglected. In the calculation of transmittivity through the quantum well states, the mixing effects are intrinsically included in our model by using the Luttinger-Kohn Hamiltonian in the transfer matrix approach. For the tunneling times, we have adopted the phase delay time. The phase delay time can be calculated from the energy derivative of the total phase shift of the wave function upon tunneling,

$$t_{\text{delay}} = \hbar \frac{d\delta}{dE} , \quad (7)$$

where δ is the total phase of the transfer function. The transmission coefficient can be written as $Te^{i\theta}$. Therefore, the total phase shift upon tunneling is

$$\delta = k_z d + \theta , \quad (8)$$

where k_z is the hole momentum in the direction of growth and d represents the distance traveled. The approach outlined above, in which a steady state quantity (phase shift) is related to the delay time, avoids time-consuming numerical computations using wave packets or application of effective masses. Other methods of calculating time delay have been proposed. Since no clear agreement exists regarding when and how to use these methods, we have, thus far, been concerned only with phase delay time and any reference to time or delay time should be interpreted as such.

Applying our model to a double-barrier GaAs/AlAs heterostructure, we have found that the hole tunneling time is very sensitive to the parallel momentum. As k_y is increased, mixing increases as a

result of off-diagonal terms in the Luttinger-Kohn Hamiltonian. The first (second) resonant state is originally a hh (lh) state; i.e., only the hh (lh) to hh (lh) transition is allowed without mixing. However, when mixing is considered, other possibilities (channels) arise and all of the hh to hh, hh to lh, lh to lh, lh to hh channels are present. In general, we have observed that the time delays for the first (second) resonant state decrease (increase) with increased $k_{\parallel}$. As $k_{\parallel}$ increases, the hh resonant state becomes more and more lh-like in nature and the lh resonant state becomes more hh-like. As a result, the tunneling time for the first state decreases while it increases for the second state. Our results indicated that mixing has a more pronounced effect on the time delay associated with the original hh (first) state than the original lh (second) state. This could be explained by the fact that heavy holes have a much longer lifetime (i.e., stay longer) in the quantum well. It has also been found that the mixing effects are much more important for samples with larger barrier thicknesses. Figure 4 shows the tunneling time for the hh to hh transition in the first resonant state for barrier thicknesses of 10 Å and 20 Å in GaAs/AlAs double-barrier structures. As can be seen, the hh tunneling time is reduced more drastically for a thicker barrier. Since mixing increases with barrier thickness due to the larger lifetime of the quasibound level in the quantum well, the case with thick barriers can exhibit a greater reduction in the hh tunneling time for non-zero $k_{\parallel}$.

In an effort to compare our results with experiments, we consider the double barrier structure used by Jackson et al. [13]. In their experiment, it was concluded that the heavy holes and electrons tunnel through the structure at comparable rates and the measured value represents the delay time for both carriers. With $k_{\parallel}=0.03 \text{ Å}^{-1}$ which gives $E_{\parallel}=k_{\parallel}T$ at 80 K, our calculated values of hole tunneling times show good agreement with their experiment. The difference between our results and the measured values ranges from ~ 30 % for the 16 Å barrier to an order of magnitude for the 34 Å barrier; our results are consistently larger than the measured values. This is a significant improvement from conventional approaches considering that the results with $k_{\parallel}=0$ (i.e., effective mass results without band

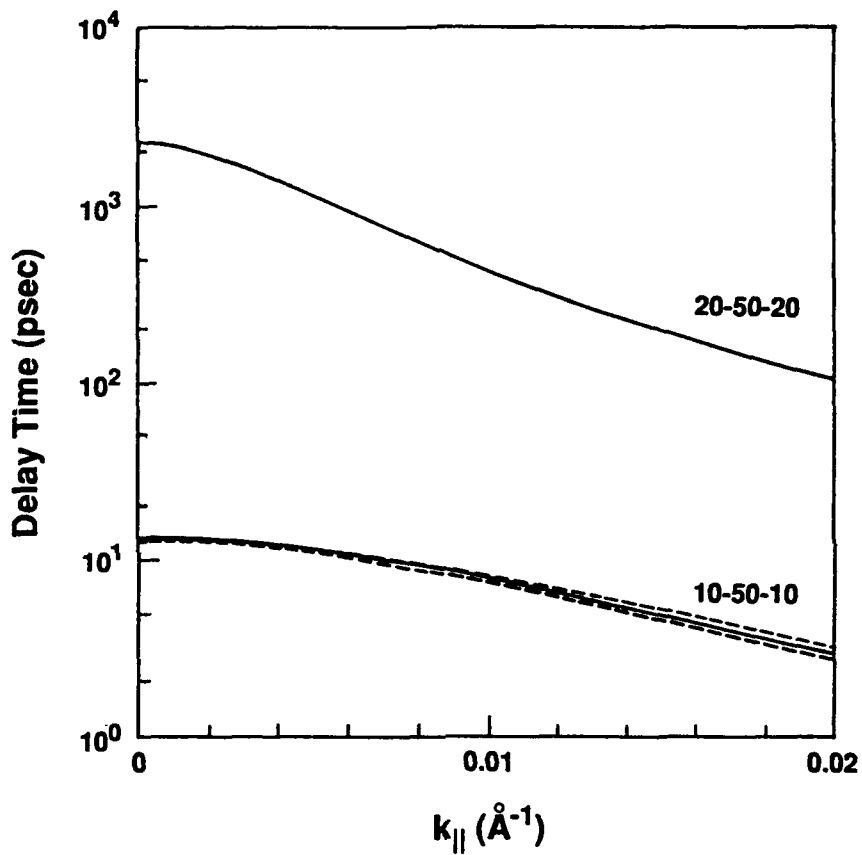


Figure 4. Heavy hole to heavy hole tunneling time for the first resonant state for barrier thicknesses of 10 $\text{\AA}$ and 20 $\text{\AA}$ in a GaAs/AlAs double-barrier heterostructure. The well is 50 $\text{\AA}$ thick in both cases. The solid lines show the delay time without a field. For the 10 $\text{\AA}$ -barrier structure, the tunneling times obtained with an applied electric field (40 kV/cm) are shown by the dashed lines.

mixing) are ~ 50 times (for $16 \text{ \AA}$) and 4 orders of magnitude (for $34 \text{ \AA}$) greater than the measured data, respectively. Moreover, the difference between our results and the measured values can be reconciled further when the uncertainties in the thicknesses are considered, in which case, the calculated results fall within the given experimental range. One should also notice that, in estimating $k_{\parallel}$ only the effect of temperature was considered, but not that of carrier concentration. Other effects such as scattering, impurities, quantum well charging and band bending may be effective in determining tunneling times. These are not expected to be as important compared with the mixing effects. We have simulated the effect of an electric field as well by using a simple staircase potential consisting of flat potentials in each region. The breaking of inversion symmetry due to the electric field causes two solutions for a finite $k_{\parallel}$. As can be seen from Fig. 4, the field does not alter the general tendency of delay time reduction with finite $k_{\parallel}$. Although the staircase approximation of the electric field does not provide a quantitative understanding of the delay time accurately, the results with an electric field will be, on average, close to those without; thus, the basic attributes of the delay vs $k_{\parallel}$ curve remain the same. As a result, it is expected that our findings apply well for the biased structure used in practice.

Multi-band theory of Bloch electron dynamics in homogeneous electric fields

Bloch electron dynamics in a homogeneous electric field has been a subject of great interest dating back to the earliest applications of quantum mechanics to solid state physics. During the past contract period, we have developed a novel multi-band theory of Bloch electron dynamics in homogeneous electric fields of arbitrary strength. In this formalism, the electric field has been described through the use of the vector potential based on the methodology previously developed by Iafrate and co-workers [1]. The coupling between bands has been treated in the Wigner-Weisskopf (W-W) approximation [14]. A classic approach for describing the time decay from an occupied quasi-stationary state, the W-W approximation allows analysis of the long-time, time-dependent tunneling characteristics of an electron transition out of an initially occupied band due to the power absorbed by the electric field,

while preserving conservation of total transition probability over the complete set of excited bands. The Wannier representation has been chosen as the basis set in our theory to accommodate the inherent localization manifest for Bloch dynamics in strong electric fields. In a homogeneous field, the transport picture leads to localization, with hopping transport from site to site. From this theory, we have derived a generalized tunneling time in terms of the applied electric field and the relevant band parameters.

In the localized Wannier representation, the Schrödinger equation for a Bloch electron in the presence of a homogeneous electric field is given by [1]

$$i\hbar \frac{\partial f_n(\vec{r},t)}{\partial t} = \epsilon_n(-i\vec{\nabla} - \frac{e}{\hbar c} \vec{A}_0) f_n(\vec{r},t) - e\vec{E}_0 \cdot \sum_{n'} \vec{R}_{nn'}(-i\vec{\nabla} - \frac{e}{\hbar c} \vec{A}_0) f_{n'}(\vec{r},t), \quad (9)$$

where $\epsilon_n(\vec{K})$ is the n -th Bloch energy band, $\vec{A}_0$ is the vector potential of the electric field, and $\vec{R}_{nn'}$ is the interband coupling term due to the electric field. In the vector potential gauge, the Wannier envelope function can be expressed as

$$f_n(\vec{r},t) = \frac{1}{\sqrt{N}} \sum_{\vec{K}} e^{-\frac{i}{\hbar} \int_0^t \epsilon_n(\vec{K} - \frac{e}{\hbar c} \vec{A}_0) dt} e^{i\vec{K} \cdot \vec{r}} A_n(\vec{K},t), \quad (10)$$

where the expansion coefficient $A_n(\vec{K},t)$ satisfies a set of coupled equations derived from Eq. (9). As mentioned above, the interband couplings were treated by using the W-W approximation. From this approximation, an integro-differential equation was obtained for $A_n(\vec{K},t)$ of the band of interest (or the initial band " n_0 "). When this integro-differential equation was solved through the use of Laplace transform, the solution for the initial band " n_0 " was found to be

$$A_{n_0}(\vec{K},t) = A_{n_0}(\vec{K},0) e^{[i\Delta\epsilon_{n_0}(\vec{K}_\perp) - \gamma_{n_0}(\vec{K}_\perp)/2]t}, \quad (11)$$

where $A_{n_0}(\vec{K},0)$ is determined by the initial state of the system, $\vec{K}_\perp$ is the component of $\vec{K}$ perpendicular to the direction of the electric field, and

$$\Delta\omega_{n_0}(\vec{K}_\perp) = \left(\frac{eE_0}{\hbar}\right)^2 \sum_{n \neq n_0} \sum_{l_x} |D_{n_0 n}(l_x, \vec{K}_\perp)|^2 P \left[\frac{1}{-\omega_B l_x + \omega_{n_0 n}(\vec{K}_\perp)} \right], \quad (12)$$

$$\gamma_{n_0}(\vec{K}_\perp) = 2 \frac{\pi}{\omega_B} \left(\frac{eE_0}{\hbar}\right)^2 \sum_{n \neq n_0} |D_{n_0 n}(l_{n_0 n}(\vec{K}_\perp), \vec{K}_\perp)|^2, \quad (13)$$

$$|D_{n_0 n}(l_x, \vec{K}_\perp)| = \frac{q}{4} e^{-q_{n_0 n} |l_x|}, \quad (14)$$

where $l_{n_0 n}(\vec{K}_\perp) = \omega_{n_0 n}(\vec{K}_\perp)/\omega_B$. In these equations, $\omega_{n_0 n}(\vec{K}_\perp) = \epsilon_{n_0 n}(\vec{K}_\perp)/\hbar$ with $\epsilon_{n_0 n}(\vec{K}_\perp)$ the average value of energy gap in the direction of electric field between the bands " n_0 " and " n ", ω_B is the Bloch frequency, and $q_{n_0 n} = |q|$ with q determined by $\epsilon_{n_0}(q, \vec{K}_\perp) = \epsilon_n(q, \vec{K}_\perp)$. It is noted that $\Delta\omega_{n_0}$ and γ_{n_0} are the $\vec{K}_\perp$ -dependent parameters that include the couplings between the band of interest and all other bands. The exponentially decaying terms of the initial band indicate the irreversible decay into the upper bands of the crystal due to the power absorbed by the electric field. The excited state envelope functions exhibit an electric field enhanced broadening of the excited state probability amplitudes, thus resulting in spatial lattice delocalization and smearing of the on-set of discrete, Stark-ladder and band-to-band transitions due to the presence of the electric field.

The analysis of the envelope functions for the initial state shows Bloch oscillatory temporal behavior in the direction of the electric field, damped by the Zener decay rate. The excited state envelope functions show a clear electron delocalization upon excitation to the excited state if the electron was initially localized in the lowest band. The Bloch oscillatory behavior is suppressed after Zener tunneling due to the accompanying delocalization and broadening. From the W-W approximation, a generalized Zener tunneling time has been derived in terms of the applied uniform electric field and the relevant band parameters, which can be written as

$$\tau_z = \frac{1}{\Gamma(0)}, \quad (15)$$

where $\Gamma(0)$ is the total Zener transition rate for a Bloch electron transition out of initial " n_0 ". This rate

is given by

$$\Gamma(0) = \frac{\pi}{8} \omega_B \sum_{\vec{K}} |A_{n_0}(\vec{K}, 0)|^2 \sum_{n \neq n_0} e^{-2a_{n_0 n}(\vec{K}_\perp) \epsilon_{n_0 n}(\vec{K}_\perp) e E_0}. \quad (16)$$

It is noted that the total transition rate for a Bloch electron tunneling out of its initial band depends on the initial condition of the electron, and the sum of $n \neq n_0$ couples the initial band with all other bands.

The combined use of the vector potential gauge and, therefore, the concomitant use of time-dependent accelerated states and the W-W approximation have allowed the temporal analysis of Bloch electron dynamics covering a time span from several Bloch oscillations to times well beyond the Zener tunneling time. Although Zener tunneling times have been derived for a general periodic potential, a specific example of the use of this analysis was put forth using a nearest-neighbor tight-binding model. Zener tunneling times derived using our model have identical parametric dependence on electric field but different dependence on band structure parameters compared to those of the well known Kane's two-band model in the effective mass limit.

Calculation of minority carrier mobilities in the dielectric function formalism

During the 1991-92 contract period, we had reported 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 framework of the random phase approximation (RPA) or the self-consistent field (SCF) approach. By modifying an approach proposed by Mermin for the free electron gas [15], we had formulated the dielectric response function which properly incorporates the finite particle lifetime in heavily-doped zincblende semiconductors (denoted as the Lindhard-Mermin dielectric function hereinafter) and have obtained accurate inelastic scattering rates in such media [16]. Last year, as an expansion of this effort, we have developed a new approach for the calculation of minority carrier mobilities based on the Lindhard-Mermin dielectric function formalism.

Minority electron mobility in a heavily-doped p-type semiconductor is an important macroscopic quantity in many applications and several issues concerning this physical property of semiconductors remain to be resolved. Evaluation of minority carrier mobility is a non-trivial problem, both experimentally and theoretically. Increasing data for minority electron mobility have become available in the past few years, especially for GaAs. These data have been obtained from sophisticated experiments such as the time-of-flight measurement and the common-emitter cutoff frequency measurement with adequately-fabricated heterojunction bipolar devices. Experiments for another important semiconductor material Si are fewer in number. For theoretical calculations of minority electron transport, one must consider carefully the appropriate application of many body theory. The significant many body effects are dynamical screening and collective excitations. Very recently, Lowney and Bennett showed a refined calculation of majority- and minority-carrier mobilities for GaAs [17] and Si [18]. They incorporated plasmon scattering in the variational method, and applied phase shift corrections beyond the Born approximation for ionized impurity scattering and minority carrier-majority carrier scattering. Also, Fischetti reported a detailed study of the effects of plasmon scattering on the majority- and minority-carrier mobilities along with a phase shift analysis for ionized impurity scattering in Si [19]. In these calculations, the effects of interband transition of holes were neglected and the Bohm and Pines approach of introducing a wavevector cutoff was adopted for the electron-hole interaction. However, in heavily-doped p-type semiconductors, the definition of a cutoff wavevector for hole plasmons becomes highly ambiguous due to the extended and complicated Landau damping region. The dynamical response of a hole gas is significantly affected by interband transitions between the heavy hole band and the light hole band. In addition, the collision damping of coupled collective excitations due to finite hole lifetime is important as discussed in our earlier work [16].

An effective method to describe minority carrier transport in a heavily-doped semiconductor is to extend the dielectric response function formalism to an appropriate transport theory. Although there are limitations, the RPA or SCF method is a tractable and reasonable approach for describing the many

body effects in heavily-doped semiconductors. By evaluating the frequency- and wavevector-dependent dielectric response functions for majority holes, we have developed a more comprehensive method for the calculation of minority electron transport. The transport theory we have adopted in our approach uses the iterative method [20] to solve the Boltzmann transport equation since the relaxation time approximation cannot be applied when non-randomizing inelastic scattering mechanisms dominate. Under weak-field conditions, we can apply the first-order Legendre polynomial expansion of the full distribution function:

$$f(\vec{k}) = f_0(E_{\vec{k}}) - eFv(\vec{k})\phi(E_{\vec{k}})\frac{\partial f_0(E_{\vec{k}})}{\partial E_{\vec{k}}}\cos\theta, \quad (17)$$

where θ is the angle between velocity $\vec{v}(\vec{k})$ and electric field $\vec{F}$. Here, we assume a spherical conduction band incorporating first-order nonparabolicity, i.e., the energy-momentum relation is given by

$$\frac{\hbar^2 k^2}{2m^*} = \gamma(E_{\vec{k}}) = E_{\vec{k}}(1 + \alpha E_{\vec{k}}), \quad (18)$$

where m^* is the effective mass at the bottom of the conduction band. The nonparabolicity factor α has a moderate effect on mobility at room temperature. The electron velocity is given by

$$\vec{v}(\vec{k}) = \frac{\hbar \vec{k}}{m^*(1 + 2\alpha E_{\vec{k}})}. \quad (19)$$

We assume nondegenerate statistics for the minority carrier distribution. By applying the trial solution [i.e., Eq. (17)] to the Boltzmann equation, the iterative form for $\phi(E_{\vec{k}})$ in our case is given by

$$\phi(E_{\vec{k}}) = \frac{1 + \Gamma(\phi, E_{\vec{k}})}{1/\tau(E_{\vec{k}}) + \Gamma_0(E_{\vec{k}})}, \quad (20)$$

where $\tau(E_{\vec{k}})$ is the relaxation time for elastic scattering:

$$\frac{1}{\tau(E_{\vec{k}})} = \frac{1}{8\pi^3} \int W_{\vec{k}\vec{k}'}^{\text{el}} [1 - \cos\Theta] d\vec{k}'. \quad (21)$$

Here, $W_{\vec{k}\vec{k}'}^{\text{el}}$ is the elastic scattering rate from $\vec{k}$ to $\vec{k}'$ and Θ is the angle between $\vec{k}$ and $\vec{k}'$. Also, $\Gamma_0(E_{\vec{k}})$ and $\Gamma(\phi, E_{\vec{k}})$ are defined by the following integrals:

$$\Gamma_0(E_{\vec{k}}) = \frac{1}{8\pi^3} \int W_{\vec{k}\vec{k}'}^{\text{in}} d\vec{k}', \quad (22)$$

$$\Gamma(\phi, E_{\vec{k}}) = \frac{1}{8\pi^3} \int W_{\vec{k}\vec{k}'}^{\text{in}} \phi(E_{\vec{k}'}) \frac{v(\vec{k}')}{v(\vec{k})} \cos\Theta d\vec{k}'. \quad (23)$$

In these equations, $W_{\vec{k}\vec{k}'}^{\text{in}}$ is the inelastic scattering rate from $\vec{k}$ to $\vec{k}'$; thus, $\Gamma_0(E_{\vec{k}})$ is the total inelastic scattering rate. Retaining first-order nonparabolicity, the minority carrier mobility can be obtained as:

$$\mu = \frac{2e}{3k_B T m^*} \frac{\int_0^\infty \phi(E_{\vec{k}}) E_{\vec{k}}^{3/2} (1 - \frac{1}{2} \alpha E_{\vec{k}}) \exp(-E_{\vec{k}}/K_B T) dE_{\vec{k}}}{\int_0^\infty E_{\vec{k}}^{1/2} (1 + \frac{5}{2} \alpha E_{\vec{k}}) \exp(-E_{\vec{k}}/K_B T) dE_{\vec{k}}}. \quad (24)$$

In Eqs. (21)-(23), $W_{\vec{k}\vec{k}'}^{\text{el}}$ (by ionized impurity scattering) and $W_{\vec{k}\vec{k}'}^{\text{in}}$ are obtained from our analysis of the Lindhard-Mermin dielectric response function [16]. For this purpose (i.e., to obtain the dielectric response function in p-type materials), the heavy hole and light hole bands are assumed to be parabolic. Then, by using Eq. (20), the solutions for $\phi(E_{\vec{k}})$ and μ can be calculated iteratively.

We have applied our model to study the minority electron mobilities in heavily-doped p-type GaAs and Si. Figure 5 shows electron mobility in GaAs at 300 K as a function of hole concentration with the hole lifetime $\hbar/\tau_h$ as a parameter (solid line for $\hbar/\tau_h = 0.02$ eV and dashed line for 0.05 eV), along with experimental data from the literature. The dotted-dashed line is the result including the multi-ion screening correction, which will be discussed later. In general, as doping density becomes higher, hole mobility becomes smaller, resulting in a larger damping constant $\hbar/\tau_h$. Although the experimental data are highly scattered, overall agreement is satisfactory, especially for hole concentrations up to 10^{19} cm^{-3} . The tendency of the U-shaped curve qualitatively agrees with the experimental results of Furuta et al. Near the minimum of the curve (around $3 \times 10^{18} \text{ cm}^{-3}$), coupled collective exci-

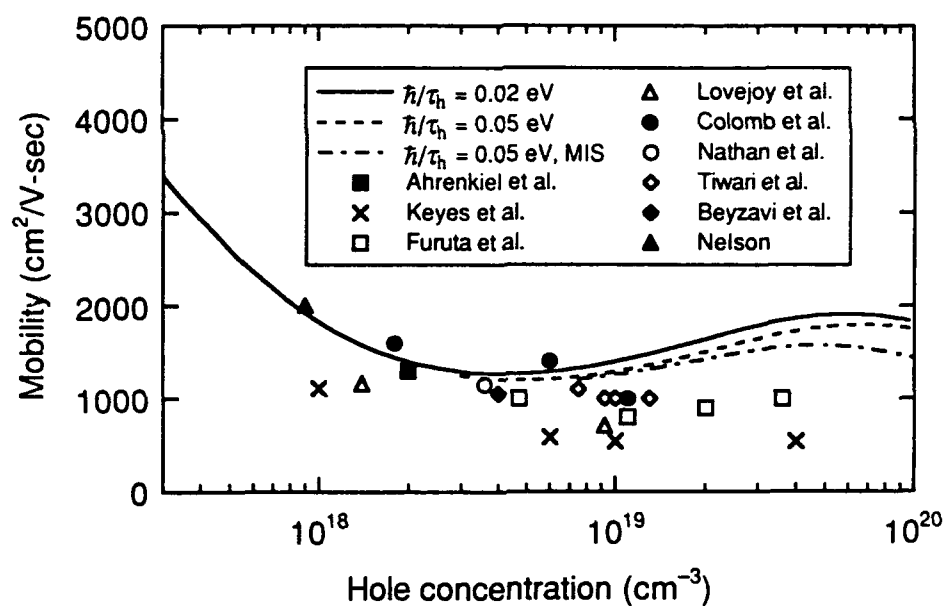


Figure 5. Electron mobilities for GaAs as a function of hole concentration evaluated at 300 K. The theoretical values (lines) are compared with experimental data available in the literature (points). The dotted-dashed line denotes the results with multi-ion screening (MIS) correction [21].

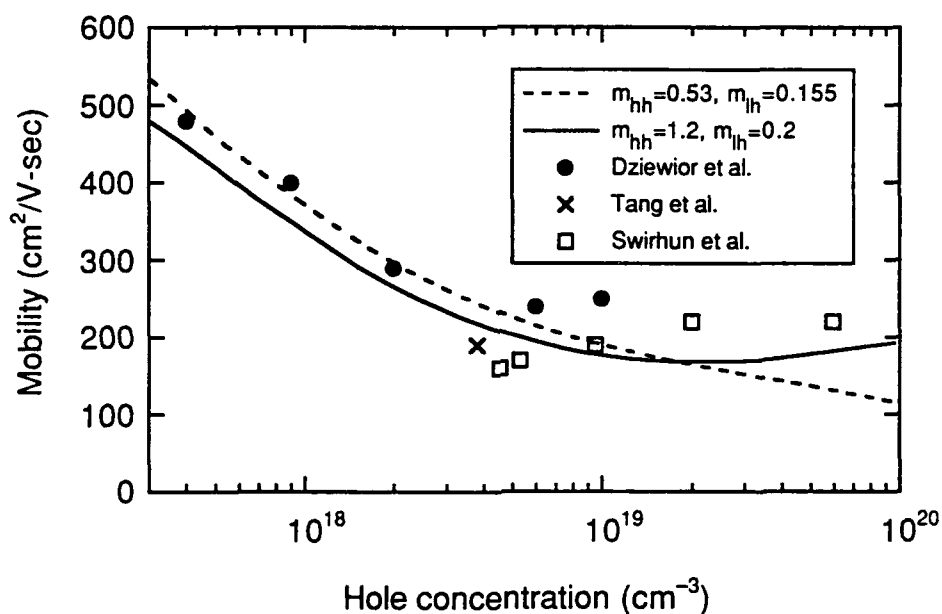


Figure 6. Electron mobilities for Si as a function of hole concentration evaluated at 300 K. Two sets of heavy hole (m_{hh}) and light hole (m_{hl}) effective masses are used for calculation. The theoretical values (lines) are compared with experimental data available in the literature (points).

tations interact most effectively with thermally injected electrons. As hole concentration becomes larger than this value, the interaction between minority electrons and coupled modes becomes less effective and impurity scattering dominates. This is due to the fact that the plasmon energy becomes too large to interact with thermally injected electrons, and also the LO-phonon mode is strongly screened by higher frequency plasmons. At very high hole concentrations, the momentum relaxation rates due to total inelastic scattering becomes even smaller than those for bare LO-phonon scattering. These effects result in an increase of minority carrier mobilities for hole concentration above about $3 \times 10^{18} \text{ cm}^{-3}$. However, the mobility decreases again for the very heavily-doped conditions due to the increase of dominant impurity scattering rates. The deviation of our results from experimental data in Fig. 5 becomes larger for the larger hole concentrations, even when we adopt a larger collision damping constant (e.g., $\hbar/\tau_h = 0.05 \text{ eV}$). In this regime, where ionized impurity scattering dominates with strong screening by majority holes, improvements in our theory are needed. For example, the Born approximation in our theory may not be adequate. Also, our basic assumption for inelastic scattering by collective excitations is that the electrons are weakly coupled to the many particle system, which is true for fast electrons. Thus, it may be essential in this regime (with the hole concentration greater than 10^{19} cm^{-3}) to go beyond the Born approximation, not only for ionized impurity scattering, but also for collective excitations. We plan to pursue this more complete and accurate treatment in the future. Here, an effort has been made to improve accuracy within the current formalism. We have applied the multi-ion screening (MIS) correction for ionized impurity scattering discussed by Meyer and Bartoli [21]. The MIS correction further improves the agreement with experimental values as shown in Fig. 5.

Figure 6 shows minority carrier mobility in Si as a function of hole concentration calculated with two sets of hole effective mass ratios. Here, we have assumed a single value of damping constant of $\hbar/\tau_h = 0.01 \text{ eV}$. In our theory, the choice of appropriate hole effective mass values is important and other corrections cause only secondary effects. The major differences of electron scattering

mechanisms in Si from those in GaAs are the absence of the polar LO-phonon scattering and the contribution of other scattering mechanisms. Acoustic phonon scattering and intervalley phonon scattering play moderate roles in the reduction of mobility only at small doping densities although they can never be neglected. Screening for acoustic phonon scattering is small for hole concentrations below 10^{18} cm^{-3} while it is significant for higher concentrations where other scattering mechanisms dominate. The agreement between the dashed line (with smaller effective hole mass values) and the experimental data is excellent below the hole concentration of 10^{19} cm^{-3} , while this line is monotonically decreasing and deviates from experimental values at larger hole concentrations. At very heavily-doped conditions, we believe that the ionized impurities are strongly screened by "very heavy" holes, which is qualitatively explained by the better fit by the solid line (with larger effective mass values). The strong nonparabolicity of the valence bands is important and, thus, responsible for large average hole effective mass ratios in this region. We have obtained a minimum in the solid line similar to that observed for GaAs. The shallowness (or even the absence in the dashed line) of this minimum is attributed to the absence of polar phonon interaction. In polar semiconductors, the coincidence of the uncoupled LO-phonon and plasmon frequency provides a turning point, where the effects of "anti-screening" and "screening" for LO-phonon modes take turns. In Si, there is no such point and "uncoupled" plasmon scattering plays a moderate role in the reduction of minority carrier mobilities for small hole concentrations. At higher hole concentrations, ionized impurity scattering plays a major role in determining mobility.

2.3 Publications and Presentations

During the last year, this program has resulted in ten refereed publications in the literature, three additional manuscripts are currently in press, and one more has been submitted to a major technical journal. Six 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

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 Thermal Broadening of the Exciton Linewidth in GaAs/Ga_{0.7}Al_{0.3}As Single Quantum Wells," *Appl. Phys. Lett.* 61, 1411 (1992).

T. Kaneto, K. W. Kim, and M. A. Littlejohn, "Dielectric Response Functions of Heavily-Doped Zincblende Semiconductors with Finite Particle Lifetime," *J. Appl. Phys.* 72, 4139 (1992).

M. A. Stroscio, K. W. Kim, A. R. Bhatt, G. J. Iafrate, M. Dutta, and H. L. Grubin, "Reduction of Inelastic Longitudinal-Optical Phonon Scattering in Narrow Polar-Semiconductor Quantum Wells," *Proc. SPIE* 1675, 237 (1992).

M. A. Stroscio, G. J. Iafrate, K. W. Kim, M. A. Littlejohn, A. R. Bhatt, and M. Dutta, "Confined and Interface Optical Phonons in Quantum Wells and Quantum Wires," *Proc. SPIE* CR45, 341 (1993).

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," *J. Appl. Phys.* 73, 2338 (1993).

T. Kaneto, K. W. Kim, and M. A. Littlejohn, "Calculation of Minority Carrier Mobilities in Heavily-Doped p-Type Semiconductors in the Dielectric Function Formalism," *Phys. Rev. B* 47, 16257 (1993).

M. U. Erdogan, K. W. Kim, and M. A. Stroscio, "Effects of Band Mixing on Hole Tunneling Times in GaAs/AlAs Double-Barrier Heterostructures," *Appl. Phys. Lett.* 62, 1423 (1993).

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," *Appl. Phys. Lett.* 63, 48 (1993).

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," in *Phonon Scattering in Condensed Matter VII*, edited by M. Meissner and R. O. Pohl (Springer-Verlag, Berlin, 1993), Springer Series in Solid-State Sciences, Vol. 112, p. 341.

M. A. Stroscio and K. W. Kim, "Piezoelectric Scattering of Carriers from Confined Acoustic Modes in Cylindrical Quantum Wires," *Phys. Rev. B* 48, 1936 (1993).

M. U. Erdogan, K. W. Kim, M. A. Strosio, and M. Dutta, "An Extension of Kronig-Penney Model for Γ -X Mixing in Superlattices," accepted for publication in *J. Appl. Phys.*

A. R. Bhatt, K. W. Kim, M. A. Strosio, and J. M. Higman, "Simplified Microscopic Model for Electron-Optical-Phonon Interactions in Quantum Wells," accepted for publication in *Phys. Rev. B*.

M. A. Strosio and K. W. Kim, "Generalized Piezoelectric Scattering Rate for Electrons in a Two-Dimensional Electron Gas," accepted for publication in *Solid-State Electron.*

Jun He and Gerald J. Iafrate, "Multi-Band Theory of Bloch Electron Dynamics in Homogeneous Electric Field," submitted to *Phys. Rev. B*.

B. Conference Presentations

V. Mitin, R. Mickevicius, M. A. Strosio, G. J. Iafrate, and K. W. Kim, "Electron Scattering and Transport in Multisubband Quantum Wires," presented at the 8th Vilnius Symp. on Ultrafast Phenomena in Semiconductors (September, 1992, Vilnius, Lithuania).

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

M. A. Strosio, G. J. Iafrate, K. W. Kim, M. A. Littlejohn, A. R. Bhatt, and M. Dutta, "Confined and Interface Optical Phonons in Quantum Wells and Quantum Wires (Invited)," presented at the SPIE Intl. Symp. on Optoelectronic Packaging and Interconnects (January, 1993, Los Angeles, Calif.).

K. W. Kim, A. R. Bhatt, and M. A. Strosio, "Microscopic Model for Confined and Interface Longitudinal Optical Phonons in Polar Semiconductor Nanostructures," presented at the March Meeting of the American Physical Society (March, 1993, Seattle, Washington).

M. A. Strosio, G. J. Iafrate, K. W. Kim, A. R. Bhatt, M. Dutta, and C.-J. Chiu, "Interface Longitudinal Optical Phonon Modes in Polar Semiconductor Nanostructures," presented at the March Meeting of the American Physical Society (March, 1993, Seattle, Washington).

M. A. Strosio, G. J. Iafrate, K. W. Kim, M. A. Littlejohn, A. R. Bhatt, and M. Dutta, "Confined and Interface Phonons in Quantum Wells and Quantum Wires," presented at the 2nd Workshop on Optical Properties of Mesoscopic Semiconductor Structures (April, 1993, Snow Bird, Utah).

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3. PERSONNEL

Three faculty members; Dr. K. W. Kim, Dr. G. J. Iafrate, and Dr. M. A. Stroschio, 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 MOS-FETs 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. Dr. M. A. Stroschio 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 phonon modes in heterostructures, especially the effects of reduced dimensionality.

Dr. Iafrate and Dr. Stroschio 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. Stroschio related to this program 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. Strosio, 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. Strosio, 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. Strosio, 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).
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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 Int. Semiconductor Device Research Symp.*, pp. 235-238, 1991.
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14. K. W. Kim, M. A. Littlejohn, M. A. Strosio, 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. Strosio, "Electron High-Field Transport in Multi-Subband Quantum Wire Structures," *Semicond. Sci. Technol.* 7, B299 (1992).

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25. A. R. Bhatt, K. W. Kim, M. A. Stroschio, G. J. Iafrate, M. Dutta, H. L. Grubin, R. Haque, and X. T. Zhu, "Reduction of Interface Phonon Modes Using Metal-Semiconductor Heterostructures," *J. Appl. Phys.* **73**, 2338 (1993).
26. T. Kaneto, K. W. Kim, and M. A. Littlejohn, "Calculation of Minority Carrier Mobilities in Heavily-Doped p-Type Semiconductors in the Dielectric Function Formalism," *Phys. Rev. B* **47**, 16257 (1993).
27. M. U. Erdogan, K. W. Kim, and M. A. Stroschio, "Effects of Band Mixing on Hole Tunneling Times in GaAs/AlAs Double-Barrier Heterostructures," *Appl. Phys. Lett.* **62**, 1423 (1993).
28. 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," *Appl. Phys. Lett.* **63**, 48 (1993).
29. M. A. Stroschio, 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," in *Phonon Scattering in Condensed Matter VII*, edited by M. Meissner and R. O. Pohl (Springer-Verlag, Berlin, 1993), Springer Series in Solid-State Sciences, Vol. 112, p. 341.
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32. A. R. Bhatt, K. W. Kim, M. A. Strosio, and J. M. Higman, "Simplified Microscopic Model for Electron-Optical-Phonon Interactions in Quantum Wells," accepted for publication in *Phys. Rev. B*.
33. M. A. Strosio and K. W. Kim, "Generalized Piezoelectric Scattering Rate for Electrons in a Two-Dimensional Electron Gas," accepted for publication in *Solid-State Electron*.
34. Jun He and Gerald J. Iafrate, "Multi-Band Theory of Bloch Electron Dynamics in Homogeneous Electric Field," 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 1992-93 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) 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," *Appl. Phys. Lett.* 61, 1411 (1992).
- 2) T. Kaneto, K. W. Kim, and M. A. Littlejohn, "Dielectric Response Functions of Highly-Doped Zincblende Semiconductors with Finite Particle Lifetime," *J. Appl. Phys.* 72, 4139 (1992).
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- 5) 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," *J. Appl. Phys.* 73, 2338 (1993).
- 6) T. Kaneto, K. W. Kim, and M. A. Littlejohn, "Calculation of Minority Carrier Mobilities in Heavily-Doped p-Type Semiconductors in the Dielectric Function Formalism," *Phys. Rev. B* 47, 16257 (1993).
- 7) M. U. Erdogan, K. W. Kim, and M. A. Stroscio, "Effects of Band Mixing on Hole Tunneling Times in GaAs/AlAs Double-Barrier Heterostructures," *Appl. Phys. Lett.* 62, 1423 (1993).
- 8) 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," *Appl. Phys. Lett.* 63, 48 (1993).
- 9) 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," in *Phonon Scattering in Condensed Matter VII*, edited by M. Meissner and R. O. Pohl (Springer-Verlag, Berlin, 1993), Springer Series in Solid-State Sciences, Vol. 112, p. 341.
- 10) M. A. Stroscio and K. W. Kim, "Piezoelectric Scattering of Carriers from Confined Acoustic Modes in Cylindrical Quantum Wires," *Phys. Rev. B* 48, 1936 (1993).

Size dependence of the thermal broadening of the exciton linewidth in GaAs/Ga_{0.7}Al_{0.3}As single quantum wells

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We have studied the temperature dependence of the linewidth, $\Gamma(T)$, of the fundamental absorption edge in bulk GaAs and four GaAs/Ga_{0.7}Al_{0.3}As single quantum wells of different well width using photoreflectance. As a result of the size dependence of the exciton-longitudinal optical phonon interaction, the thermal broadening of the linewidth diminishes as the dimensionality and size of the system are reduced.

The coupling between photons and elementary excitations such as electrons and excitons is an important parameter in determining many of the electronic and optical properties of semiconductor microstructure. There has recently been considerable interest in the electron (exciton)-optical phonon coupling in reduced dimensional polar semiconductor systems such as heterojunctions,¹ quantum wells,²⁻¹² quantum wires,¹³ quantum boxes,³ and nanospheres.^{14,15} In these systems the electron (exciton)-optical phonon (Frohlich) interaction is affected not only by changes in the particle wave function due to the confining potential but also by changes in the longitudinal optical (LO) phonon modes caused by phonon confinement. Although there have been a number of theoretical treatments,^{1-5,10} there have been relatively few experimental results.⁶⁻¹² The time-dependent Raman scattering results of Kim and Yu⁶ and Tsen *et al.*⁷ on GaAs/GaAlAs multiple quantum wells (MQWs) of different well widths (L_z) were explained in terms of confinement of both the electrons and optical phonons in the quantum wells. Interband relaxation in GaAs/GaAlAs MQWs has been detected by an infrared bleaching technique.¹⁰ The size dependence of the exciton-LO phonon coupling in CdSe¹⁴ and CuCl¹⁵ nanospheres has been reported.

Coupling to LO phonons also can be evaluated by studying the temperature dependence (thermal broadening) of the linewidth, $\Gamma(T)$, of the fundamental absorption edge in reduced dimensional systems.^{8,9,11,12} In both bulk¹⁶⁻¹⁸ and low-dimensional systems^{5,8,9,11,12,18-21} the dominant mechanism for thermal broadening is the interaction with the LO phonon. Thus, $\Gamma(T)$ can be described by a Bose-Einstein relation which contains a coupling constant (Γ_{ep}) and an occupation number.^{5,8,9,16-21} Several workers have measured $\Gamma(T)$ for the fundamental conduc-

tion to heavy-hole intersubband excitonic transition (11H) in GaAs/GaAlAs MQWs^{8,9,19,20} and an In_{0.21}Ga_{0.79}As/GaAs²¹ single quantum well (SQW), and have extracted values of Γ_{ep} . However, these authors did not present firm conclusions concerning the dimensionality dependence of Γ_{ep} . This is probably because these studies were (a) not systematic and (b) Γ_{ep} for the bulk constituent material of the well was not known. In II-VI quantum wells a dimensionality dependent reduction in Γ_{ep} was observed when the exciton binding energy became larger than the LO-phonon energy.^{11,12}

In this letter we report a systematic photoreflectance (PR)²² study of the temperature dependence ($10\text{ K} < T < 500\text{ K}$) of $\Gamma(T)$ of the fundamental absorption edge of bulk GaAs (E_0) and 11H of four molecular-beam-epitaxy-grown GaAs/Ga_{0.7}Al_{0.3}As SQWs with different L_z . We have observed a monotonic decrease of Γ_{ep} with reduced dimensionality and size. The value of Γ_{ep} for E_0 of bulk GaAs is considerably larger than Γ_{ep} of our four GaAs/GaAlAs SQWs and the GaAs/GaAlAs MQWs reported in Refs. 8, 9, 19, and 20. In our four GaAs/GaAlAs SQW samples, it is found that Γ_{ep} scales linearly with L_z . We interpret our observations as evidence for the size dependence of the electron (exciton)-LO phonon interaction in reduced dimensional systems.

Shown by the solid lines in Fig. 1(a) are the photoreflectance (PR) traces of bulk GaAs in the region of E_0 for $T = 10, 80, 293$, and 465 K . To facilitate comparison of the spectra at different temperatures, we have taken the zero of energy of each scan to lie at the energy of E_0 . The dashed lines are least-squares fits to a first-derivative Gaussian line shape (FDGL) function.²² This fit has enabled us to accurately determine E_0 , as indicated by the arrows, as well as the quantity of interest, $\Gamma(T)$. The numbers next to the arrows are E_0 in meV. The first-derivative nature of the line shape is indicative of an exciton;²³ band-to-band transistors would produce a third-derivative spectrum.²²

The PR signals from the SQW with $L_z = 60\text{ \AA}$ in the

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Dielectric response functions of heavily doped zincblende semiconductors with finite particle lifetime

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The dielectric response functions in the valence bands and in the conduction band of heavily doped zincblende semiconductors have been evaluated using the self-consistent field method and incorporating the *finite* lifetime of particles in the relaxation time approximation. Scattering rates of injected electrons are calculated with the Born approximation in the dielectric response function formalism at *finite* temperature. The finite particle lifetime introduces significant modifications to the spectral density function $\{\text{Im}[-1/\epsilon(q, \omega)]\}$ at small q , where collective excitations (i.e., coupled phonon-plasmon modes) are heavily damped due to collisions. However, these modifications are small at large q . At the same time, the scattering rates of injected electrons are strongly affected by the temperature dependence of these effects, which are particularly significant for *p*-type semiconductors.

I. INTRODUCTION

A heavily doped semiconductor is an important medium for studying a many particle system since its effective interparticle radius (r_e) is usually smaller than that for metals, even though the particle density is also much smaller. Correct models of hot carrier relaxation and electron transport in a many particle system are important for emerging optical and high speed electronic devices. For example, electron transport in the base region is one of the critical factors which limits the maximum switching speed of heterojunction bipolar transistors (HBTs) and hot electron transistors. Quasiballistic electron transport in such devices has been reported recently.¹⁻³

It is well known that the dynamic response of a free electron gas is described by the Lindhard dielectric function in the random phase approximation (RPA) or in the self-consistent field (SCF) approach when the electron lifetime is infinite ($\tau = +\infty$).^{4,5} In polar semiconductors, the coupling between longitudinal-optical (LO) phonons and the free carrier system is fundamental to carrier relaxation, carrier transport, and optical phenomenon.⁶ The electron gas-LO phonon coupling has been studied extensively by many authors and theoretical modeling in this context has been applied to a variety of electron device simulations.⁶⁻¹¹ Also, properties of the electron-phonon interaction have been studied experimentally by Raman scattering¹² and far-infrared reflectivity measurements.¹³

On the other hand, the dielectric response function for a hole gas has not been widely studied due to the difficulty of achieving an exact formulation for the valence bands which have $p^{3/2}$ -like symmetry in zincblende semiconductors. In most calculations, simplified models have been adopted which assume either a single valence band (which neglects the light hole band and the $p^{3/2}$ -like symmetry), or another "damped plasmon" model which includes a phe-

nomenological model for the Landau damping.¹⁴ Actually, interband transitions within the valence band have a significant effect on the dielectric function, particularly for degenerate conditions.¹⁵⁻¹⁷ Recently, Yevic and Bardyszewski evaluated the Lindhard dielectric function for a *p*-type semiconductor at finite temperature using the first order $k \cdot p$ expansion in the two-valence-band model.^{18,19} These authors showed that the structure of the spectral density function at elevated temperatures is quite different from that at zero temperature. They also showed that the scattering rates of minority electrons are dramatically increased at lower energies due to the energy absorption process at higher temperature.

However, prior to our current study, the dielectric response function has not been evaluated properly with a finite particle lifetime. The usual method uses $\tau = +\infty$ as in Ref. 4, even for finite temperature where scattering is usually important. This approximation is invalid, especially when dealing with heavily doped semiconductors, since the Lindhard function does not give a correct dc conductivity which is characterized by a (rather small) relaxation time. This inconsistency can be neglected only when we are treating the high frequency regime, such as a high energy plasmon in metals. Inherently, the Lindhard dielectric function incorporates the effects of single particle excitation (Landau damping) including both intraband and interband transitions. However, it does not account for the finiteness of particle lifetime (i.e., a finite mean time between collisions) resulting from, e.g., impurity scattering and phonon scattering. At finite temperature, these effects are very important since broadening of states due to collisions act to relax momentum conservation in intraband and interband transitions, resulting in significant changes in the dynamic response function. In heavily doped semiconductors, impurity scattering plays a major role in decreasing the particle lifetime at low temperature, while phonon scattering is important at higher temperature. In either case, the collision rate for a quasiparticle is quite frequent ($> 10^{13} \text{ s}^{-1}$) and in general this value tends to

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Reduction of inelastic longitudinal-optical phonon scattering in narrow
polar-semiconductor quantum wells

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ABSTRACT

In this paper, it is demonstrated that establishing metal-semiconductor interfaces at the heterojunctions of polar semiconductor quantum wells introduces a set of boundary conditions that dramatically reduces or eliminates unwanted carrier energy loss caused by interactions with interface longitudinal-optical (LO) phonon modes.

1. INTRODUCTION

It is now generally known that interface LO phonons, also known as surface-optical (SO) phonons, are established at the semiconductor-semiconductor boundaries of quantum wells.^{1,2} Furthermore, for carrier energies in excess of the interface LO-phonon energy, recent findings³ indicate that the inelastic scattering caused by carrier-interface-phonon interactions dominates over other scattering mechanisms when quantum-well confinement occurs on a scale of about 100 Å or less. Motivated by the predicted enhancement in carrier-interface-phonon coupling as well as by the recently demonstrated technology for the epitaxial growth of metals in intimate contact with polar-semiconductors,⁴⁻⁶ Stroscio et al.⁷ have applied the dielectric continuum model of interface phonon modes to determine the carrier-interface-phonon interaction Hamiltonian near a semi-infinite metal-polar-semiconductor interface.^{1,2} Detailed microscopic calculations of interface modes in polar semiconductors indicate that the dielectric continuum model provides an accurate formalism for modeling carrier-interface phonon modes.⁸ Based on this dielectric continuum model for LO phonons in polar-semiconductor quantum wells, it is demonstrated that inelastic carrier-interface-phonon scattering is dramatically reduced for narrow (less than 100 Angstroms) polar-semiconductor quantum wells with metal-semiconductor heterointerfaces. The dramatic reduction in carrier-interface-phonon scattering reported in this paper is expected to be important in a variety of nanoscale and mesoscopic devices which incorporate quantum-well elements.

**Confined and interface optical phonons in
quantum wells and quantum wires**

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ABSTRACT

As device dimensions in nanoscale structures and mesoscopic devices are reduced, the characteristics and interactions of dimensionally-confined longitudinal-optical (LO) phonons deviate substantially from those of bulk polar semiconductors. This account emphasizes the properties of LO-phonon modes arising in polar-semiconductor quantum wells and quantum wires. In particular, this review highlights recent results of both microscopic and macroscopic models of LO phonons in polar-semiconductor quantum wells and quantum wires with a variety of cross sectional geometries. Emphasis is placed on the dielectric continuum model of confined and interface phonons. In addition, this review provides brief discussions of how carrier-LO-phonon interactions change in the presence of dynamical screening. Finally, the use of metal-semiconductor heterointerfaces to reduce unwanted inelastic scattering in nanoscale electronic and optoelectronic structures is discussed.

1. INTRODUCTION

In nanoscale and mesoscopic systems, the effects of confinement on carriers have been studied extensively. However, to properly model carrier energy loss

Reduction of interface phonon modes using metal-semiconductor heterostructures

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Based on a simplified analysis of perfectly conducting metals, it has been suggested qualitatively that establishing metal-semiconductor interfaces at the heterojunctions of polar semiconductor quantum wells introduces a set of boundary conditions that dramatically reduces or eliminates unwanted carrier energy loss caused by interactions with interface longitudinal-optical (LO) phonon modes. In this article, it is theoretically demonstrated that comparable reductions in LO phonon scattering strengths may be achieved for metal-semiconductor structures with metal having realistic conductivities and Thomas-Fermi screening lengths.

I. INTRODUCTION

In recent years it has become clear that carrier interactions with longitudinal-optical (LO) phonon modes in heterostructures are strongly affected by the changes in the Frölich Hamiltonian caused by phonon confinement and localization.¹⁻⁶ Of special importance to the field of nanoscale device physics is the discovery that carrier-LO phonon scattering in narrow quantum wells may be determined by the interaction between carriers and interface LO phonons established near heterojunctions.⁷⁻¹⁰ Indeed, for typical phonon wave vectors of $0.02 \text{ \AA}^{-1}$, carrier scattering by interface LO phonons may dominate over that by confined LO phonons in multiple quantum well structures for well widths of about $100 \text{ \AA}$ or less.⁷ In numerous nanoscale structures and devices, the trends to greater complexity and higher speed lead to the simultaneous requirements for reduced structural dimensions and minimal inelastic scattering. The enhancement of inelastic carrier-interface-phonon scattering with decreasing structural size is contrary to the desired trend for a wide class of nanoscale structures.^{11,12}

Recent advances in epitaxial growth technologies for metallic and compound semiconductor structures have made possible the fabrication of nanostructures containing metal-semiconductor heterojunctions with highly uniform interfaces.¹³⁻¹⁶ As an example, these techniques have been applied to fabricate metallic quantum wells surrounded with barriers composed of polar semiconductors.^{13,14} These techniques open the way to grow a wide variety of nano-

scale structures which incorporate metal-semiconductor interfaces.

Motivated by the recently demonstrated technology for epitaxial growth of metals in intimate contact with polar semiconductors, Stroscio *et al.*^{10,17} have applied the dielectric continuum model of interface phonons to determine the carrier-interface-phonon interaction Hamiltonian for carriers in a polar semiconductor near the interface between a semiconductor and an ideal metal with infinite conductivity and vanishing Thomas-Fermi screening length. Based on this model, it has been demonstrated that phonon modes may be tailored through the judicious use of metal-semiconductor interfaces in such a way as to reduce unwanted inelastic scattering due to interface LO phonons.

In this article, the previous qualitative model for interface LO phonons at heterojunctions between semiconductors and ideal metals^{10,17} is extended through an approximate mathematical treatment to the case of metals with finite conductivity and finite, frequency-independent Thomas-Fermi screening lengths. It is demonstrated for the first time that the previous model does indeed provide useful approximate results. Specific results presented in this article include the interface LO phonon potentials and dispersion relations for metal-semiconductor-metal (M-S-M) structures. In this article the GaAs-metal system has been used to illustrate the concept of reducing the strength of interface LO phonons through the use of metal-semiconductor boundaries; in practice, however, other polar semiconductor-metal combinations such as InAs-Al may be more attractive for applications since the Fermi

Calculation of minority-carrier mobilities in heavily doped *p*-type semiconductors in the dielectric-function formalism

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An alternative approach for the calculation of minority-carrier mobilities is proposed. This approach is based on the self-consistent-field (SCF) method, and it combines elementary excitation theory with an appropriate transport theory beyond the relaxation-time approximation. Detailed information on elementary excitations of majority holes at *finite* temperature is obtained from the spectral density function ($\text{Im}[-1/\epsilon(q, \omega)]$) derived by the SCF method. Also, the *finite* lifetime of holes has been incorporated and a suitable form for the coupling of longitudinal-optical phonons, plasmons, and single-particle excitations is described. We have calculated minority-carrier mobilities for *p*-type GaAs and *p*-type Si, which show excellent agreement with available experimental data for a wide range of hole concentrations. Suggestions for improvements to this approach are described.

I. INTRODUCTION

Minority electron mobility in heavily-doped semiconductors is an important macroscopic quantity in many applications and several issues concerning this physical property of semiconductors remain to be resolved. Evaluation of minority-carrier mobility is a nontrivial problem, both experimentally and theoretically. Increasing data for minority electron mobility have become available in recent years, especially for GaAs. These data have been obtained from sophisticated experiments such as the time-of-flight measurement¹⁻⁵ and the common-emitter cutoff frequency measurement with adequately fabricated heterojunction bipolar devices,⁶⁻⁸ in addition to other experimental methods.⁹⁻¹¹ Experiments for Si are fewer in number.¹²⁻¹⁴

Theoretical calculations of the minority electron mobility for GaAs were first made by the variational method.¹⁵ Recently, Monte Carlo simulations have also been applied.¹⁶⁻¹⁸ However, as pointed out by Beyzavi *et al.*, the calculated mobility does not agree well with their experimental data, either at room temperature or at low temperature.⁸ At room temperature, the observed minority electron mobility is as much as a factor of 2 below the ionized impurity-dominated value. As temperature decreases, the experimental mobility increases much more sharply than the theoretical prediction. The variational method and Monte Carlo simulations are both effective for the calculation of carrier mobilities when the scattering mechanisms are described correctly. In earlier theories, electron-hole scattering was calculated by the same formula as that used for ionized impurity scattering in the center-of-mass coordinate system, and plasmon scattering was neglected. This approximation loses validity for fully degenerate conditions since hole transitions are strongly prohibited by the Pauli exclusion principle, while the collective excitation (i.e., plasmon) comes into play.

Minority electron transport should be described by the appropriate application of the many-body theory. The

significant many-body effects are dynamical screening and collective excitations. Very recently, Lowney and Bennett showed a refined calculation of majority- and minority-carrier mobilities for GaAs (Ref. 19) and Si.²⁰ They incorporated plasmon scattering in the variational method, and applied phase-shift corrections beyond the Born approximation for ionized impurity scattering and minority-carrier-majority-carrier scattering, where the Pauli exclusion principle for majority carriers was approximated by removing those states with energies below the Fermi energy. Also, Fischetti reported a detailed study of the effects of plasmon scattering on the majority- and minority-carrier mobilities along with a phase-shift analysis for ionized impurity scattering in Si.²¹ In these calculations, the effects of interband transition of holes were neglected and the Bohm and Pines approach of introducing a wave-vector cutoff²² was adopted for the electron-hole interaction. As pointed out by Rorison and Herbert in their study of the electron-electron interaction using the random-phase approximation (RPA), the concept of wave-vector cutoff in *n*-type semiconductors becomes invalid as the carrier density is lowered.²³ In heavily-doped *p*-type semiconductors, the definition of a cutoff wave vector for hole plasmons becomes more ambiguous due to the extended and complicated Landau damping region. The dynamical response of a hole gas is significantly affected by interband transitions between the heavy-hole band and the light-hole band.^{24,25} In addition, our recent work²⁶ has demonstrated the importance of collision damping of coupled collective excitations due to finite hole lifetime, i.e., the short interval time between scattering events. The resulting damped plasma modes are coupled to longitudinal-optical (LO) phonons in zinc-blende semiconductors. Coupling of hole-plasmon-LO-phonon modes and the broadening of these modes in *p*-type GaAs have been observed experimentally by Raman scattering.²⁷⁻²⁹ Major issues which need to be addressed in minority electron mobility calculations include (i) electron-hole interactions related to the interband hole transitions within the valence bands and (ii) the

Effects of band mixing on hole tunneling times in GaAs/AlAs double-barrier heterostructures

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The tunneling time of holes in GaAs/AlAs double-barrier heterostructures is calculated within the envelope function approximation, including band-mixing effects. The phase delay time is obtained from the energy derivative of the total phase shift of the wave function upon tunneling. The results show clearly that mixing plays a very important role in hole tunneling. In particular, our study suggests that the conventional effective mass models (without band mixing) can significantly overestimate the heavy hole tunneling time and thus are not suitable for estimation of the hole tunneling time. It is also demonstrated that the effect of band mixing on hole tunneling times becomes more important for thicker barriers.

The properties of double-barrier structures have received much attention since they were first proposed by Tsu and Esaki.¹ These structures are potentially useful as ultrahigh speed devices for application in high frequency detection, mixing, and oscillations.² The time associated with the tunneling of carriers has been an important issue because the ultimate device response appears to be directly related to it.³⁻⁵ Up to now, most of the attention in tunneling devices has been paid to electrons due to their expected fast response compared to holes. However, it is important to understand the tunneling time of holes in optoelectronic devices, such as coupled quantum well modulators,⁶ since both electrons and holes are involved in the operation. The device speed is limited by the transfer time of the slowest carrier. Thus, it is holes, not electrons, that dominate the frequency response in these devices. At the same time, hole tunneling is a physically interesting subject due to the degeneracy at the top of the valence band and the resulting complicated band structure, which gives rise to band mixing and tunneling through different channels originating from heavy hole (hh) and light hole (lh) states.

In the theoretical treatment of tunneling, it is generally assumed that transmission properties for nonzero $k_{\parallel}$ (the carrier momentum component in the plane of layers) are the same as for $k_{\parallel}$ equal to zero. Unlike the case for electrons, however, the tunneling time estimated for holes from conventional independent effective mass models do not agree with the experimental results. While the simple theories predict much longer tunneling time due to the large effective mass of heavy holes, experiments show that tunneling times for holes are comparable to those of electrons.^{7,8} This discrepancy may be explained by using a more realistic band structure which considers band-mixing effects for holes.⁹ The assumption of $k_{\parallel} = 0$ is not appropriate due to the strong mixing of hh and lh states in the presence of sizable nonzero $k_{\parallel}$ (on the order of lattice thermal energy $k_B T$ or Fermi wave vector). In this letter, we present a calculation of phase tunneling times for heavy

holes and light holes in double-barrier resonant tunneling heterostructures with a realistic (valence) band obtained by a $\mathbf{k} \cdot \mathbf{p}$ method. Our study emphasizes the importance of realistic band structure and band mixing in hole tunneling and demonstrates that the conventional theories with effective mass are not suitable for the calculation of tunneling times for holes.

For band structure calculations in a double-barrier heterostructure, we use the Luttinger-Kohn Hamiltonian in the envelope-function approach.¹⁰⁻¹² By applying a unitary transformation, the 4×4 Luttinger-Kohn Hamiltonian is block diagonalized with two 2×2 matrices. For a symmetric structure, the solutions for both upper and lower blocks are degenerate and, therefore, we need to solve only one of the following 2×2 Hamiltonians:

$$H^{U,L} = \begin{bmatrix} P \pm Q + V(z) & \bar{R} \\ \bar{R}^\dagger & P \mp Q + V(z) \end{bmatrix}, \quad (1)$$

where U (or L) refers to the upper (or lower) signs, and

$$\begin{aligned} P &= (\hbar^2 \gamma_1 / 2m) (k_x^2 + k_y^2 + k_z^2), \\ Q &= (\hbar^2 \gamma_2 / 2m) (k_x^2 + k_y^2 - 2k_z^2), \\ R &= -(\hbar^2 \gamma_2 / 2m) \sqrt{3} (k_x^2 - k_y^2) + i(\hbar^2 \gamma_3 / 2m) 2\sqrt{3} k_x k_y, \\ S &= (\hbar^2 \gamma_3 / 2m) 2\sqrt{3} (k_x - ik_y) k_z, \\ \bar{R} &= |R| - i|S|. \end{aligned} \quad (2)$$

In this treatment, $V(z)$ is the potential for each region including the external field; γ_1 , γ_2 , and γ_3 are the Luttinger parameters; m is the free electron mass; and k_x , k_y , and k_z are the hole momentum components in each direction. The z -axis is chosen as the growth direction. For a given $k_{\parallel}$ and E , eigenfunctions of the Luttinger-Kohn Hamiltonian in each region are calculated. After taking a linear combination of the bulk solutions, continuity and current conserving boundary conditions are applied. For $k_{\parallel} = 0$ (i.e., $k_x = k_y = 0$), the Hamiltonian is diagonal and, as a result, there is no mixing between the light holes and heavy holes.

A comparison of minority electron transport in $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ and GaAs

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The electron transport properties of heavily doped p -type $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ and GaAs have been investigated and the applications in heterojunction bipolar transistors (HBTs) are emphasized. Using the dielectric function formalism, we have characterized minority electron transport in terms of mean-free path and diffusivity. These parameters quantify the nonequilibrium (ballistic) and near-equilibrium (diffusive) transport in the p -type base region of HBTs. Our calculations demonstrate that electron energies above 300 meV provide no benefit for ballistic transport in p -type InGaAs in terms of momentum relaxation mean-free path. Especially for very heavily doped cases ($\sim 10^{20} \text{ cm}^{-3}$), low-energy electron injection into the p -type InGaAs base is more advantageous for base transport, as well as the succeeding transport in the base-collector depletion region. When diffusive transport is dominant, p -type InGaAs exhibits superior performance over GaAs for a wide range of doping concentrations.

Heterojunction bipolar transistors (HBTs) using $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ (abbreviated as InGaAs in this letter) for the base have achieved cutoff frequencies as high as 165 GHz.¹ This impressive performance is attributed to the effective electron injection and transport in the base and base-collector regions of the device. Two typical conditions for minority electron transport in the p -type base regions of HBTs are ballistic transport and diffusive transport. When the abruptness of the emitter-base junction is completely removed by grading, electrons are thermally injected into the base region and their "diffusivity" is important. On the other hand, if all or part of the conduction-band discontinuity is present, electrons are launched ballistically with high forward momentum, and the transit time in the base region is expected to be reduced.² The well-known advantages of InGaAs over GaAs are the smaller Γ -valley effective mass, the larger Γ - L energy band separation, and the smaller surface recombination rates.²

Electron transport in p -type semiconductors is complicated by the dynamical response of the hole gas, which involves interband transitions between the heavy-hole band and the light-hole band.³ The coupling of hole plasmons and longitudinal-optical (LO) phonon modes and the resultant broadening of these modes in p -type GaAs and AlGaAs have been observed by Raman scattering experiments.⁴ The dielectric function formalism is best suited for describing such complex mode coupling behavior. Evaluation of the valence-band dielectric function at finite temperature was first done by Yevic and Bardyszewski for p -type GaAs.⁵ Recently, we have developed a more realistic dielectric function for the valence bands, which incorporates collision damping of coupled collective excitations due to finite hole lifetime.⁶ In addition, a new approach for the calculation of minority carrier mobility has been proposed by combining elementary excitation theory and appropriate transport theory.⁷

The ballistic and diffusive nature of minority electron

transport in the base region can be characterized in terms of mean-free path (for nonequilibrium transport) and diffusivity (for near-equilibrium transport), respectively. The momentum relaxation mean-free path (MMFP) is defined by $l_m(E_k) = v(k)\tau_m(E_k)$, where $v(k)$ is the electron velocity, $\tau_m(E_k)$ is the momentum relaxation time, and E_k is the electron energy in the conduction band. Electron velocity is given by $v(k) = \hbar k / m^*(1 + 2\alpha E_k)$, which is obtained from the spherical band approximation with first-order nonparabolicity, i.e., $\hbar^2 k^2 / 2m^* = \gamma(E_k) = E_k(1 + \alpha E_k)$, where m^* is the effective mass at the bottom of the conduction band and α is the band nonparabolicity parameter. Here, we have assumed that $m^* = 0.041m_0$ ($0.07m_0$) and $\alpha = 1.33$ (0.64) eV^{-1} for InGaAs (GaAs), respectively. The momentum relaxation time $\tau_m(E_k)$ is defined as

$$\frac{1}{\tau_m(E_k)} = \frac{1}{8\pi^3} \int W_{kk'} \left(1 - \frac{v(k')}{v(k)} \cos \theta \right) dk', \quad (1)$$

where $W_{kk'}$ is the scattering rate from k to k' and θ is the angle between k and k' .

The dominant scattering mechanisms in p -type polar semiconductors are ionized impurity scattering and inelastic scattering due to the coupled LO-phonon-plasmon excitation and single hole excitation (i.e., Landau damping). We have also considered acoustic phonon scattering⁸ and alloy scattering⁹ (in InGaAs) for completeness. Thus, the total momentum relaxation time is given as the sum of the individual contributions, i.e., $1/\tau_m(E_k) = \sum_i [1/\tau_i(E_k)]$. In the Born approximation, the momentum relaxation time due to ionized impurities is given by

$$\frac{1}{\tau_{\text{imp}}(E_k)} = \frac{4\pi N_i e^4 m^*(1 + 2\alpha E_k)}{\hbar^3 k^3} \int_0^1 \frac{d\eta}{\eta [\epsilon(2k\eta, 0)]^2}, \quad (2)$$

where $\epsilon(q, 0)$ is the static dielectric function, N_i is the density of ionized impurities, and $\eta = \sin \theta/2$ [θ is as defined in Eq. (1)]. We assume the compensation ratio is zero, i.e., $p = N_i$. The spectral density function {i.e., $\text{Im}[-1/\epsilon(q, \omega)]$ } is used to describe the inelastic scattering due to the excitation of the whole system coupled between the LO phonon and the hole gas. The momentum relaxation rate

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Reduction in the Longitudinal-Optical Phonon Emission Rate in Polar-Semiconductor Quantum Wires and Quantum Wells

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1. Introduction

This work addresses how confined and interface LO phonons in mesoscopic devices 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.

2. Longitudinal-Optical Phonons in Metal-Semiconductor Systems

As originally proposed by Sakaki [1], the predicted high mobilities of quasi-one-dimensional wire-like regions of semiconducting material underlie many proposed quantum-wire system concepts [2,3], and have resulted in pioneering efforts leading to the actual fabrication of quantum wires [4,5]. Recently, however, theoretical studies of the interaction between longitudinal-optical (LO) phonons and carriers in a polar-semiconductor quantum wire [6] have revealed the presence of discrete LO phonon modes similar to those identified earlier for polar-semiconductor quantum wells [7-9]. As for the case of quantum wells [9,10], interface LO phonons are established at the semiconductor-semiconductor boundaries of quantum wires [11]. In addition, for carrier energies in excess of the interface LO-phonon energy, the inelastic scattering caused by carrier-interface-phonon interactions dominates over other scattering mechanisms when quantum-well [12] or quantum-wire [11] confinement occurs on a scale for about 50 Å or less. Herein, it is indicated that establishing a metal-semiconductor interface at the lateral boundaries of confined polar-semiconductor dramatically reduces or eliminates unwanted carrier energy loss caused by the interactions with interface LO-phonon modes.

Motivated by the recently demonstrated technology for the epitaxial growth of metals in intimate contact with polar-semiconductors [13], Strosio et al. [14] have applied the dielectric continuum model of interface phonon modes [9,10] to determine the carrier-interface-phonon interaction Hamiltonian for carriers in a polar-semiconductor near a metal-semiconductor interface. It is demonstrated that [14] only those confined and interface modes of odd potential satisfy the correct boundary conditions at the metal-semiconductor interface. Hence, only those quantized LO phonon modes with vanishing potential at $z=0$ in a polar semiconductor slab bounded for $z < -a/2$ and for $z > a/2$ by polar semiconductors will be present in a polar semiconductor slab bounded for $z < 0$ by a perfect metal and for

Piezoelectric scattering of carriers from confined acoustic modes in cylindrical quantum wires

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Confined acoustic modes are derived for a free-standing nanometer-scale cylindrical polar semiconductor quantum wire. The piezoelectric scattering Hamiltonian is calculated for the interaction of charge carriers with the lowest-order azimuthally symmetric torsional modes in such nanometer-scale quantum wires.

Many proposed applications of mesoscopic electronic structures involve carrier transport at low temperatures and low carrier energies; frequently, the regime of interest is one where dimensional confinement modifies the phase space substantially. In this low-temperature, low-energy regime,¹⁻⁶ acoustic phonons play an enhanced role in carrier scattering and may dominate over the scattering of carriers by optical phonons. Furthermore, in nanometer-scale structures it is possible that phase-space restrictions may weaken or forbid optical-phonon scattering processes that would normally dominate in bulk structures. In recent years, there has been extensive literature on the role of dimensional confinement in modifying optical-phonon modes and their interactions with charge carriers (see, for example, Refs. 7-11 and the numerous references therein). However, there are relatively few treatments dealing with the role of dimensional confinement in modifying acoustic-phonon modes and their interactions with charge carriers.²⁻⁴ While there is extensive literature on the theory of acoustic modes in conventional waveguides, resonators and related structures,⁵ no efforts have been reported to formulate a theory of acoustic phonons in nanometer-scale structures where both phonon confinement and a quantum-mechanical treatment of phonon normalization are both essential; Constantinou has, however, discussed the unnormalized acoustic-phonon modes in cylindrical polar semiconductor quantum wires.¹²

In this paper, the general piezoelectric polarization vector is derived in terms of the acoustic-phonon mode displacements in free-standing cylindrical quantum wires fabricated of zinc-blende polar semiconductors. By taking an approach analogous to the dielectric continuum theory of confined optical phonons, the proper quantum-mechanical technique of normalizing such acoustic-phonon modes is illustrated and the piezoelectric scattering Hamiltonian is calculated for the interaction of charge carriers with the lowest-order azimuthally symmetric torsional modes in nanometer-scale quantum wires of both infinite and finite length (i.e., quantum dots or boxes).

The piezoelectric tensor relating the piezoelectric polarization vector and the acoustic strain tensor may be expressed in matrix notation⁵ for the case of a zinc-blende crystal in rectangular coordinates as

$$\tilde{\epsilon} = \begin{pmatrix} 0 & 0 & 0 & e_{x4} & 0 & 0 \\ 0 & 0 & 0 & 0 & e_{x4} & 0 \\ 0 & 0 & 0 & 0 & 0 & e_{x4} \end{pmatrix}.$$

The piezoelectrically induced electric polarization vector $\mathbf{P}$ is given in terms of $\tilde{\epsilon}$ by the matrix equation,

$$\mathbf{P} = \tilde{\epsilon} \mathbf{S},$$

where $\mathbf{P}$ is a three-component vector,

$$\mathbf{P} = \begin{pmatrix} P_1 \\ P_2 \\ P_3 \end{pmatrix},$$

and $\mathbf{S}$ is the six-component strain vector with components,⁵

$$S_1 = S_{rr} = \frac{1}{i\omega} \frac{\partial v_r}{\partial r},$$

$$S_2 = S_{\phi\phi} = \frac{1}{i\omega} \left[\frac{v_r}{r} + \frac{1}{r} \frac{\partial v_\phi}{\partial \phi} \right],$$

$$S_3 = S_{zz} = \frac{1}{i\omega} \frac{\partial v_z}{\partial z},$$

$$S_4 = 2S_{z\phi} = \frac{1}{i\omega} \left[\frac{\partial v_\phi}{\partial z} + \frac{1}{r} \frac{\partial v_z}{\partial \phi} \right] = 2S_{\phi z},$$

$$S_5 = 2S_{rz} = \frac{1}{i\omega} \left[\frac{\partial v_r}{\partial z} + \frac{\partial v_z}{\partial r} \right] = 2S_{zr},$$

$$S_6 = 2S_{r\phi} = \frac{1}{i\omega} \left[\frac{1}{r} \frac{\partial v_r}{\partial \phi} + \frac{\partial v_\phi}{\partial r} - \frac{v_\phi}{r} \right] = 2S_{\phi r},$$

where $\mathbf{v}$ is the velocity associated with the acoustic-phonon displacement $\mathbf{u}$ and ω is the harmonic frequency assumed for the phonon field; that is, $\mathbf{v} = i\omega \mathbf{u}$. To cast $\tilde{\epsilon}$ into a form suitable for a cylindrical quantum wire, it is necessary to express $\tilde{\epsilon}$ in a more general form where the coordinate axes are rotated with respect to the principal axes of the crystal. Upon applying the rotation transformation matrices of Auld⁵ to the case of rotation by an angle ϕ about the z axis ([100] axis),