Microscopic calculation of electric field effects in GaAs/$Al_xGa_{1-x}As$/GaAs tunnel structures

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The combined effects of an applied electric field and the inherent crystal band structure on the tunneling of electrons through $Al_xGa_{1-x}As$ barriers between field-free regions of GaAs are presented. A microscopic pseudopotential-based calculation is used. It includes the effect of all the higher conduction-band minima. We find that a finite field changes the electron tunneling probabilities and produces intervalley transfers if the energy of the tunneling particle is near a conduction-band minimum. The net result for direct-band-gap barriers is small, but for indirect-band-gap barriers a field-dependent transition region between a Γ behavior and an X behavior is found, with the electron transferred from an evanescent Γ state to a propagating X state in the barrier. The exact rate of transfer and proportion of the Γ and the X states' contributions to the total wave function is found to be strongly dependent on the exact composition of the barrier material.

The behavior of electronic states in semiconductor heterostructures with an electric field is of considerable interest, since in any experimental study or electronic device application of these systems voltage biases are required. In addition, electric field effects associated with the Γ-X mixing of the electronic states have recently been observed in optical[1-4] and transport[5-7] measurements in GaAs/$Al_xGa_{1-x}As$ structures. This Γ-to-X transfer (or indeed X-to-Γ) may occur either at a heterojunction interface[8-10] or be the result of an applied potential since in both cases the translational symmetry of the system is broken. In a heterostructure system it has been suggested[11] that this real-space intervalley transfer may change the electron inelastic-scattering rate. For the purposes of the production of ballistic transport devices the understanding of this combined band-structure and electric field effect is important, especially with the growing evidence of unusually long electron inelastic mean free paths, of the order of 1000 Å, in III-V heterostructures.[11,12] Also the possibilities of a type-I–to–type-II transition under the application of even a small bias potential[1] may result in some interesting optical behavior in superlattice systems.

Theoretically, however, the understanding of the band-structure contributions to the electronic states in semiconductor heterostructures has relied on calculations carried out in the flat-band field-free limit.[8-10,13,14] When the electric fields are included the analysis has been restricted to continuum or effective-mass models,[15-17] where the full band structure of the material is absent. In fact, there appears to be very little theoretical work on the combined effects of a macroscopic electrostatic potential and a microscopic crystal potential on the electronic states in heterostructures or bulk materials. The principal difficulty of any such analysis is how to incorporate an electrostatic potential which extends over the entire system and maintain a microscopic description of the crystal potential, since the latter's characteristic length scale is only a few angstroms. Superlattice "supercell" calculations are inappropriate, since there is no natural periodicity with an applied electric field, and only superlattice eigenstates are obtained. Standard transfer-matrix methods are also unsuitable since in order to maintain numerical stability they must truncate the growing exponential solutions.[9,13,14] Yet what one is interested in is just how these exponentially growing and decaying states may couple to the propagating states to produce a real-space intervalley transfer.

In this paper we present the results of a microscopic analysis of the combined band structure and electric field effects on the electronic states in single GaAs/$Al_xGa_{1-x}As$/GaAs tunneling barriers. The effects of electric fields in multiple-barrier systems and in superlattices will be presented elsewhere. We concentrate here on single wide-barrier systems for both direct- and indirect-band-gap materials, so that the crossover points of the different band-structure minima may be clearly separated.

The method we use is based on a combination of an empirical pseudopotential calculation from which the III-V materials' complex band structure are obtained,[8,9,13,14] and a scattering-matrix formulation for connecting the electronic states through the heterostructure.[8,14] The scattering-matrix formalism has the advantage that it remains stable for very large systems without having to truncate any growing exponentials. Thus the macroscopic length scale associated with wide barriers and finite electric fields no longer conflicts with the microscopic scale length of the electronic wave functions and the need to maintain numerical stability. The full details of the pseudopotential band-structure calculation and of the scattering-matrix formalism have already been published.[8,9,13,14] Briefly, the system is divided into a large number of sections and for a given electron energy the wave function is obtained as a superposition of the set of complex wave-vector Bloch states with that energy in each section. These are then matched at the interfaces between sections using a scattering-matrix formalism. We have used 26 basis states in each section in the construction of the total wave function. Electric fields are

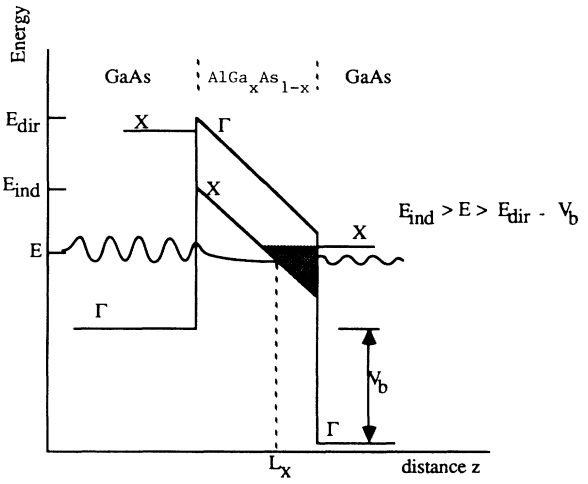

FIG. 1. Schematic representation of the tunneling situation, showing the relative positions of the energy bands for an indirect-band-gap $Al_xGa_{1-x}As$ barrier with an electron tunneling with energy in the intervalley transfer region (see text). The X well in the $Al_xGa_{1-x}As$ is shown as the shaded region in the diagram.

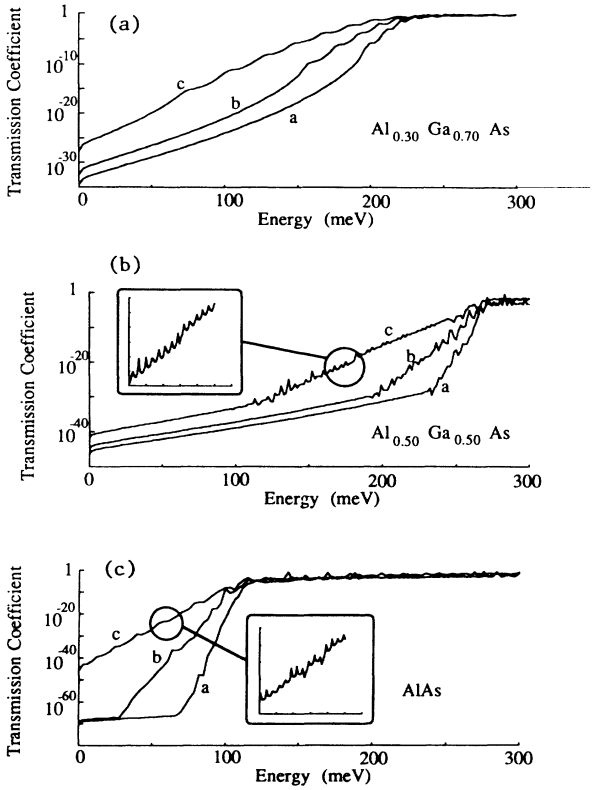

FIG. 2. Transmission coefficients vs energy for an electron tunneling through a single barrier with three different bias voltages, calculated using a many-band pseudopotential model. The barrier width is 100 layers (565 Å), the bias voltages are (a) 50, (b) 100, and (c) 200 meV. The results for a direct-band-gap barrier $Al_{0.30}Ga_{0.70}As$ and two indirect-band-gap barriers $Al_{0.50}Ga_{0.50}As$ and AlAs are shown.

treated in the calculation by dividing the electrostatic potentials into a number of energy steps. This method has been used successfully within the very much simpler effective-mass framework.[17] With the full pseudopotential basis we find that a typical potential-energy step size of ~ 8 meV is sufficient for the transmission coefficient and wave function to converge. In the calculations presented here we have used step sizes ranging from 1–5 meV.

Figure 1 illustrates the typical lineup of the energy bands for the tunneling structure, with an indirect-band-gap barrier shown. With a direct-band-gap barrier the positions of the Γ and the X bands in the barrier will be reversed. Remembering that the electronic states are evanescent for energies below the conduction-band edge and propagating otherwise, the tunneling situation may be divided into three regions. First, for low incident energies, $E < E_c - V_b$, where E_c is the lowest conduction-band offset ($E_c = E_{\text{ind}}$ for the situation shown in Fig. 1) and V_b is the bias voltage across the barrier, the energy of the particle will remain below the conduction-band edge of the barrier material throughout the barrier. A purely tunneling behavior is therefore expected with no finite field-induced intervalley transfer. Secondly, particles with energies in the range $E_c - V_b < E < E_c$ will cross the conduction-band edge of the barrier (in Fig. 1 this is at $z = L_X$). At the crossover point the tunneling particle changes from an evanescent state to a propagating state. It may then interfere with its reflection from the GaAs interface, producing structures in the electronic transmission. In addition, for an indirect-band-gap material as shown in Fig. 1, there will be an electric-field-induced intervalley transfer from an evanescent Γ state to a propagating X state at the crossover point. And since the X minima in GaAs are at a higher energy there will usually be a region where the X states will be quasiconfined in the alloy layer (the shaded region in Fig. 1). It would therefore be possible for resonant tunneling to occur via the quasibound barrier X levels. The transmission through the barrier will therefore depend on both the Γ and X states. If the bias voltage is sufficiently large there can be a further crossover with a higher conduction-band minimum. For a direct band gap the electron will be crossing the X minima, and for an indirect-band-gap barrier it will be crossing the Γ minimum. Again, at the crossover point, an intervalley transfer is possible. Finally, for electron energies above the conduction-band edge ($E > E_{\text{ind}}$ in Fig. 1) propagating states will be available throughout the system and the electron will no longer be "tunneling" through the barrier. Consequently, near-unit transmission is expected.

We begin with the electronic transmission through a single 565-Å-wide $Al_xGa_{1-x}As$ barrier sandwiched between GaAs contacts. The transmission coefficient, defined as usual to be the ratio between the total transmitted current to the incident current, is plotted in Fig. 2 for different aluminum concentrations. The results for three different voltage biases across barriers, of 50, 100, and 200 meV, labeled a, b, and c, respectively, are shown for each system.

The results for the direct-band-gap material, $Al_{0.30}Ga_{0.70}As$, show the the electronic transmission increases monotonically for low electron energies, corre-

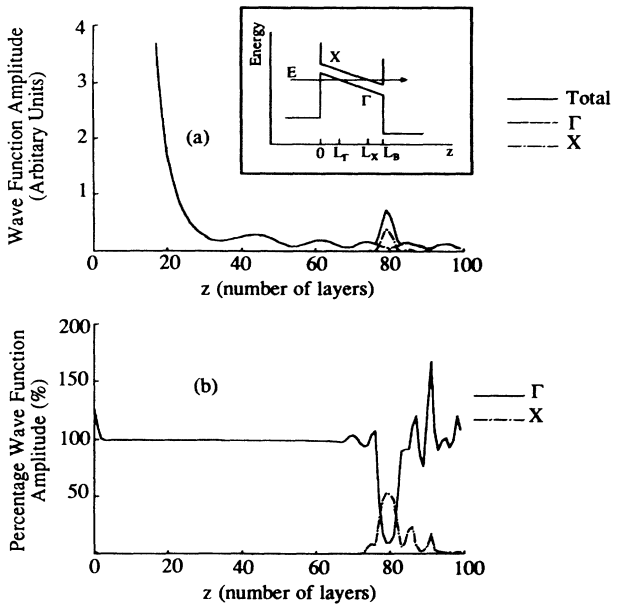

FIG. 3. (a) Wave-function amplitude in the barrier region for an electron tunneling through a single $Al_{0.30}Ga_{0.70}As$ barrier. The barrier width is 100 layers, and the bais voltage is 200 meV. The inset shows the relative positions of the energy bands, and L_Γ and L_X are at $z=30$ and 78 layers, respectively. (b) Percentage wave-function-amplitude contributions from the Γ and X states.

sponding to the purely tunneling regime previously discussed. For higher energies we find a set of shoulders in the transmission. From our band structure this system has a band offset $E_{\rm dir}$ of 230 meV. The energies of these shoulders all lie in the range $E > E_{\rm dir} - V_b$ and thus correspond to the second possibility considered previously, when the tunneling particle crosses the conduction band in the barrier. The shoulders therefore originate from the interference of the propagating state in the barrier with its reflection from the GaAs interface. Finally, for elec-

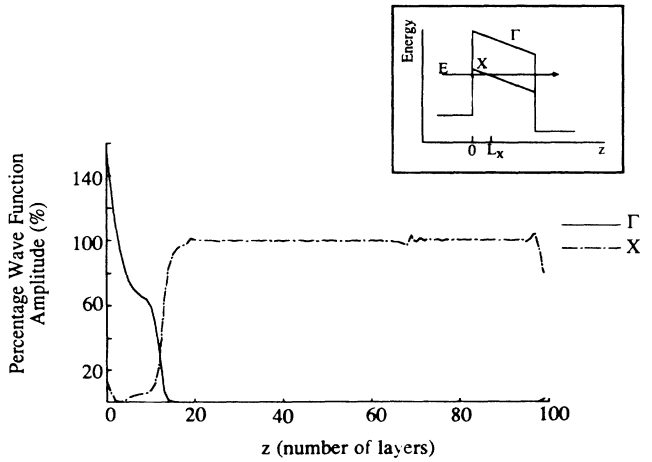

FIG. 4. The percentage wave-function-amplitude contributions from the Γ and X states for the wave function in an AlAs barrier. The inset shows the corresponding positions of the energy bands, with L_X occurring at $z=13$ layers.

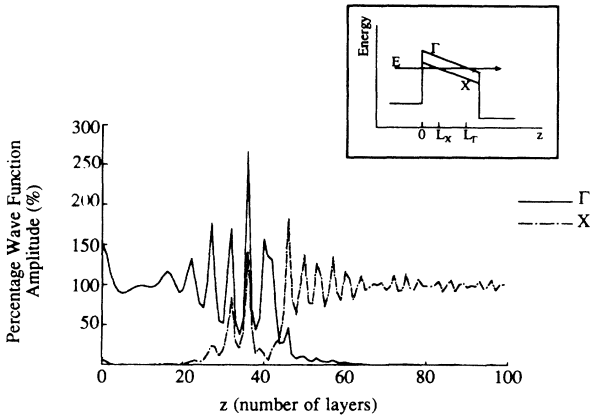

FIG. 5. The percentage wave-function-amplitude contributions from the Γ and X states for the wave function in an $Al_{0.50}Ga_{0.50}As$ barrier. The inset shows the corresponding positions of the energy bands, with L_X and L_Γ occurring at $z=12$ 50 layers, respectively.

tron energies greater than the barrier height ($E > E_{\rm dir}$) there is always a propagating state in the barrier and near-unit transmission is obtained. A comparison with a single nonparabolic band calculation using only the Γ state shows that the results of a single-band analysis are in good agreement with the many-band results presented here. Thus the behavior of the electronic transmission for a direct-band-gap barrier with a finite field is well described by a single-band model.

For the indirect-band-gap barriers, namely $Al_{0.50}Ga_{0.50}As$ and AlAs, we find a clear division of the electronic transmission into the three different regions discussed. For low incident energies ($E < E_{\rm ind} - V_b$) the results show a slow monotonic increase in the transmission coefficient which corresponds to the purely tunneling regime. Comparison with a nonparabolic single-band model shows that the behavior in this region is accurately reproduced by considering the evanescent Γ state only. The transition to the next region ($E_{\rm ind} - V_b < E < E_{\rm ind}$) is indicated by a sharp change in the gradient of the transmission coefficient. The size of this region, as expected, grows with increasing bias. Electrons tunneling with energy lying in this regime cross the X minima of the alloy material somewhere in the barrier and a finite field-induced Γ-to-X transfer is produced. In addition, the now propagating barrier X state is quasiconfined in the barrier layer (see Fig. 1) and the particle may resonantly tunnel via the quasibound X states. The result is a set of closely separated resonant peaks in the transmission, which are resolved and shown in the insets. The electronic states in this energy range are therefore a combination of the evanescent Γ and the propagating X states. Finally, for energies $E > E_{\rm ind}$ an X-dominated behavior is found with near total transmission, since the particle is no longer tunneling through the alloy layer.

Thus from the results in Fig. 2 we find that for a direct-band-gap barrier the field dependence of the electronic transmission is single-band-like, with a Γ-state dependence maintained throughout, even for high voltage biases where an X-minima crossover may be possible. For the indirect-band-gap barriers there is a clear transi-

tion region between the single-band Γ behavior for low electron energies and an X-dominated behavior for high electron energies. This region corresponds to the energy range where a tunneling Γ to a propagating X transfer may occur in the alloy material.

Since the actual degree of real-space intervalley transfer is better determined from the wave function of the electronic state in the barrier than from the transmission coefficient, we have shown in Fig. 3(a) the total wave-function amplitude of the electronic state at an energy of 170 meV in an $Al_{0.30}Ga_{0.70}As$ barrier where a bias of 200 meV is applied. We have also plotted with the dashed line the Γ-state wave-function amplitude and with the dotted-dashed line the X-state wave-function amplitude. The energy of the tunneling particle in relation to the various band-structure minima is given diagrammatically in the inset. The result shows that throughout most of the barrier region the particle's wave function is composed entirely of the Γ state, with an initial exponential decay corresponding to the tunneling region for $z < L_\Gamma$, leading to an oscillatory behavior with a decreasing amplitude for $z > L_\Gamma$. This is simply the type of behavior one expects.[18] At the crossover point with the barrier material's X minima ($z = L_X$) there is an enhanced amplitude to the total wave function. This is due to a peak in the X wave-function amplitude which until now has been negligible. Thus, at the crossover point with the X minima, the X states in the barrier are indeed strongly excited. However, as shown by the percentage contribution of the Γ and X states to the total wave-function amplitude [Fig. 3(b)], we find that once beyond the crossover point the Γ state remains dominant. The total amplitude is not given by the simple sum of the different states' amplitudes, indicating that the propagating Γ and X states still interfere strongly with each other. That is, the wave function beyond the crossover point is no longer described by a single state.

For the indirect-band-gap situations the particle will first cross the band-structure X minima. This is examined in Fig. 4 where the percentage contributions of the Γ and X states through an AlAs barrier with 200-meV bias are plotted. The electron energy is 89 meV. Again, the corresponding energy-band diagram is shown in the inset. We find that for the first layer or so of the barrier material the X states contribute about 10% to the total wave-function amplitude due to a Γ-to-X transfer at the interface. However, as a result of the large decay constant of the X states, within a few layers from the interface this X amplitude has decreased to zero, leaving only the Γ state to contribute to the particle's wave function. As we move across the barrier the tunneling particle's energy traverses the X minima of the AlAs (at $z = L_X$ in the inset) and a very sharp transition occurs. The wave function changes over in a region of two to three layers from being totally Γ-dominated to being totally X-dominated. The applied electric field has therefore induced an intervalley transfer of the tunneling electron. And because the Γ state in the AlAs is still evanescent for this energy throughout the barrier, the tunneling electron is entirely transferred into the propagating X state. Only at the far interface does a Γ contribution reappear, due again to interfacial scattering.

With a lower direct-band offset E_{dir} the situation becomes more complicated. This is illustrated in Fig. 5 where we have considered the $Al_{0.50}Ga_{0.50}As$ barrier. We have chosen an electron energy of 138 meV and a bias potential of 292 meV, so that as well as crossing the alloy X minima the tunneling particle also crosses the conduction-band Γ minimum in the barrier (see inset to Fig. 5). The results again show a 10% X-state contribution to the wave function at the first interface at $z = 0$, which then rapidly decays to zero. And as the X minima are approached, that is, for $z \approx L_X$, the X state is again excited as a result of the electric-field-induced intervalley transfer. The X states' contribution to the total wave function in this case increases gradually over a much larger distance, of the order of 20 layers (~ 100 Å), because of the slower decay rate of the Γ state and because the coupling between the Γ and X states leads to the interference oscillations observed. At the crossover with the Γ minimum at $z = L_\Gamma$ the electron wave function is almost entirely X-like and no appreciable transfer back to the Γ state in the barrier region is observed.

In conclusion, we have performed a fully microscopic calculation on the combined effects of the crystal band structure and finite electric fields on the electronic state in wide single-barrier heterostructures. We have found that electric-field-induced intervalley transfer occurs if the energy of the tunneling particle crosses a minimum in the band structure. For a direct-band-gap barrier, the electron is transferred from a propagating Γ state to a propagating X state, with the X-state excitation significant only at the crossover point. Since the spatial region where the crossover can occur decreases with increasing bias for direct-band-gap barriers, electric-field-induced intervalley transfer will be significant for low bias voltages only. For indirect-band-gap barriers the transfer is from an evanescent Γ state to a propagating X state. The rate of transfer is strongly dependent on the decay rate of the evanescent Γ wave function, with a very sharp transition if the Γ state decays rapidly. Ultimately the tunneling particle is transferred into the lowest band-structure minimum. The subsequent traversal of higher minima has little effect.

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[1]M.-H. Meynandier, R. E. Nahory, J. M. Worlock, M. C. Tamargo J. L. de Miguel, and M. D. Sturge, Phys. Rev. Lett. **60**, 1338 (1988).
[2]R. T. Phillips, N. R. Couch, and M. J. Kelly, Semicond. Sci. Technol. **2**, 828 (1987).
[3]M. Naganuma, T. Ishibashi, and Y. Horikoshi, J. Appl. Phys. **62**, 644 (1987).
[4]G. Danan, F. R. Ladan, F. Mollot, R. Planel, Appl. Phys. Lett. **51**, 1605 (1987).
[5]A. R. Bonnefoi, T. C. McGill, R. D. Burnham, and G. B. Anderson, Appl. Phys. Lett. **50**, 344 (1987).
[6]N. R. Couch, M. J. Kelly, T. M. Kerr, E. G. Britton, and W. M. Stobbs, Semicond. Sci. Technol. **2**, 244 (1987).
[7]E. E. Mendez, W. I. Wang, E. Calleja, and C. E. T. Gonçalves da Silva, Appl. Phys. Lett. **50**, 1263 (1987).
[8]D. Y. K. Ko, and J. C. Inkson, Semicond. Sci. Technol. **3**, 791 (1988).
[9]A. C. Marsh, Semicond. Sci. Technol. **1**, 320 (1986).
[10]H. Akera, S. Wakahara, and T. Ando, in Proceedings of the Seventh International Conference on Electronic Properties of Two-Dimensional Systems, Santa Fe, New Mexico, 1987 [Surf. Sci. **196**, 694 (1988)].
[11]J. R. Hayes, P. England, and J. P. Harbison, Appl. Phys. Lett. **52**, 1578 (1988).
[12]U. K. Reddy, J. Chen, C. K. Peng, and H. Morkoç, Appl. Phys. Lett. **48**, 1799 (1986).
[13]D. Y. K. Ko, and J. C. Inkson, J. Phys. C **20**, 4213 (1987).
[14]D. Y. K. Ko, and J. C. Inkson, Phys. Rev. B (to be published).
[15]K. F. Brennan, and C. J. Summers, J. Appl. Phys. **61**, 614 (1987).
[16]J. Bleuse, G. Bastard, and P. Voisin, Phys. Rev. Lett. **60**, 220 (1988).
[17]A. Harwit and J. S. Harris, Jr., J. Appl. Phys. **60**, 3211 (1986).
[18]See, for example, L. D. Landau, and E. M. Lifshitz, *Quantum Mechanics (Non-Relativistic Theory)* (Pergamon, Oxford, 1977), Sec. 24.