Time-dependent formalism for interband tunneling application to the $In_xGa_{1-x}As$ system

V. Sankaran and J. Singh
Department of Electrical Engineering and Computer Science, 2234 EECS Building, University of Michigan, Ann Arbor, Michigan 48109-2122

(Received 16 September 1992; accepted for publication 14 December 1992)

A formalism is presented to study interband tunneling which involves a direct, numerical solution of the time-dependent Schrödinger equation, employing the tight-binding representation for electronic states with an eight-element (sp^3) basis. Using this explicitly time-dependent formalism, one can study the dynamics of interband tunneling in the presence of complicated space- and time-dependent electric field profiles encountered in many devices. This technique is well suited to study interband tunneling in heterostructures since the tight-binding method describes their band structure adequately. In conjunction with deformation potential theory, it can be applied to strained systems as well. The technique is applied to the important semiconductor system of $In_xGa_{1-x}As$.

Zener tunneling is the important phenomenon responsible for the anomalous current-voltage characteristics of Esaki diodes under forward and reverse bias. The negative differential resistance exhibited under forward bias is exploited in microwave devices, such as oscillators and mixers. Zener tunneling can be an important limiting factor in semiconductor devices for high power applications. In narrow band gap semiconductor alloys, such as $In_xGa_{1-x}As$, the band gap can range from 1.5 to 0.4 eV as the In content increases and interband tunneling can dominate the breakdown process.

The theory of Zener tunneling in a uniform electric field, as well as its adaptation to the *p-n* junction geometry, has been formulated by several authors (see Refs. 1 and 2 for reviews). The diode current density $J(V)$ at a dc bias V is conventionally calculated from the following formula:

$$J=\frac{2e}{\hbar}\int_{-\infty}^{\infty} dE[f(E)-f(E+eV)]\int \frac{d^2k_{\parallel}}{(2\pi)^2},T(E,k_{\parallel}). \tag{1}$$

The energy E and parallel wave vector $k_{\parallel}$ are conserved in direct tunneling. $f(E)$ is the Fermi–Dirac function. All formulations of Zener tunneling yield a tunneling probability, $T(E, k_{\parallel})$, of the general form (Ref. 1, Sec. 6c):

$$T(E,k_{\parallel})=T_0\exp\left(-\frac{E_{\parallel}}{\tilde{E}_{\parallel}}\right),$$
$$E_{\parallel}\equiv\hbar^2(k_{\parallel}-k_{0\parallel})^2/2m^*. \tag{2}$$

Here, $\tilde{E}_{\parallel}$ is a measure of the reduction in tunneling probability due to parallel momentum. $E_{\parallel}$ is the energy of transverse motion and k_0 is the point of band extrema. The probability T_0 for zero parallel momentum is independent of energy for the constant field case. It is given by

$$T_0=D_0\exp[-c_0(m^*)^{1/2}E_G^{3/2}/\hbar F], \tag{3}$$

where D_0 and c_0 are numerical coefficients of the order of unity whose exact value depends on the theoretical formulation. The constant field F is usually taken to be the maximum value of the field at the junction. E_G denotes the band gap and m^* is related to the effective masses of the conduction and valence bands in a two-band model.

Derivations leading to these formulas[2–6] rely on the two-band $\mathbf{k}\cdot\mathbf{p}$ model of the band extremum, which accounts only for the coupling between the light-hole valence band and the conduction band. They cannot be extended in any straightforward manner to take complete account of valence band degeneracy.[2] They are valid, moreover, only for moderate values of the electric field in which the perturbation treatment of interband coupling terms can be expected to hold. Another source of error lies in the use of uniform field analyses to calculate tunneling current in *p-n* junctions, since the junction field could change appreciably over short distances.

These formulations are also based on the time-dependent Schrödinger equation and are not well suited to study the dynamics of the tunneling process. We have developed a time-dependent technique to investigate interband tunneling in the presence of complicated space- and time-dependent electric field profiles, devoid of the limitations of existing models mentioned earlier. If the procedure is implemented in the tight-binding representation, interactions between bands and interband coupling are retained accurately in the tight-binding Hamiltonian. This technique is appropriate for studying Zener tunneling in heterostructures, since the tight-binding method describes their band structure adequately. In conjunction with deformation potential theory, it can be applied to strained systems as well. The dependence of the tunneling probability on parallel momentum can be investigated accurately without the assumption of an isotropic effective mass that leads to Eq. (2).

The basic idea is to construct a wave packet out of Bloch functions confined to a single band and then to study its propagation across the band gap. The transmitted and reflected components of this wave packet yield the interband tunneling probabilities. Although the technique is applicable to arbitrary electric field profiles, we have chosen the uniform field profile shown schematically in Fig. 1 to facilitate the comparison with existing theory. We construct a wave packet out of Bloch states from the conduc-

 0003-6951/93/080849-03$06.00

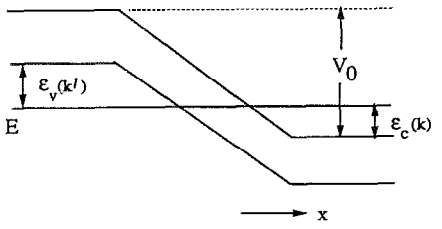

FIG. 1. Deformed band diagram of a *p-n* junction under uniform electric field for interband tunneling calculations.

tion band localized initially in the field-free region on the *n* side of the junction and constructed so as to propagate towards the junction. Thus, the wave packet may be expressed as

$$\psi(\mathbf{r},0)=\int dK\,\mathbf{A}(\mathbf{k})\phi_c(\mathbf{k},\mathbf{r}) \tag{4}$$

in terms of the conduction band Bloch states $\phi_c(\mathbf{k},\mathbf{r})$ of the unperturbed crystal. The envelope $A(\mathbf{k})$ has a narrow spread in k space around a mean value $\mathbf{k}_0$. Such a wave packet moves in the field-free region with a group velocity given by

$$v_g=\frac{1}{\hbar}\frac{d\epsilon_c(\mathbf{k})}{d\mathbf{k}},$$

where $\epsilon_c(\mathbf{k})$ is the band energy function.

The tight-binding form of the wave packet is obtained by using the bulk tight-binding eigenstates[7] for the Bloch functions in Eq. (4):

$$\psi(\mathbf{r},0)=\int d\mathbf{k}A(k)\sum_{\nu}b_{c,\nu}(\mathbf{k})\sum_{l}e^{i\mathbf{k}\cdot(\mathbf{R}_l+\mathbf{r}_\nu)}\times\xi_\nu[\mathbf{r}-(\mathbf{R}_l+\mathbf{r}_\nu)], \tag{5}$$

where: l indexes Bravais lattice sites of the crystal, $\mathbf{R}_l$ being the corresponding lattice translation, ν indexes distinct atomic orbitals in the tight-binding basis, $\mathbf{r}_\nu$ being the relative position of the corresponding ion within the primitive cell, $\xi_\nu(\mathbf{r}-\mathbf{r}_\nu)$ are the atomic orbitals, and $b_{n,\nu}(\mathbf{k})$ are the expansion coefficients.

Expressing the time-dependent wave function in the form

$$\psi(\mathbf{r},t)=\sum_{\nu}\sum_{l}c_\nu(\mathbf{R}_l+\mathbf{r}_\nu,t)\xi_\nu[\mathbf{r}-(\mathbf{R}_l+\mathbf{r}_\nu)], \tag{6}$$

we define "envelope functions" $c_\nu(\mathbf{R}_l+\mathbf{r}_\nu,t)$, one for each distinct orbital in the basis.

We have recently established a general numerical procedure[8-11] to study the dynamical evolution of a quantum system, which involves successive solution of the equation

$$(1+iH\delta t/2\hbar)\,|\psi(t+\delta t)\rangle=(1-iH\delta t/2\hbar)\,|\psi(t)\rangle, \tag{7}$$

where H is the Hamiltonian of the system and $|\psi(t)\rangle$ the time-dependent state vector. In the tight-binding representation, we substitute form 6 for the wave function, so that this equation becomes

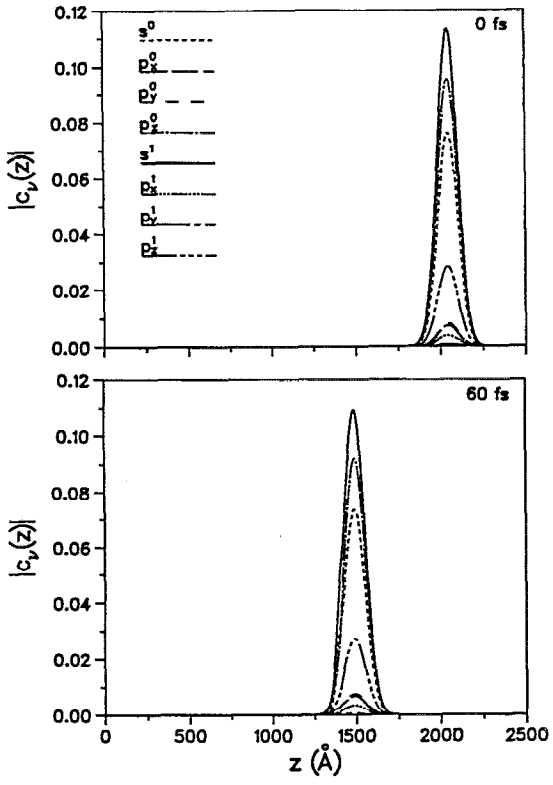

FIG. 2. Transmission and reflection of an electron in an $In_{0.80}Ga_{0.20}As$ *p-n* junction with a uniform junction field of 10^3 kV/cm. The transmitted part consists of two distinct wave packets arising from the split-off valence band and the light-hole band.

$$(1+iH\delta t/2\hbar)\sum_{\nu}\sum_{l}c_\nu(\mathbf{R}_l+\mathbf{r}_\nu,t+\delta t)\xi_\nu[\mathbf{r}-(\mathbf{R}_l+\mathbf{r}_\nu)]=(1-iH\delta t/2\hbar)\sum_{\nu}\sum_{l}c_\nu(\mathbf{R}_l+\mathbf{r}_\nu,t)\xi_\nu[\mathbf{r}-(\mathbf{R}_l+\mathbf{r}_\nu)]. \tag{8}$$

Taking the scalar product in this equation successively with distinct orbitals yields simultaneous equations for the coefficients at time $t+\delta t$ in terms of their values at t and the known tight-binding parameters of the bulk material.[11]

As illustrative examples, we have applied the wave packet technique to calculate interband tunneling probabilities over a range of electric field strengths in *p-n* junctions of bulk $In_{0.53}Ga_{0.47}As$ and $In_{0.80}Ga_{0.20}As$. Figures 2 and 3 depict the propagation of an electron wave packet across the $In_{0.80}Ga_{0.20}As$ *p-n* junction, when the junction field is 10^3 kV/cm. The envelope functions are identified with their orbitals in the legend to the figures, with subscripts 0 and 1 denoting cation and anion, respectively. Spin-orbit coupling has been included in these simulations.[12] The wave packet was constructed with mean wave vector $k_x=0$, $k_y=0$, and $k_z=-0.12$ (units $Å^{-1}$). It propagates initially in the field-free region at a velocity of 10 Å/fs, which coincides with the group velocity computed from the band structure. The transmitted part consists of two distinct wave packets which propagate at different velocities. It was ascertained from the composition and group

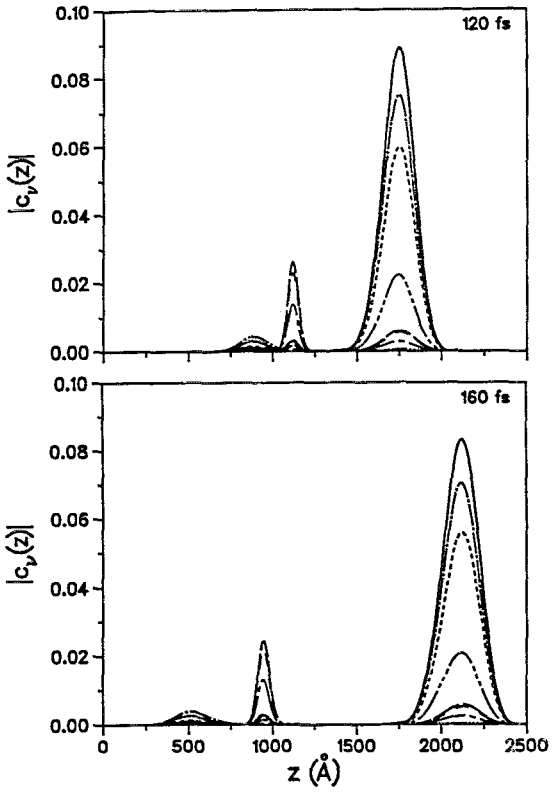

FIG. 3. Transmission and reflection of an electron in an $In_{0.80}Ga_{0.20}As$ *p-n* junction, continued.

velocities of these wave packets that the faster one arises from the split-off band and the slower one from the light-mass band.

Tunneling probabilities are plotted in Fig. 4 against the inverse of the electric field strength. The linearity of the plots suggests that the functional form 3 is valid over the range of field strengths depicted. As noted earlier, this formula is derived on the basis of a two-band model. Since we can explicitly perceive tunneling from the conduction band into the light-hole band and into the split-off band, the two-band model is not appropriate. We may still fit the computed tunneling probabilities to the functional form 3, but treat m^* in the exponent as the free-electron mass.

In conclusion, we have established a viable, time-dependent technique to investigate interband tunneling in semiconductor heterostructures, which is well suited to

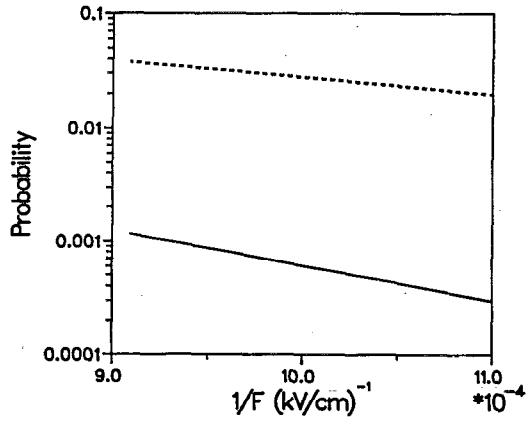

FIG. 4. Uniform-field interband tunneling probabilities in $In_xGa_{1-x}As$ *p-n* junctions plotted as a function of inverse field strength. The solid line is for $In_{0.53}Ga_{0.47}As$ while the dashed line is for $In_{0.8}Ga_{0.2}As$.

study the dynamics of the tunneling process in the presence of space- and time-dependent electric field profiles. The procedure may be implemented in the tight-binding representation, where interactions between bands and interband coupling are fully retained in the tight-binding Hamiltonian. The effect of strain can be incorporated and the dependence of tunneling probability on parallel momentum can be investigated accurately. The feasibility of the method was demonstrated by calculating interband tunneling probabilities in $In_{0.53}Ga_{0.47}As$ and $In_{0.80}Ga_{0.20}As$ *p-n* junctions.

This work was supported by the U. S. Army Research Office under the URI program (Grant No. DAAL03-92-G-0109).

[1] C. B. Duke, in *Solid State Physics*, edited by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic, New York, 1969), Chap. Supp. 10.
[2] P. J. Price, *Electron Tunneling in Semiconductors*, Research Report RC 17634 (No. 77579) (IBM Research Division, T. J. Watson Research Center, Yorktown Heights, NY, 1992).
[3] C. Zener, Proc. R. Soc. London Ser. A **145**, 523 (1934).
[4] E. O. Kane, J. Phys. Chem. Solids **12**, 181 (1959).
[5] E. O. Kane, J. Appl. Phys. **32**, 83 (1961).
[6] P. N. Argyres, Phys. Rev. **126**, 1386 (1962).
[7] J. C. Slater and G. F. Koster, Phys. Rev. **94**, 1498 (1954).
[8] V. Sankaran and J. Singh, Appl. Phys. Lett. **58**, 1509 (1991).
[9] V. Sankaran and J. Singh, Phys. Rev. B **44**, 3175 (1991).
[10] V. Sankaran and J. Singh, Appl. Phys. Lett. **59**, 1963 (1991).
[11] V. Sankaran, Ph.D. thesis, University of Michigan, Ann Arbor, MI 48109-2122 (1992).
[12] M. D. Jaffe and J. Singh, Solid State Commun. **62**, 339 (1987).