Tadayon), and funding from IBM, AT&T, Rockwell International, Brush Wellman, and Spectrum Technology. This work was performed in part at Howard University.

[1]G. Metze and A. Calawa, Appl. Phys. Lett. 42, 818 (1983).
[2]Y. Horikoshi, M. Kawashima, and H. Yamaguchi, Jpn. J. Appl. Phys. 27, 169 (1988).
[3]B. Tadayon, S. Tadayon, W. Schaff, M. Spencer, G. Harris, P. Tasker, C. Wood, and L. Eastman, Appl. Phys. Lett. 55, 59 (1989).
[4]P. M. Enquist, L. M. Lunardi, D. F. Welch, G. W. Wicks, J. R. Shealy, L. F. Eastman, and A. R. Calawa, Inst. Phys. Conf. Ser. 74, 599 (1985).
[5]B. Tadayon, S. Tadayon, M. G. Spencer, G. L. Harris, L. Rathbun, J. T. Bradshaw, W. J. Schaff, P. J. Tasker, and L. F. Eastman, Appl. Phys. Lett. 53, 2664 (1988).
[6]H. Shtrikman, M. Heiblum, K. Seo, D. E. Galbi, and L. Osterling, J. Vac. Sci. Technol. B 6, 670 (1988).
[7]F. Smith, H. Le, V. Diadiuk, M. Hollis, A. Calawa, S. Gupta, M. Frankel, D. Dykaar, G. Mourou, and T. Hsiang, Appl. Phys. Lett. 54, 890 (1989).
[8]J. Gerard, J. Marzin, B. Jusserand, F. Glas, and J. Primot, Appl. Phys. Lett. 54, 30 (1989).
[9]R. Katsumi, H. Ohno, H. Ishii, K. Matsuzaki, Y. Akatsu, and H. Hasegawa, J. Vac. Sci. Technol. B 6, 593 (1988).
[10]J. Kim, J. Liu, G. Radhakrishnan, J. Katz, S. Sakai, S. Chang, and N. El-Masry, Appl. Phys. Lett. 53, 2435 (1988).
[11]A. Salokatve, J. Varrio, J. Lammasniemi, H. Asonen, and M. Pessa, Appl. Phys. Lett. 51, 1340 (1987).
[12]G. Abstreiter, E. Bauser, A. Fischer, and K. Ploog, Appl. Phys. 16, 345 (1978).
[13]G. W. Wicks, Ph.D. thesis, Cornell University, 1981.

Improved boundary conditions for the time-dependent Schrödinger equation

R. K. Mains and G. I. Haddad
Center for High-Frequency Microelectronics, Department of Electrical Engineering and Computer Science, The University of Michigan, Ann Arbor, Michigan 48109

(Received 3 July 1989; accepted for publication 15 September 1989)

An improved boundary condition treatment for the time-dependent Schrödinger equation applied to resonant-tunneling diode simulation has been developed. This treatment is half-implicit, or centered in time, and allows larger time steps than the previous explicit treatment. The method does not complicate the time-dependent calculation since the resulting matrix is still tridiagonal.

Realistic quantum transport modeling of semiconductor devices using the time-dependent Schrödinger equation requires the formulation of open-system boundary conditions. Typically time-dependent Schrödinger calculations[1,2] have avoided the boundary condition problem by terminating the simulation before disturbances reach the boundaries, which precludes the establishment of a steady-state solution. A method of extracting outgoing waves has been used for a quantum MESFET calculation,[3] however, details of the boundary condition method were not given.

Previously a method has been presented for applying open-system boundary conditions to the time-dependent Schrödinger equation for resonant-tunneling diode modeling.[4] This method is purely explicit and limited to a maximum time step of $(1–2)\times 10^{-16}$ s. In this communication, a half-implicit treatment is presented which allows time steps of 5×10^{-16} s or larger.

From Ref. 4, the wave function at the LHS (x_0) for waves incident from the left is expressed as

$$\psi(x_0) = Ae^{ikx_0} + B(x_0)e^{-ikx_0}, \qquad (1)$$

where A is constant with x and $B(x)$ is taken to be linear. The boundary update for this case is:

$$\psi^f(x_0) \approx \psi(x_0)e^{-iE\Delta t/\hbar} + \frac{\hbar k}{m^*}\frac{\partial B(x_0)}{\partial x}e^{-ikx_0}\Delta t, \qquad (2)$$

where superscript f refers to quantities at $t+\Delta t$. In the previous treatment,[4] $\partial B(x_0)/\partial x$ in Eq. (2) was evaluated at the present time t. A better method is the following:

$$\frac{\partial B(x_0)}{\partial x} \approx \frac{1}{2}\left[\left(\frac{\partial B(x_0)}{\partial x}\right)_t + \left(\frac{\partial B(x_0)}{\partial x}\right)_{t+\Delta t}\right]. \qquad (3)$$

Values of $B(x)$ are obtained as follows:

$$\begin{aligned} B(x_0) &= (\psi_1 - Ae^{ikx_0})e^{ikx_0},\\ B(x_0+\Delta x) &= (\psi_2 - Ae^{ik(x_0+\Delta x)})e^{ik(x_0+\Delta x)},\\ B^f(x_0) &= (\psi_1^f - A^f e^{ikx_0})e^{ikx_0},\\ B^f(x_0+\Delta x) &= (\psi_2^f - A^f e^{ik(x_0+\Delta x)})e^{ik(x_0+\Delta x)}, \end{aligned} \qquad (4)$$

where ψ_1 is the leftmost wave-function value. Equation (3) becomes, in finite-difference form:

$$\frac{\partial B(x_0)}{\partial x} \approx \frac{1}{2}\left(\frac{B(x_0+\Delta x) - B(x_0)}{\Delta x} + \frac{B^f(x_0+\Delta x) - B^f(x_0)}{\Delta x}\right). \qquad (5)$$

Substituting Eqs. (5) and (4) into Eq. (2) yields the following equation involving future values of ψ at the left-hand boundary:

$$\psi_1^f\left(1 + \frac{\hbar k\Delta t}{2m^*\Delta x}e^{-ikx_0}\right) + \psi_2^f\left(\frac{-\hbar k\Delta t}{2m^*\Delta x}e^{ik\Delta x}\right) = b_1, \qquad (6)$$

where

$$b_1 = \psi_1\left(e^{-iE\Delta t/\hbar} - \frac{\hbar k\Delta t}{2m^*\Delta x}e^{-ikx_0}\right) + \psi_2\left(\frac{\hbar k\Delta t}{2m^*\Delta x}e^{ik\Delta x}\right)$$

$$+\frac{\hbar k\Delta t}{2m^*\Delta x}e^{ikx_0}(1-e^{2ik\Delta x})(A+A^f). \quad (7)$$

Since Eq. (6) involves only the first two values of the wave function at $t+\Delta t$, the tridiagonal property of the matrix is preserved.

Roache[5] has given a tridiagonal matrix solution routine. In his notation, Eq. (6) may be expressed as a Robbin's condition in the following form:

$$\psi_1^f + p_1[(\psi_2^f - \psi_1^f)/\Delta x] = q_1, \quad (8)$$

where

$$p_1 = \frac{(-\hbar k\Delta t/2m^*)e^{ik\Delta x}}{1+(\hbar k\Delta t/2m^*\Delta x)(e^{-ikx_0}-e^{ik\Delta x})},$$

$$q_1 = \frac{b_1}{1+(\hbar k\Delta t/2m^*\Delta x)(e^{-ikx_0}-e^{ik\Delta x})}. \quad (9)$$

For waves incident from the left, the wave functions at the RHS outflow boundary (x_{max}) are of the form[4]:

$$\psi(x_{max}) = C(x_{max})e^{ik_0x_{max}}, \quad (10)$$

and the boundary update is given by

$$\psi^f(x_{max}) \approx \psi(x_{max})e^{-iE_0\Delta t/\hbar} - \frac{\hbar k_0}{m^*}\frac{\partial C(x_{max})}{\partial x}e^{ik_0x_{max}}\Delta t. \quad (11)$$

Values of C are determined from

$$\begin{aligned} C(x_{max}) &= \psi_N e^{-ik_0x_{max}}, \\ C(x_{max}-\Delta x) &= \psi_{N-1}e^{-ik_0(x_{max}-\Delta x)}, \\ C^f(x_{max}) &= \psi_N^f e^{-ik_0x_{max}}, \\ C^f(x_{max}-\Delta x) &= \psi_{N-1}^f e^{-ik_0(x_{max}-\Delta x)}, \end{aligned} \quad (12)$$

where N represents the last value of ψ on the RHS. The quantity $\partial C/\partial x$ is evaluated as follows:

$$\frac{\partial C(x_{max})}{\partial x} \approx \frac{1}{2}\left[\left(\frac{\partial C(x_{max})}{\partial x}\right)_t + \left(\frac{\partial C(x_{max})}{\partial x}\right)_{t+\Delta t}\right]. \quad (13)$$

Substituting Eqs. (12) and (13) into Eq. (11) yields the following RHS outflow boundary equation:

$$\psi_{N-1}^f\left(\frac{-\hbar k_0\Delta t}{2m^*\Delta x}e^{ik_0\Delta x}\right) + \psi_N^f\left(1+\frac{\hbar k_0\Delta t}{2m^*\Delta x}\right) = b_N, \quad (14)$$

where

$$b_N = \frac{\hbar k_0\Delta t e^{ik_0\Delta x}}{2m^*\Delta x}\psi_{N-1} + \psi_N\left(e^{-iE_0\Delta t/\hbar} - \frac{\hbar k_0\Delta t}{2m^*\Delta x}\right). \quad (15)$$

Again, since Eq. (14) involves only the last two ψ^f values, the tridiagonal property is preserved.

In Roache's notation,[5] this is expressed as a Robbin's condition:

$$\psi_N^f + p_M[(\psi_N^f - \psi_{N-1}^f)/\Delta x] = q_M, \quad (16)$$

where

$$p_M = \frac{(\hbar k_0\Delta t/2m^*)e^{ik_0\Delta x}}{1+(\hbar k_0\Delta t/2m^*\Delta x)(1-e^{ik_0\Delta x})},$$

$$q_M = \frac{b_N}{1+(\hbar k_0\Delta t/2m^*\Delta x)(1-e^{ik_0\Delta x})}. \quad (17)$$

In a similar manner, boundary equations have been derived for waves incident from the right; only the results are given here. In this case, the outflow boundary equation at x_0 is

$$\psi_1^f\left(1-\frac{\hbar k_0\Delta t}{2m^*\Delta x}\right) + \psi_2^f\left(\frac{\hbar k_0\Delta t}{2m^*\Delta x}e^{-ik_0\Delta x}\right) = b_1, \quad (18)$$

where

$$b_1 = \psi_1\left(e^{-iE_0\Delta t/\hbar} + \frac{\hbar k_0\Delta t}{2m^*\Delta x}\right) - \frac{\hbar k_0\Delta t}{2m^*\Delta x}e^{ik_0\Delta x}\psi_2. \quad (19)$$

In Roache's notation:

$$p_1 = \frac{(\hbar k_0\Delta t/2m^*)e^{-ik_0\Delta x}}{1+(\hbar k_0\Delta t/2m^*\Delta x)(e^{-ik_0\Delta x}-1)},$$

$$q_1 = \frac{b_1}{1+(\hbar k_0\Delta t/2m^*\Delta x)(e^{-ik_0\Delta x}-1)}. \quad (20)$$

The inflow boundary equation at x_{max} is

$$\psi_{N-1}^f\left(\frac{\hbar k\Delta t}{2m^*\Delta x}e^{-ik\Delta x}\right) + \psi_N^f\left(1-\frac{\hbar k\Delta t}{2m^*\Delta x}\right) = b_N, \quad (21)$$

where

$$b_N = \frac{-\hbar k\Delta t}{2m^*\Delta x}e^{-ik\Delta x}\psi_{N-1} + \left(e^{-iE\Delta t/\hbar} + \frac{\hbar k\Delta t}{2m^*\Delta x}\right)\psi_N + \frac{\hbar k\Delta t}{2m^*\Delta x}e^{ikx_{max}}(A+A^f)(e^{-2ik\Delta x}-1). \quad (22)$$

In Roache's notation:

$$p_M = \frac{(-\hbar k\Delta t/2m^*)e^{-ik\Delta x}}{1+(\hbar k\Delta t/2m^*\Delta x)(e^{-ik\Delta x}-1)},$$

$$q_M = \frac{b_N}{1+(\hbar k\Delta t/2m^*\Delta x)(e^{-ik\Delta x}-1)}. \quad (23)$$

Figure 1 shows the switching transients that result when the bias voltage is instantaneously switched from the peak current to the valley current value (solid curve), and in the opposite direction (dashed curve) for a 28 Å barrier–45 Å well GaAs–$Ga_{0.7}Al_{0.3}As$ device at room temperature (incident waves from the cathode contact only were included in

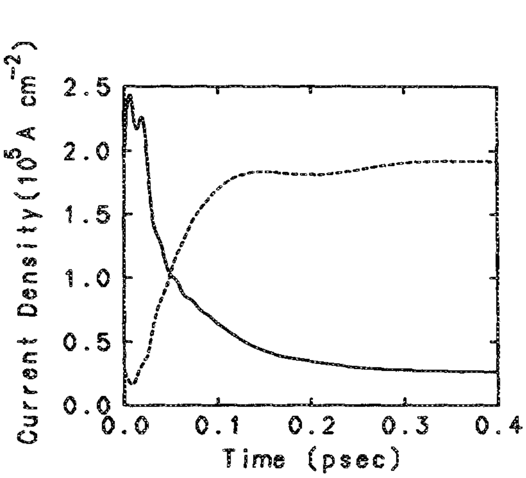

FIG. 1. Turnoff (solid curve) and turnon (dashed curve) transients for a 28 Å barrier–45 Å well GaAs–$Ga_{0.7}Al_{0.3}As$ device at room temperature.

this calculation). The effective masses used in the calculation were $m^* = 0.09m_0$ inside the barriers and $m^* = 0.067m_0$ outside. The barrier height was 0.246 eV. In the turnoff transient, the initial oscillations are due to the electron distribution in the well reflecting between the barriers. The calculations of Fig. 1 utilize the boundary condition treatment described in this communication, and a time step of 5×10^{-16} s was used with no sign of instability in the results. Larger time steps were also successfully tried for this calculation. For this device, the maximum allowable time step is limited by the time scale of processes occurring during the switching transient rather than numerical instability. Time steps greater than 10^{-15} s are possible but details of the switching transients are lost. Thus, time step limitations of this method are expected to be a function of device structure and biasing conditions.

This work was supported by the US Army Research Office under the URI program, Contract No. DAAL03-87-K-0007.

[1]H. Guo, K. Diff, G. Neofotistos, and J. D. Gunton, Appl. Phys. Lett. **53**, 131 (1988).
[2]S. C. Kan and A. Yariv, J. Appl. Phys. **64**, 3098 (1988).
[3]M. C. Yalabik, J. D. Gunton, G. Neofotistos, and K. Diff, Superlattices and Microstructures 3, 463 (1987).
[4]R. K. Mains and G. I. Haddad, J. Appl. Phys. **64**, 3564 (1988).
[5]P. J. Roache, *Computational Fluid Dynamics* (Hermosa, Albuquerque, NM, 1976).

The effect of interface roughness and island scattering on resonant tunneling time

H. C. Liu
Laboratory for Microstructural Sciences, Division of Physics, National Research Council, Ottawa, Ontario K1A 0R6, Canada

(Received 13 January 1989; accepted for publication 27 September 1989)

The effect of interface roughness and island scattering on resonant tunneling time in double-barrier structures is investigated theoretically. The scattering process degrades the resonant tunneling peak current, broadens the resonance, and hence shortens the resonant tunneling time. For thin barrier structures, the tunneling time enhancement due to the scattering is relatively small, while the resonance width is dominated by the scattering for thick barrier samples.

The major driving force for studying the resonant tunneling phenomenon comes from the possibility of high-speed device applications.[1,2] There have been many publications dealing with the issue of the ultimate response time of resonant tunneling in double-barrier structures.[3–5] Inelastic scattering (e.g., by phonons) broadens the resonance,[6] although the relative importance of inelastic scattering is not clear yet.[7] Epitaxial-growth-related interface roughnesses and islands are unavoidable in samples grown by today's advanced technologies such as molecular-beam epitaxy.[8] We have studied interface roughness and island effects on tunneling probabilities and tunneling currents in quantum well structures theoretically.[9] We have shown that interface roughnesses and islands reduce and broaden the resonant transmission, degrade the peak current, and increase the valley current.[9] In this communication, we consider the effect of interface roughnesses and islands on the resonant tunneling time.

The physical interpretation of tunneling times is still an open question.[10] We employ the formalism by Pollak and Miller.[11] A complex time for scattering process involving in-state i to out-state j is defined as

$$\tau_{ij} = -i\hbar \frac{\partial}{\partial E}(\ln S_{ij}), \qquad (1)$$

where S is the scattering matrix. For resonant scattering, the matrix element S_{ij} is related to a Breit–Wigner-like form:

$$S_{ij} = S^0_{ij} e^{i\delta_{ij}} \frac{\Gamma_{ij}}{(E - E_0) + i\Gamma_{ij}}, \qquad (2)$$

where the amplitude S^0_{ij} is real, δ_{ij} is a real phase and is assumed to have a weak (nonresonance) dependence on energy E, E_0 is the resonant energy, and Γ_{ij} is the resonant width. We concentrate on the tunneling time at the maximum transmission $E = E_0$, i.e., the on-resonance tunneling time in which case the imaginary part of τ_{ij} vanishes ($\partial |S_{ij}|/\partial E = 0$ at $E = E_0$) and the real part is the well-known time delay (or phase time):

$$\tau^\phi_{ij} = \mathrm{Re}(\tau_{ij}) = \hbar \frac{\partial \phi_{ij}}{\partial E}, \qquad (3)$$

where ϕ_{ij} is the phase shift defined by $S_{ij} = |S_{ij}|\exp(i\phi_{ij})$. For double-barrier resonant tunneling structures the above time delay is the longest because $\tau^\phi_{ij} = \hbar\Gamma_{ij}/[\Gamma^2_{ij} + (E - E_0)^2]$, and we take this time $\hbar/\Gamma_{ij}$ as the intrinsic ultimate limit of the device response time.[1,4] It should be pointed out that such a definition of the ultimate response is only an estimate. A time-dependent approach should be employed to determine the device frequency re-

 0021-8979/90/010593-03$03.00