Observation of intrinsic bistability in resonant tunneling diode modeling

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Intrinsic bistability has been observed experimentally and attributed to the effect on the potential profile from stored charge in the quantum well through Poisson's equation. This effect leads to two possible current states corresponding to a single voltage within the negative resistance region. In this letter a simulation method is presented which clearly shows bistability in the current-voltage curve of a resonant tunneling diode. This method self-consistently combines a Thomas–Fermi equilibrium model for the electron concentrations outside the double-barrier structure with a quantum calculation for the concentration inside the structure.

Experimental results have been presented[1,2] indicating that resonant tunneling diodes exhibit intrinsic bistability when biased within the negative resistance region of the current-voltage (I-V) curve. It has also been shown[3] that observed bistabilities may be due to device-circuit oscillations, i.e., dynamic bistable effects. Intrinsic bistability has been observed theoretically[4,5] using a sequential tunneling model where expressions for tunneling current between an energy continuum and a quantum well are combined with Poisson's equation.

In this letter, a self-consistent model for calculating the dc behavior of resonant tunneling diodes is presented. The contact regions outside the double-barrier structure are treated using a Thomas–Fermi equilibrium model, i.e., constant Fermi levels within each region and equilibrium Fermi–Dirac statistics are assumed. Within the double-barrier structure, electron concentrations are obtained from the time-independent Schrödinger equation using the methods of Ref. 6. The concentrations obtained inside the device are then self-consistently coupled to the Thomas–Fermi model through matching conditions connecting the two contact regions.

Results for a particular $In_{0.53}Ga_{0.47}As$-$In_{0.52}Al_{0.48}As$-$In_{0.53}Ga_{0.47}As$ structure are presented which clearly show bistability in the dc I-V curve. It is shown that the origin of bistability is the buildup of charge inside the quantum well during resonant tunneling.

This section describes the method used to simulate the contact regions outside the double-barrier structure. Let mesh points $1,..., N_L$ be the points in the left-hand contact, and points $N_L + 1,...,N$ be in the right-hand contact. Constant Fermi levels E_{FL} and E_{FR} are associated with the contacts, such that $E_{FR} - E_{FL} = qV_{app}$, where V_{app} is the applied bias voltage. Using equilibrium Fermi–Dirac statistics, the electron concentration is given by

$$n(x) = \frac{2N_c}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{y}\,dy}{1 + e^{(y - \eta(x))}}, \tag{1}$$

where N_c is the effective density of electrons in the conduction band and

$$\eta(x) = [E_{FR,L} - E_c(x)]/k_B T. \tag{2}$$

Note from Eq. (2) that the concentration is related to the difference between the local conduction band edge $E_c(x)$ and the Fermi level E_{FR} or E_{FL}, depending in which contact the expression is applied.

Equation (1) is a mapping between η and the local electron concentration. It cannot be evaluated in closed form, and the usual approximation of Boltzmann statistics is not valid for this case since degenerate doping levels are typically found in the contact regions. However, Eq. (1) can be accurately approximated by retaining the first two terms in the Joyce–Dixon approximation[7,8]:

$$\eta(x) = \frac{E_{FR,L} - E_c(x)}{k_B T} \approx \log\left(\frac{n(x)}{N_c}\right) + \frac{n(x)}{\sqrt{8}N_C}. \tag{3}$$

The condition band edge is related to the potential by

$$E_C(x) = E_C(\pm\infty) - q[V(x) - V(\pm\infty)], \tag{4}$$

where the upper sign applies to the right-hand contact and the lower sign to the left.

The potential variation is determined from Poisson's equation, discretized at point x_i as follows:

$$V_{i+1} - 2V_i + V_{i-1} = (q\Delta x^2/\epsilon)[n_i - N_{di}], \tag{5}$$

where N_{di} is the doping density.

Combining Eqs. (3) and (4) yields the following discrete equation for n_i:

$$\log\left(\frac{n_i}{N_c}\right) + \frac{n_i}{\sqrt{8}N_C}$$
$$= \frac{E_{FR,L} - E_C(\pm\infty) - qV(\pm\infty) + qV_i}{k_B T}. \tag{6}$$

Equations (5) and (6) are solved at all interior mesh points for n_i and V_i.

In addition, matching conditions must be applied at mesh points N_L and $N_L + 1$, at the left and right boundaries of the double-barrier structure. These matching conditions express the fact that the discontinuity of electric field is related to the integral of the charge inside the structure, and that the potential discontinuity is related to this charge as well as the boundary electric fields. The first condition is expressed as

$$E_R - E_L = \frac{V_{NL+1} - V_{NL+2} + V_{NL} - V_{NL-1}}{\Delta x}$$

$$= D_E = \frac{q}{\epsilon} \int_{x_L}^{x_R} [N_d(x) - n(x)] \, dx, \tag{7}$$

where x_L and x_R are the positions at the left and right boundaries. The condition on potential discontinuity across the structure may be written as

$$V_{NL+1} - V_{NL} = \frac{-(x_R - x_L)}{\Delta x}(V_{NL-1} - V_{NL}) + \bar{D}_V, \tag{8}$$

where $\bar{D}_v$ is given by

$$\bar{D}_V = \frac{q}{\epsilon} \int_{x_L}^{x_R} dx' \int_{x_L}^{x'} dx'' [n(x'') - N_d(x'')]. \tag{9}$$

The quantities D_E and $\bar{D}_V$ are the means by which the quantum calculation for the electron concentration inside the double-barrier structure is coupled to the Thomas–Fermi calculation. Note that these quantities would be zero if charge in the quantum well were ignored.

In addition, Dirichlet boundary conditions are set at mesh points 1 and N on the potential using the applied bias voltage, and on the concentration using the contact doping.

The overall numerical procedure may now be described. An initial guess is generated for the potential and electron concentrations in the contacts, and the quantum well concentration is initially assumed zero. The Newton–Raphson iterative method is used to solve Eqs. (5)–(9), which constitute a set of nonlinear equations. At each iteration, a quantum calculation is performed using the methods of Ref. 6 to calculate the quantities D_E and $\bar{D}_V$ required for the matching conditions. This process is repeated until the maximum fractional change of potential and carrier density predicted by the Newton–Raphson method for each iteration is below a specified tolerance. It is necessary to introduce numerical damping techniques for this procedure to converge, wherein full steps are not taken at every iteration.

After convergence is obtained, the device current density is calculated by solving the time-independent Schrödinger equation using the methods of Ref. 6.

The procedure described above was applied to an $In_{0.53}Ga_{0.47}As\text{-}In_{0.52}Al_{0.48}As$ barrier-$In_{0.53}Ga_{0.47}As$ well structure with 23.2 Å barriers and a 43.5 Å well. The doping in the $In_{0.53}Ga_{0.47}As$ contacts was 2×10^{18} cm^{-3}, and 50 Å undoped spacer layers were placed adjacent to each barrier. The effective mass used was $0.042m_0$ in the contacts and well, and $0.075m_0$ in the barrier. The barrier height was 0.53 eV.

Figure 1(a) shows the static I-V curves obained for this device. For the solid curve, the bias voltage was started at 0 V and swept positive. For the dashed curve (which coincides with the solid curve except in the bistable region), the bias voltage was started at 0.8 V and swept downward toward 0 V. It is seen that a bistable region exists where different dc current states may be assumed depending upon the direction of the bias voltage sweep.

Figures 1(b) and 1(c) show two bistable solutions at the bias point $V_{dc} = 0.55$ V in Fig. 1(a), within the bistable

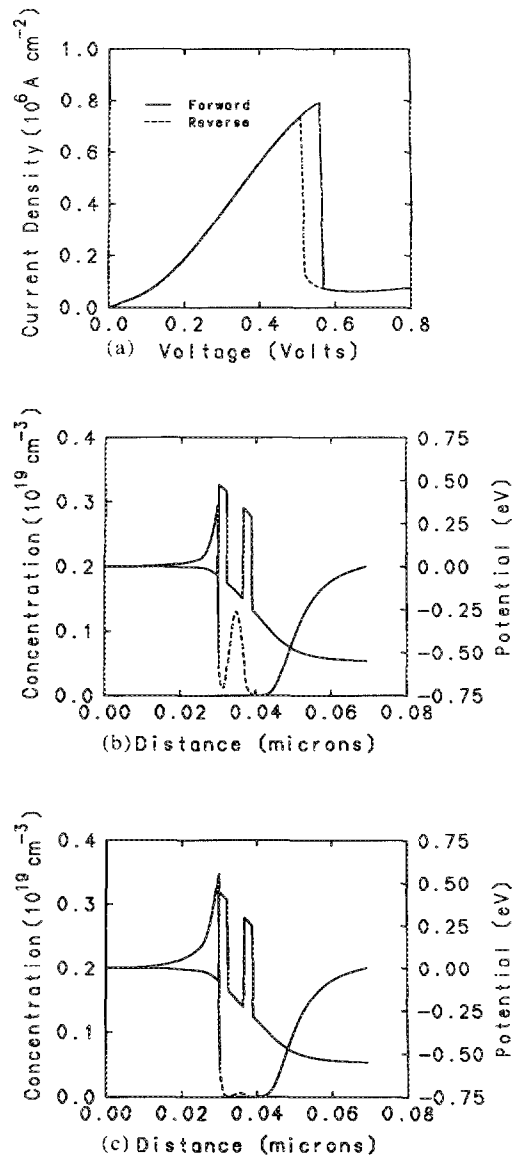(a) Voltage (Volts)

(b) Distance (microns)

(c) Distance (microns)

FIG. 1. (a) I-V curves for the $In_{0.53}Ga_{0.47}As\text{-}In_{0.52}Al_{0.48}As\text{-}In_{0.53}Ga_{0.47}As$ structure starting from 0 V (solid curve) and starting from 0.8 V (dashed curve), and solutions at $V_{dc} = 0.55$ V (b) corresponding to the solid curve or high-current state, and (c) corresponding to the dashed curve or low-current state.

region. Figure 1(b) corresponds to the high-current state along the solid curve. The solid curves in 1(b) show the electron concentrations in the contacts obtained from the Thomas–Fermi calculation, while the dashed curve shows the electron concentration within the double-barrier structure obtained from the quantum calculation. Since the solution is near the peak current point on the I-V curve, an appreciable resonant buildup of electrons in the first quasi-bound state of the well is observed. In Fig. 1(c), the charge in the well is much reduced and a corresponding buildup of charge in the accumulation region of the left contact is observed. The interpretation of these results is as follows. In Fig. 1(c), a greater voltage drop exists across the left-hand accumulation region than in Fig. 1(b). This places the double-barrier structure at a lower (electron) potential than is the case in Fig. 1(b). Because of this, the resonant energy level in the well drops below the conduction band edge in the left-hand contact. This in turn is responsible for the reduced charge in

the well, since the condition in Fig. 1(c) is off resonance. It can be appreciated that once this redistribution of charge between left-hand accumulation region and quantum well is initiated, a regenerative action causes the device to behave as a bistable switch.

A simulation method has been presented for modeling the dc behavior of resonant tunneling devices taking into account self-consistency and quantum mechanical effects inside the double-barrier structure (this method does not include nonequilibrium quantum effects outside the structure). The method is relatively stratightforward to implement, compared to a full quantum mechanical treatment. Important effects such as bistability are clearly observed. It is shown that dual states in the bistable region are due to the repartition of electrons from the well at resonance to the contact accumulation layer off resonance.

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