Microscopic Model for Sequential Tunneling in Semiconductor Multiple Quantum Wells.

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We propose a selfconsistent microscopic model of vertical sequential tunneling through a multi-quantum well. The model includes a detailed description of the contacts, uses the Transfer Hamiltonian for expressions of the current and it treats the Coulomb interaction within a mean field approximation. We analyze the current density through a double well and a superlattice and study the formation of electric field domains and multistability coming from the Coulomb interaction. Phase diagrams of parameter regions (bias, doping in the heterostructure and in the contacts, etc) where different solutions exist are given.

Coulomb interaction in heterostructures with large area wells is a small effect compared with the energy difference between non-interacting eigenstates of the structure. Therefore a mean field model gives, for many purposes a good description of the system. Among features of the transport properties having their origin in Coulomb interaction, intrinsic bistability has great importance. This physical phenomenon arises from the non-linear effect of the electric charge on the induced electrostatic potential, and it has been predicted and observed in double barrier structures (DB) [1–4]. Furthermore in the presence of a laser polarized in the sample growth direction, new bistability regions have been theoretically predicted [3]. In this paper we deal with the statics and dynamics of vertical transport through biased heterostructures whose main mechanism is sequential tunneling. This is a topic which has attracted a great deal of attention in recent times. In weakly coupled superlattices, multistability due to domain formation has been much studied both theoretically and experimentally, [1–4]. When the charge in the superlattice is small due to lower doping in the wells, self-sustained current oscillations and chaos due to domain dynamics are possible [10, 12]. So far, the most successful modeling of these phenomena use discrete rate equations for the electron density and electric field in each well, plus constitutive laws for the current, bias, boundary and initial conditions, [7, 13]. The laws may be phenomenological [8] or obtained from microscopic considerations, [7, 10, 14, 15]. In all cases cited, the boundary conditions were selected in a more or less ad hoc manner by using the available information from experiments. This is particularly annoying because the boundary conditions select the relevant dynamics of electric field domains in the oscillatory regime [13]. In this paper we present a microscopic model which includes in a natural way boundary conditions due to the emitter and collector regions of a multiwell structure (MW). We then solve it for the cases of a double quantum well (DQW) and a superlattice (SL). The presence of intrinsic bistability is demonstrated through phase diagrams and I-V characteristics obtained by numerical simulation and by means of numerical continuation of stationary solution branches. The main ingredients of our model are as follows: we assume that the characteristic time of intersubband relaxation due to scattering (about 0.1 ps for optical phonon scattering [17]) is much smaller than the tunneling time (less than 0.5 ns), which is in turn much smaller than the dielectric relaxation times responsible for reaching a steady state (about 10 ns for the 9nm/4nm GaAs/AlAs superlattices of Ref. [10]). This separation of time scales, as well as the configuration of a typical sample allows us to consider that only the ground state of each well is populated and that the tunneling processes are stationary. Our assumptions then justify using rate equations for the electron densities at each well with relations for the currents calculated by means of the Transfer Hamiltonian (TH) [18]. The rate equations for the electron densities imply that the interwell currents and the currents from the emitter and to the collector are all equal to the total current in the stationary case (a form of Ampère’s law may be derived in the time-dependent case). Furthermore, since no current is created or destroyed in the MW, the total charge in it (emitter and collector included) is zero. Finally, the electrostatics is simplified by assuming that the charges are concentrated on 2D planes located at the wells, emitter and collector regions, as indicated in Fig. 1 and further explained below.

The Hamiltonian for independent electrons in a MW under dc bias is:

\[ H = \sum_{k_i, i \in \{L,R\}} E_{k_i} c_{k_i}^\dagger c_{k_i} + \sum_{i=1}^{N} \sum_{k_i} E_{k_i} d_{k_i}^\dagger d_{k_i} \]
Here $c^\dagger_{k_i}(c_{k_i})$ are the creation (annihilation) operators in the leads and $d^\dagger_{k_i}(d_{k_i})$ are the creation (annihilation) operators in the wells, and $T_{k_i,k_j}$ are the tunneling matrix elements. The latter depend on the local electric field and must be calculated self-consistently for each bias. Applying the TH under the assumptions listed before, we obtain the following expressions for the tunneling currents where $J_{e,1}$ and $J_{N,c}$ are the currents in the contacts and $J_{i,i+1}$ the interwells currents:

$$J_{e,1} \equiv J_{0,1} = \frac{2 e k_B T}{\pi^2 h} \sum_{j=1}^{n} \int A_{Cj}^1(\epsilon) T_1(\epsilon) \times \ln \left[ \frac{1 + e^{\frac{\epsilon - E_d}{k_B T}}}{1 + e^{\frac{\epsilon + E_d}{k_B T}}} \right] d\epsilon,$$

$$J_{i,i+1} = \frac{2 e k_B T}{\pi^2 m^*} \sum_{j=1}^{n} \int A_{Cj}^i(\epsilon) A_{Cj}^{i+1}(\epsilon) T_{i+1}(\epsilon) \times \ln \left[ \frac{1 + e^{\frac{\epsilon - E_d}{k_B T}}}{1 + e^{\frac{\epsilon + E_d}{k_B T}}} \right] d\epsilon,$$

$$J_{N,c} \equiv J_{N,N+1} = \frac{2 e k_B T}{\pi^2 h} \sum_{j=1}^{n} \int A_{C1}(\epsilon) A_{C1}^N(\epsilon) T_{N+1}(\epsilon) \times \ln \left[ \frac{1 + e^{\frac{\epsilon - E_d}{k_B T}}}{1 + e^{\frac{\epsilon + E_d}{k_B T}}} \right] d\epsilon,$$

where $i = 1, \ldots, N-1$, $N$ is the number of wells, $n$ is the number of subbands in each well $i$ with energies $\epsilon_j$ (referred with respect to the origin of potential drops), and $T_i$ are the transmission coefficients through the $i$th barrier. The spectral functions of the wells are Lorentzians whose widths correspond to the LO phonon lifetimes ($\approx 1-10$ meV): $A_{Cj}(\epsilon) = \frac{\gamma}{(\epsilon - \epsilon_{Cj})^2 + \gamma^2}$ for the $i$th well. Of course this model can be improved by calculating microscopically the self-energies, which could include other scattering mechanisms (e.g. interface roughness, impurity effects [7]) or even exchange-correlation effects (which affect the electron lifetime in a self-consistent way [8]). We have assumed that the electrons in each well are in local equilibrium with Fermi energies $\epsilon_{\omega_i}$ which define the electronic densities $n_i$. For a given set $\{\epsilon_{\omega_i}\}$ the densities evolve according to the following rate equations:

$$\frac{d n_i}{d t} = J_{i-1,i} - J_{i,i+1} \quad i = 1, \ldots, N.$$

In these equations $J_{i,i+1} \equiv J_{i,i+1}(\epsilon_{\omega_i}, \epsilon_{\omega_{i+1}}, \Phi)$, $J_{e,1} \equiv J_{e,1}(\epsilon_{\omega_1}, \Phi)$, and $J_{N,c} \equiv J_{N,c}(\epsilon_{\omega_N}, \Phi)$, where $\Phi$ denotes the set of voltage drops through the structure which are calculated as follows. The Poisson equation yields the potential drops in the barriers, $V_i$, and the wells, $V_{wi}$ (see Fig. 1):

$$\frac{V_{wi}}{w} = \frac{V_i}{d} + \frac{n_i(\epsilon_{\omega_i}) - eN_D^w}{2\varepsilon},$$

$$\frac{V_{i+1}}{d} = \frac{V_i}{d} + \frac{n_i(\epsilon_{\omega_i}) - eN_D^w}{\varepsilon},$$

where $\varepsilon$ is the GaAs static permittivity, $n_i(\epsilon_{\omega_i})$ is the 2D (areal) charge density at the $i$th well (to be determined), $w$ and $d$ are the well and barrier thickness respectively, and $N_D^w$ is the 2D intentional doping at the wells. The emitter and collector layers can be described by the following equations [8]:

$$\frac{\Delta_1}{\delta_1} = \frac{eV_i}{d}, \quad \sigma = 2\varepsilon \frac{V_i}{d} \simeq eN(E_F)\Delta_1 \delta_1,$$

$$\frac{\Delta_2}{\varepsilon} = \frac{V_{N+1}\delta_2}{d} - \frac{1}{2\varepsilon} eN_D \delta_2^2, \quad \delta_3 = \frac{\delta_2 E_F}{\Delta_2}.$$

To write the emitter equations [8], we assume that there are no charges in the emitter barrier. Then the electric field across $\delta_1$ (see Fig. 1) is equal to that in the emitter barrier. Furthermore, the areal charge density required to create this electric field is provided by the emitter. $N(E_F)$ is the density of states at the emitter $E_F$. To write the collector equations [8], we assume that the region of length $\delta_2$ in the collector is completely depleted of electrons [8] and local charge neutrality in the region of length $\delta_3$ between the end of the depletion layer $\delta_2$ and the collector. In order to close the set of equations we impose global charge conservation and that all voltage drops across the different regions must add up to the applied bias:

$$\sigma + \sum_{i=1}^{N} (n_i(\epsilon_{\omega_i}) - eN_D^w) = eN_D(\delta_2 + \frac{1}{2}\delta_3).$$

$$V = \sum_{i=1}^{N+1} V_i + \sum_{i=1}^{N} V_{wi} + \frac{\Delta_1 + \Delta_2 + E_F}{\varepsilon}.$$

Note that the right hand side of Eq. (8) is the positive 2D charge density depleted in the collector region. Instead of the rate equations (3), we can derive a form of Ampère’s law which explicitly contains the total current density $J(t)$. We differentiate (8) with respect to time and eliminate $n_i$ by using (3). The result is

$$\varepsilon \frac{dV_i}{dt} + J_{i-1,i} = J(t), \quad i = 1, \ldots, N+1,$$

where $J(t)$ is the sum of displacement and tunneling currents. The time-dependent model consists of the 3N + 8 equations (3) - (10) (the currents are given by
Eqs. (2)), which contain the $3N + 8$ unknowns $\epsilon_{\nu i}$, $V_{\nu j}$, $(i = 1, \ldots, N)$, $V_j$ $(j = 1, \ldots, N + 1)$, $\Delta_1$, $\Delta_2$, $\delta_k$ $(k = 1, 2, 3)$, $\sigma$, and $J$. Thus we have a system of equations which, together with appropriate initial conditions, determine completely and self-consistently our problem. The boundary conditions arise in a natural way. Notice that the charge and electric field at the boundaries cannot be set prior to the calculation of the whole structure, which all previous models did.

In this paper we are interested in analyzing the statistics of the model and the stability of the stationary solutions. One way to do this is to numerically solve the algebraic-differential system \( \mathbf{H} \cdot \mathbf{D} \) (plus appropriate initial conditions) for each bias until a stationary profile is reached. This is rather costly, so that we follow this procedure for a given value of the bias and then use a numerical continuation method to obtain all stationary solution branches in the I–V characteristic diagram. This yields both unstable and stable solution branches. Direct integration of the stationary equations (dropping the displacement current in \( \mathbf{D} \)) presents important problems of numerical convergence to the appropriate solutions in regions of multistability (see below).

We analyze a DQW (sample a) consisting of 90Å GaAs wells and 40Å Ga$_{0.5}$Al$_{0.5}$As barriers. The doping at both emitter and collector is $N_D = 2 \times 10^{18}$cm$^{-3}$, and in the wells it is $N_D^w = 1.5 \times 10^{11}$cm$^{-2}$. The half-width of the well states is $\gamma = 4$meV in Eqs. (2) and $T = 0$. We do not consider the effect of other symmetry points in the conduction band than $\Gamma$. Fig. 2 shows the DQW I–V characteristic for two different values of $N_D^w$. In Fig. 3a the low bias peak corresponds to C1C1 tunneling ($\epsilon_i$ are the conduction subbands ordered starting from that with lowest energy) between adjacent wells. At higher bias multistability of stationary solution branches sets in (three stable solutions coexist at about 0.44 V). To understand the difference between these solutions, we have depicted in Fig. 3b the potential profile of three different solutions (two stable, one unstable) corresponding to the same voltage (0.41 V). In Fig. 3b, the electrons flow from the emitter to C1 in the first well. Then there is C1C2 tunneling to the second well. A stable solution with lower current density is shown in Fig. 3c. There the C1 at the first well is below the bottom of the emitter layer, then the electrons flow to C2 at the first well instead and J is smaller. A similar situation occurs at higher bias, Figs. 3d to f. The subbands of the two wells are clearly off-resonance for the solution with lowest current, Fig. 3f. Notice that the current flowing from the emitter to the structure and the potential profile are quite different for the different solutions of our model. This shows that boundary conditions assumed in previous publications might constitute gross oversimplifications of the physical situation. In Fig. 3 we present the regions of multistability depending on the bias and the dimensionless doping inside the wells, $\nu = w N_D^w / [\epsilon (\epsilon_{C2} - \epsilon_{C1})]$, or at the emitter $s = w^2 N_D^w / [\epsilon (\epsilon_{C2} - \epsilon_{C1})]$. We see that there is a lower and upper limit for both $\nu$ and $s$ to have bistability. Then it is possible to control the presence and extent of bistability in a sample by changing the doping in the wells or at the contacts and the well widths.

In Fig. 4 we plot the I–V curve of a 90ÅGaAs/40ÅGa$_{0.5}$Al$_{0.5}$As SL with 11 barriers and 10 wells. Its doping is as in Fig. 2a. The stable branches are shown as continuous lines in Fig. 4. The inset shows three electric field profiles corresponding to three different voltages. They show the presence of domains in the SL with a domain wall which moves one well as we change the bias from one branch to the next one. Domain coexistence is also shown in the SL electrostatic potential profile; see Fig. 5 for a fixed bias $V_2 = 0.81$V. The first branch in Fig. 5 corresponds to C1C1 tunneling. As $V$ increases, C1C2 tunneling becomes possible in part of the structure and we have domain formation. This situation confirms the findings with other discrete models with ad hoc boundary conditions [7–9,13–15]. An interesting feature in Fig. 5 is that satellite peaks have a smaller current than the C1C1 peak. This agrees with the results of Ref. [13]. Another interesting feature due to the voltage drop at the contacts is that the number of branches in the I–V curve is less than the number of wells. This behaviour can be understood looking at the branch at 1.21 V where the low field domain occupies the two wells closer to the emitter. C1C2 tunneling occurs between all the wells in the branch with $V_3 = 1.48$V corresponding to a very intense peak of the current.

In summary, we have proposed and solved a microscopic selfconsistent model for the sequential current through a multilayer structure which includes the current through the contacts and appropriate boundary conditions. We have obtained the static I–V curve and phase diagrams of a DQW and a SL, which display multistability associated to domain formation. Exchange-correlation (not included in our model) has been demonstrated to reduce the bistability in a DB [19]. Including exchange-correlation effects is the aim of a future work.

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FIG. 1. Electrostatic potential profile in a SL (sample b) for $V_2 = 0.81V$.

FIG. 2. DQW I–V characteristics (sample a). The continuous (dotted) lines correspond to stable (unstable) solution branches: (a) $N_{W1}^D = 1.5 \times 10^{11} cm^{-2}$; and (b) $N_{W2}^D = 4.31 \times 10^{11} cm^{-2}$. The inset magnifies the C1C1 resonant peak, showing the region of bistability.

FIG. 3. (a) – (c) The three stationary potential profiles for the DQW structure of Fig. 2a at 0.41 V, ordered from highest to lowest current density. (d) – (f) Same for a bias $V = 0.56V$. In all cases the emitter Fermi energy and the subband energies are depicted.

FIG. 4. Phase diagrams showing the regions of multistability for the DQW (sample a): (a) dimensionless well doping $\nu$ versus voltage at $s_1 = 1.97$ ($N_D = 2 \times 10^{18} cm^{-3}$), $\nu_1 = 0.46$ corresponds to the well doping of Fig. 2b; (b) dimensionless contact doping $s$ versus voltage, at $\nu_1$.

FIG. 5. I–V characteristic curve of a SL (sample b). The inset shows the electric field distribution through the SL for three voltages: $V_1 = .69 V; V_2 = .81V; V_3 = 1.48V$. 

4
Bistability

\[ s = s_1 \]

\[ v = v_1 \]
