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Intrinsic bistability in resonant-tunneling structures

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We calculate in the effective-mass approximation the current-voltage characteristic for an $Al_xGa_{1-x}As$-GaAs-$Al_xGa_{1-x}As$ heterostructure. Our calculation includes the effect of electron-electron interaction in a self-consistent way. We show that charge accumulation in the quantum well is large enough to produce a bistability in the negative-differential-resistance region of the current-voltage curve.

Resonant tunneling in double-barrier structures (DBS) has been studied for more than fifteen years since the original work by Chang, Esaki, and Tsu.[1]

Advances in the techniques of building semiconductor heterostructures have stimulated both experimental and theoretical interest in the transport properties of these systems. Resonant tunneling in DBS is now a well-established phenomenon.[2-5] However, and despite the great activity in this field, the phenomenon still presents some aspects which are not well understood. The main interest in the study of transport properties of heterostructures and, in particular, double-barrier devices is originated by the possibility of obtaining a region of negative differential resistance (NDR) in the current-voltage (I-V) characteristics.[2]

Recently, Goldman, Tsui, and Cunningham[6] reported the observation of a bistability in the I-V curve of DBS consisting of a GaAs well between two $Al_xGa_{1-x}As$ barriers. This bistability—an hysteresis in the I-V curve—occurs in the region of NDR. There are two possible effects that could give rise to this irreversibility. On one hand an intrinsic effect originated in the accumulation of negative charge in the region of the well. On the other hand—as was pointed out by Sollner[7]—this hysteresis could also be due to the spontaneous oscillation of a circuit containing an element that exhibits NDR.[8] Although in the original experiments probably both effects were present, recent studies of the bistability in asymmetric DBS (Ref. 9) clearly show that in these systems the main source for the irreversibility is the intrinsic effect: the charge buildup in the well.

From the theoretical point of view the phenomenon has been studied using a crude estimation of the charge buildup,[10] although these estimations cannot be used to compute quantitatively the bistability, they make evident that the charge accumulation can in fact produce the hysteresis in the I-V curve. What remains to be done is a self-consistent calculation to make, if possible, quantitative estimations. Recently, Kluksdahl *et al.*[11] presented some results of a self-consistent study, using the Wigner-function approach.

The aim of this Rapid Communication is to discuss and present self-consistent results for the resonant tunneling in DBS using simultaneous solutions to the Schrödinger and Poisson equations. Consider a double-barrier diode in the usual planar-geometry configuration of layers of [n-type GaAs (emitter)]/[$Al_xGa_{1-x}As$ (first barrier)]/[GaAs (well)]/[$Al_xGa_{1-x}As$ (second barrier)]/[n^+-type GaAs (collector)]. In our calculation we included a spacer layer by taking a profile of doping in the electrodes.

In the effective-mass approximation the wave function of the tunneling electron is derived from the Γ-valley minimum of the conduction band. In this approximation the problem reduces to calculate the motion of electrons with an effective mass m^* in an effective barrierlike potential which describes the bottom of the conduction band of the diode (see Fig. 1). In order to correctly describe the redistribution of negative charge in the region of the well it is important to include also the electron-electron interaction which in the present work is computed in the Hartree approximation. The voltage applied to the junction produces an electric field in the region of barriers and well. The voltage profile is calculated in a self-consistent way by solving simultaneously the Schrödinger and Poisson equations. The partially integrated Schrödinger equation which describes the motion of the electrons in the z direction is given by

$$\left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}+U(z)\right]\psi_\epsilon^{(j)}(z)=\epsilon\psi_\epsilon^{(j)}(z)\,, \qquad (1)$$

where m^* is the electron's effective mass—assumed constant through the whole junction. The motion in the plane parallel to the interfaces is described by plane waves with

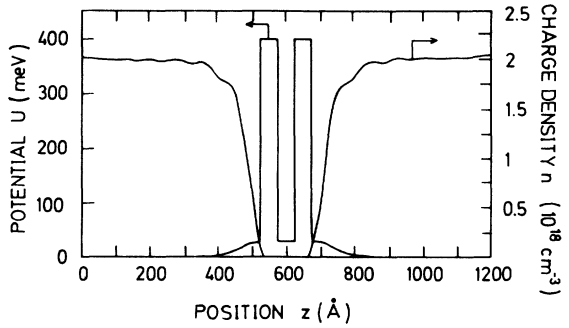

FIG. 1. Self-consistent potential $U(z)$ and electron charge-density profiles for zero bias. The parameters are barrier height 370 meV; width of the barriers, well, and spacer layers 50 Å; and dopant density in the electrodes 10^{18} donors/cm^3.

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quantum numbers k_x and k_y, and so the energy of the electron is then given by

$$E=\epsilon+\frac{\hbar^2}{2m^*}(k_x^2+k_y^2)\,. \tag{2}$$

The potential $U(z)$ has three different contributions: the square barrier potential $V_0(z)$ which modulates the bottom of the conduction band, the potential $v(z)$ created by the background of positive charge and the electron gas, and one given by the bias applied to the junction which is imposed as a boundary condition on $v(z)$.

The self-consistent potential $v(z)$ is calculated by means of the Poisson equation

$$\frac{d^2v}{dz^2}=\frac{4\pi e^2}{\mathcal{K}}[N_D(z)-n(z)]\,. \tag{3}$$

Here e is the electron charge, $\mathcal{K}$ is the dielectric constant, $N_D(z)$ is the doping profile of ionized donors, and $n(z)$ the electronic-charge-density profile.

It is convenient to separate the sample in three regions: region I ($z<0$) is the portion of the emitter far from the junction; region II ($0<z<L$) which includes the double barrier (we take the well centered at $z=L/2$); and finally region III ($L<z$) is the portion of the collector away from the interfaces. The total potential $U(z)$ is

$$U(z)=\begin{cases}0, & z<0\,, \quad (4a)\\ V_0(z)+v(z), & 0<z<L\,, \quad (4b)\\ -eV, & L<z\,. \quad (4c)\end{cases}$$

Here V is the bias voltage applied to the junction.

We solve the Schrödinger and Poisson equations [Eqs. (1) and (3), respectively] in region II taking L large enough to guarantee that in the outer regions (I and III) the potential is constant.

The solutions of Eq. (1) are of three different kinds. For $0<\epsilon<\infty$,—above the bottom of the emitter conduction band—the motion is unbounded at both ends ($z<0$ and $z>L$). These solutions far from the barriers correspond to running waves and there are two states for each ϵ, one incident from the left-hand side $\psi_\epsilon^{(+)}$ and the other incident from the right-hand side $\psi_\epsilon^{(-)}$. For $-eV<\epsilon<0$ (between the bottoms of the collector conduction band and the emitter conduction band), the motion is bounded at one end ($z<0$) and there is one solution for each ϵ, labeled $\psi_\epsilon^{(0)}$.

The electronic charge density is calculated by summing over all the states and weighting them with a Fermi factor,

$$n(z)=\frac{2}{L_xL_y}\sum_{k_x,k_y}\left[\int_{-eV}^{0}d\epsilon f((E-E_{CF})/k_BT)|\psi_\epsilon^{(0)}(z)|^2 + \int_0^\infty d\epsilon[f((E-E_{EF})/k_BT)|\psi_\epsilon^{(+)}(z)|^2+f((E-E_{CF}/k_BT)|\psi_\epsilon^{(-)}(z)|^2]\right]. \tag{5}$$

Here L_x and L_y are the transverse dimensions of the sample and $f(x)$ is the Fermi function. The chemical potential of the emitter and collector are E_{EF} and E_{CF}, respectively, T is the temperature and k_B the Boltzmann constant. The chemical potentials are calculated with the constraint that in regions I and III the system remains neutral.

Once the self-consistent solutions of Eqs. (1) and (3) are obtained, the current can be calculated using the well-known expression:[2]

$$J=\frac{em^*k_BT}{2\pi^2\hbar^3}\int_0^\infty d\epsilon\frac{k_1}{k_2}|T_\epsilon|^2\ln\left[\frac{1+\exp[(E_{EF}-\epsilon)/k_BT]}{1+\exp[(E_{CF}-\epsilon)/k_BT]}\right] \tag{6}$$

with

$$k_1=\left[\frac{2m^*\epsilon}{\hbar^3}\right]^{1/2},\quad k_2=\left[\frac{2m^*(\epsilon+eV)}{\hbar^3}\right]^{1/2},$$

and T_ϵ is the transmission coefficient of the junction.

In what follows we present results for a GaAs-$Al_xGa_{1-x}As$ double barrier in which the barriers and the well are 50 Å wide. We also include 50-Å spacer layers and a doping in the contacts of 10^{18} donors/cm^3. The other parameters of the junction are[12] $m^*=0.068m$, the barrier height $V_0=370$ meV, and the dielectric constant $\mathcal{K}=11.9$. All results were obtained with $T=5$ K.

We first present results for the case of zero bias. The electronic charge density and the potential profiles are shown in Fig. 1. Note that for the parameters used, there is no charge accumulation in the well. The resonant level lies approximately 8 meV above the chemical potential. The double-barrier structure lies on the top of a flat bump which arises from the doping profile. The effect of the spacer layer is clearly seen in this figure.

For the case of an applied bias we proceed in the following way. We made runs of the self-consistent calculation incresing the applied voltage in small amounts (typically 1 mV in the NDR region and 5 mV away from it). In each run we use the converged solution obtained with the previous bias as a seed for the calculation. Once the NDR region was observed we decrease slowly the applied voltage using the same procedure. In this way, we were able to obtain an hysteresis loop. The results for the I-V characteristics are shown in Fig. 2. For the sake of comparison we also plot in the same figure the results of the I-V curve for the flatband model (non-self-consistent).

In agreement with results of Ref. 13 and 14 our results show that the effect of the electron-electron interaction is mainly to shift the curve towards larger applied voltages. More interesting than these changes of the curve is the bistability obtained in the NDR region.

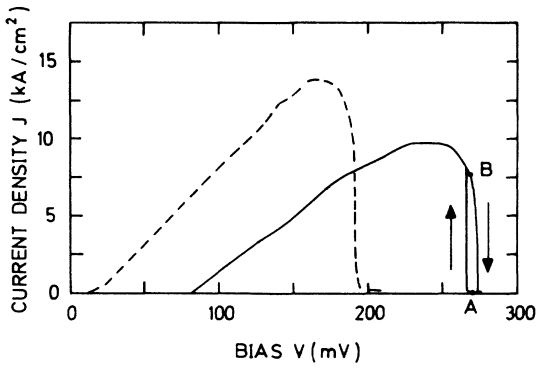

FIG. 2. Current-voltage characteristic for the heterostructure discussed in the text. All parameters are the same as in Fig. 1. Dashed line corresponds to flatband results (non-self-consistent). Continuous line is the self-consistent result. The arrows in the bistability region indicate the direction of voltage sweep. Points *A* and *B* indicate two different solutions for the same applied voltage.

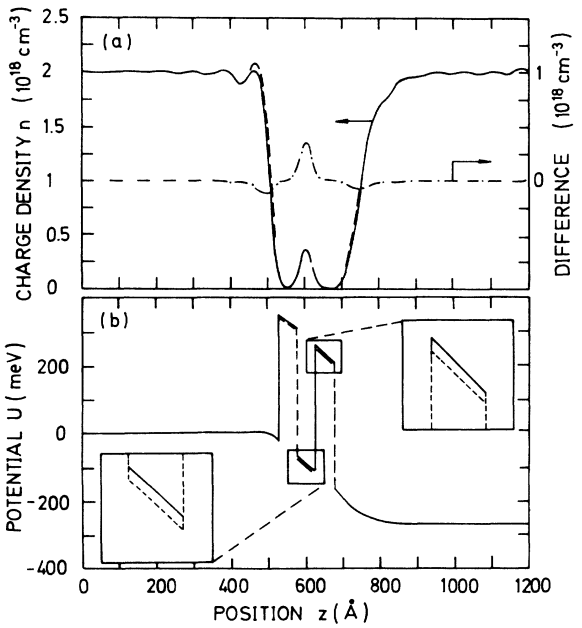

FIG. 3. (a) Charge-density profile for the two solutions corresponding to points *A* and *B* of Fig. 2. Dashed line (solution *A*) corresponds to the state without current. Continuous line (solution *B*) corresponds to the current carrying state. Dashed-dotted line is the difference between them. Note that this difference is large only in the region of the well where the charge buildup occurs. (b) Potential profile for the two solutions *A* and *B*. Insets show the effect of charge buildup at the bottom of the well and at the top of the barriers.

In order to characterize the two solutions which give rise to this bistability, we show in Fig. 3(a) the charge profile corresponding to the two solutions obtained for the same bias, points *A* and *B* indicated in Fig. 2. As expected the solution with small current—solution *A*—has no charge accumulation in the well, while the current carrying solution *B* has a buildup of charge in the well. Away from the well the charge profile remains essentially the same. In Fig. 3(b) we present the results obtained for the self-consistent potential corresponding to the same solutions. First our results show that most of the voltage drop takes place in the region of the barriers and well and not in the electrodes;[11,15] this is of course what one should expect from physical intuition. A second point that could be used to check our calculation procedure is the fact that away from the interfaces the potential and the charge-density profiles go smoothly to the constants imposed as boundary conditions; this is an indication that we have worked with a large enough *L*—the length of region II.

As indicated in the inset of Fig. 3(b) the bottom of the well is shifted according to the amount of charge buildup, and the origin of the bistability then becomes evident. When the voltage applied is such that the resonant level lies close to the bottom of the emitter conduction band, there are two possible solutions. The current carrying solution has charge accumulation in the well; if the current disappears, for example, by increasing and decreasing the voltage, the charge accumulation is highly reduced and the bottom of the well shifts down lowering the energy of the resonant level. If the new energy of this state lies below the bottom of the emitter conduction band, this situation without current will also be a self-consistent solution.

Finally, we must stress that the width of the hysteresis loop as obtained in the present work is a measure of the numerical stability of the two possible solutions and not necessarily related to the width measured in an experiment. In any case, this width is quite small for the parameters used in the present work. According to the calculation of Sheard and Toombs,[10] the width of the bistability is given by the maximum charge accumulation and the capacitance of the structure. Following these ideas, the width of the bistability in our junction should be of the order of 100 mV, six times larger than the result obtained in our self-consistent calculation. Although our calculation always tends to subestimate this width, the numbers obtained for the resonant level position and the charge buildup indicate that the maximum possible width of the bistability is of the order of 50 mV, still a factor of 2 smaller than the prediction of Ref. 10.

In summary, we have studied the *I-V* characteristics of double-barrier structure in a self-consistent way. Our results show that the charge accumulation can, in fact, produce a bistability in the NDR region of the *I-V* curve. For the parameters studied, which are not necessarily the best to produce a wide bistability, the charge density at the center of the well can be up to 20% of the charge density in the electrodes. This charge buildup is enough to produce observable effects if the resonant level is sufficiently narrow.

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[1]L. L. Chang. L. Esaki, and R. Tsu, Appl. Phys. Lett. **24**, 593 (1974).

[2]R. Tsu and L. Esaki, Appl. Phys. Lett. **22**, 562 (1973).

[3]T. C. L. G. Sollner, W. D. Goodhue, P. E. Tannenwald, C. D. Parker, and D. D. Peck, Appl. Phys. Lett. **43**, 588 (1983).

[4]E. E. Mendez, L. Esaki, and W. I. Wang, Phys. Rev. B **33**, 2893 (1986).

[5]B. Ricco and M. Ya. Azbel, Phys. Rev. B **29**, 1970 (1984).

[6]V. J. Goldman, D. C. Tsui, and J. E. Cunningham, Phys. Rev. Lett. **58**, 1256 (1987).

[7]T. C. L. G. Sollner, Phys. Rev. Lett. **59**, 1622 (1987).

[8]T. J. Foster, M. I. Leadbeater, L. Eaves, M. Henini, O. H. Hughes, C. A. Payling, F. W. Sheard, P. E. Simmonds, G. A. Toombs, G. Hill, and M. A. Pate, Phys. Rev. B **39**, 6205 (1989).

[9]A. Zaslavsky, V. J. Goldman, D. C. Tsui, and J. E. Cunningham, Appl. Phys. Lett. **53**, 1408 (1988).

[10]F. W. Sheard and G. A. Toombs, Appl. Phys. Lett. **52**, 1228 (1988).

[11]N. C. Kluksdahl, A. M. Kriman, D. K. Ferry, and C. Ringhofer, Phys. Rev. B **39**, 7720 (1989).

[12]T. Ando and S. Mori, J. Phys. Soc. Jpn. **47**, 1518 (1979).

[13]H. Ohnishi, T. Inata, S. Muto, N. Yokoyama, and A. Shibatomi, Appl. Phys. Lett. **49**, 1248 (1986).

[14]M. Cahay, M. McLennan, S. Datta, and M. S. Lundstrom, Appl. Phys. Lett. **50**, 612 (1987).

[15]In Ref. 11 the authors obtained results in which the voltage drop takes place in the emitter. We also found these types of solutions when the seed for the self-consistent calculation was very different from the final solution. However, these solutions are very sensitive to the boundary conditions, they tend to localize the voltage drop at the edge of what we called region II and give a discontinuity in the derivatives of the potential and charge profiles. We believe this type of solution to be unphysical.