

Thomas–Fermi approach to resonant tunneling in δ -doped diodes

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We study resonant tunneling in B- δ -doped diodes grown by Si-molecular beam epitaxy. A Thomas–Fermi approach is used to obtain the conduction-band modulation. Using a scalar Hamiltonian within the effective-mass approximation, we demonstrate that the occurrence of negative differential resistance (NDR) only involves conduction-band states, whereas interband tunneling effects seem to be negligible. Our theoretical results are in very good agreement with recent experimental observations of NDR in this type of diode. © 1995 American Institute of Physics.

Resonant tunneling (RT) through semiconductor diodes has recently attracted considerable attention because of its applications in ultrahigh-speed electronic devices. Their most remarkable feature is that their I - V characteristics show negative differential resistance (NDR). Most of these devices are based in double-barrier structures, where RT occurs via quasibound states within the well region in the same energy band (conduction or valence band). On the contrary, other kinds of RT devices present interband transitions as, for instance, InAs–GaSb or InAs–AlSb–GaSb structures.¹ In the later case, Kane’s parameter is not negligible as compared with band gaps and, consequently, more elaborated band structures are required to fully account for RT.

Recently, Sardela *et al.*² have observed NDR at room temperature in B- δ -doped diodes grown by Si-molecular beam epitaxy. A schematic cross section of the studied device is shown in Fig. 1. Experimental NDR peaks are seen to appear at about ± 0.2 V. However, it is not clear whether RT occurs via intraband or interband mechanisms: Indeed, the authors argued that preliminary calculations based on the static solution of the Poisson’s equation show that the whole structure only supports a very shallow quasibound state and, consequently, conduction-band modulation cannot explain the observed NDR. Hence, they claimed that the valence-band plays a major role in RT of these diodes and therefore two-band Hamiltonians³ are necessary to understand the obtained results.

In this paper we will show that scalar Hamiltonians for the conduction-band envelope functions work well to explain the results of Sardela *et al.*² Instead of using self-consistent approximations to compute the one-electron potential due to δ doping, we will concern ourselves with the nonlinear Thomas–Fermi (TF) formulation as introduced by Ioratti.⁴

This approach reproduces accurately the various subbands densities in periodically δ -doped GaAs layers at moderate and high doping⁵ and it has proved itself useful in describing the electronic structure in the presence of applied external fields.^{6,7} We thus obtain results showing the existence of several quasibound states with large lifetimes localized between the two δ layers that successfully explain the I - V characteristics previously obtained by Sardela *et al.*

We consider an electron of effective mass m^* in the δ -doped diode (see Fig. 1) in the presence of an electric field applied along the growth direction. Nonparabolicity effects are neglected so that m^* will be taken to be independent of the electron energy. The electron wave function and the total energy of the electron are given by $\Psi(\mathbf{r}, \mathbf{k}_\perp) = \exp(i\mathbf{k}_\perp \cdot \mathbf{r}_\perp) \phi(x)$ and $E(\mathbf{k}_\perp) = E + (\hbar^2 \mathbf{k}_\perp^2 / 2m^*)$, where $\phi(x)$ is the envelope function. Note that we have taken isotropic bands at the X minima, and, in fact, the band structure of Si is strongly anisotropic ($m_l^*/m_t^* \sim 5$). Hence, we should consider an *average* value m^* that would be obtained, for example, in a measurement of mobility.⁸ A similar assumption has been made in self-consistent analyses of n-type δ -doping layers and superlattices in Si.⁹ We will comment on this point in more detail later. In the effective-mass approximation the envelope function satisfies the following Schrödinger equation:

$$\left(-\frac{\hbar^2}{2m^*} \frac{d^2}{dx^2} + V_{\text{TF}}(x) - eFx \right) \phi(x) = E \phi(x). \quad (1)$$

Here F is the applied electric field and $V_{\text{TF}}(z)$ is the solution of the nonlinear TF equation (see Refs. 6 and 7 for details). As usual in scattering problems, the envelope function at the bottom electrode is a superposition of incident and reflected traveling waves, whereas at the top one there is only a transmitted wave. Hence standard numerical techniques⁶ can be used to obtain the transmission coefficient $\tau(E, V)$ for a given incident energy E and a given applied voltage $V = FL$, L being the length of the whole structure. Due to the high

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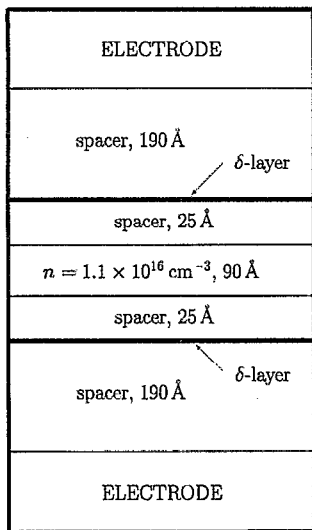


FIG. 1. Schematic cross section of a B- δ -diode grown by Si-molecular beam epitaxy, as studied in Ref. 2. The whole structure is embedded between two electrodes consisting of highly n -doped Si layers. Each δ layer is 8 Å width with an acceptor concentration $1.4 \times 10^{13} \text{ cm}^{-2}$.

doping of the electrodes, the electric field is assumed to be nonzero only within the structure. In addition, these high screening effects imply that $V_{TF}(z)$ also vanishes at the electrodes.

We have set an effective mass $m^* = 0.33$ and a dielectric constant $\epsilon = 11.7$ in Si.⁸ In the absence of external fields, the TF potential presents two peaks corresponding to the δ layers, as shown in Fig. 2. It is worth mentioning that the maximum value of the conduction-band modulation is about 20% of the band gap in Si. This value is of the same order of that obtained self-consistently in Sb- δ -doped grown by Si-molecular beam epitaxy with similar areal concentration of impurities.¹⁰ Assuming a similar profile for the valence band, we are led to the conclusion that interband RT should not play a significant role, at least at moderate electric fields. Hence, the scalar Hamiltonian (1) suffices to describe the electronic structure of the diode. In addition, since we are

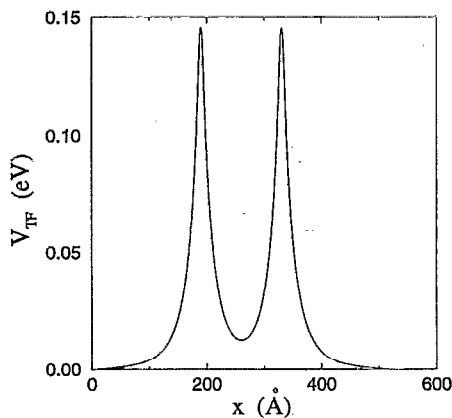


FIG. 2. Modulation of the conduction-band obtained from the Thomas-Fermi approach for the structure shown in Fig. 1 without applied electric field.

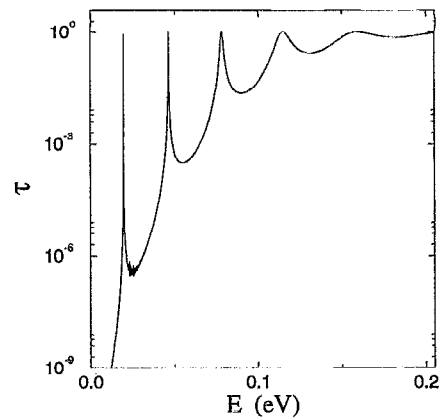


FIG. 3. Transmission coefficient without applied electric field as a function of the incident energy.

close to the conduction-band edge, parabolic subbands hold, as we assumed previously. To elucidate whether the conduction-band modulation can support narrow quasibound states, we have numerically evaluated the transmission coefficient at zero bias $\tau(E,0)$ as a function of the incident energy and results are plotted in Fig. 3. From this figure it becomes clear that four resonances (quasibound states) appear below the top of the potential. The levels are nearly equally spaced in this case: This is easy to understand if we notice that the potential profile between the two δ layers is almost parabolic. Interestingly, we thus have demonstrated that δ -doped diodes could be used to achieve equally spaced peaks in the collector characteristics, in analogous way to parabolic wells formerly proposed by Capasso and Kiehl.¹¹

The tunneling current density at a given temperature T for the diode sketched in Fig. 1 can be calculated within the stationary-state model from

$$j(V) = \frac{m^* e k_B T}{2 \pi^2 \hbar^3} \int_0^\infty \tau(E, V) N(E, V) dE, \quad (2a)$$

where $N(E, V)$ accounts for the occupation of states to both sides of the device, according to the Fermi distribution function, and it is given by

$$N(E, V) = \ln \left(\frac{1 + \exp[(E_F - E)/k_B T]}{1 + \exp[(E_F - E - eV)/k_B T]} \right). \quad (2b)$$

We show in Fig. 4 the computed $j-V$ characteristics at $T = 77 \text{ K}$ and at room temperature. The curves have been obtained taking the Fermi energy at the conduction-band edge away from the δ layers. Other values of the Fermi energy simply modify the scale of j , keeping its shape unchanged. The main NDR feature, also observable at room temperature, appears at about 0.22 V, which is very close to experimental results of Sardela *et al.*² Note that our computation predicts two separated peaks in the $j-V$ characteristics at around 0.22 V, while experiments show only a single, broader peak. Inelastic scattering mechanisms, not included in our analysis, are known to cause a broadening of the intrinsic level width, and the amount of inelastic¹² broadening makes the two separated resonances to merge into a single one, according to experimental results. Moreover, there exist

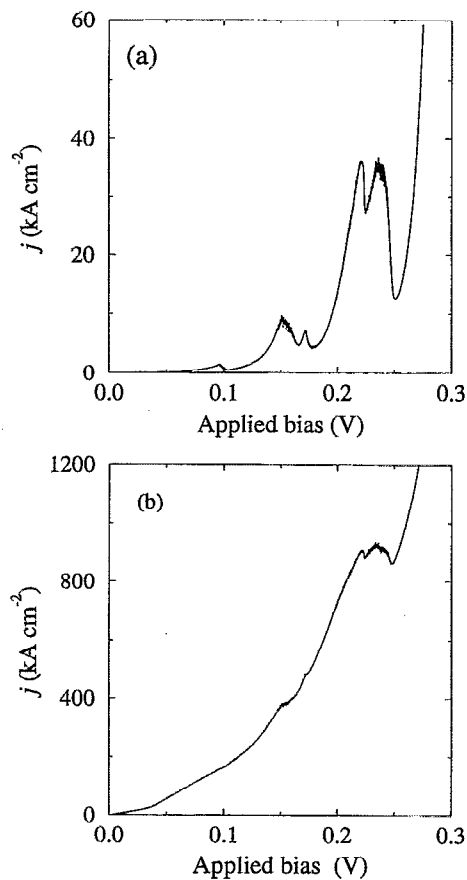


FIG. 4. Computed j - V characteristics of δ -doped diodes at (a) $T=77$ K and (b) room temperature.

smaller peaks at about 0.10 V and 0.15 V, arising from the lower resonances of the well. In experiments² such small peaks are almost unnoticeable, probably because we are overestimating its height due to the absence of inelastic effects in our model which, of course, tend to disrupt coherent tunneling. The theoretical peak-to-valley ratio of the main NDR feature is 2.8 at 77, larger than the experimental value 1.4 at the same temperature. The reason why the theoretical calculations predicts larger peak-to-valley ratios is that sequential tunneling is not being considered.

Finally, some words concerning the many valley band structure of Si and its possible effects on the present results are in order. As mentioned in Sec. II, we are assuming an isotropic effective mass m^* obtained, for instance, as the geometric average of longitudinal and transversal masses. On the other hand, it is known that level splitting arises due to anisotropic effects in δ -doped Si, and that it increases with doping concentration.⁹ However, in this paper we do not at-

tempt to estimate quantitatively this splitting in the diode because we are mainly interested in the question of whether interband coupling can significantly affect tunneling processes in the diode. What we have actually done is to estimate in part the possible influence of the many valleys by using different values of m^* in our computations. To be specific, we have repeated our calculations with $m^*=m_l^*$ and concluded that our results remain almost unchanged. For instance, the height of the TM potential changes slightly, whereas the effective mass is reduced by 50%. In addition, the main NDR peak appears at almost the same position in the j - V characteristics as that shown in Fig. 4. Hence, we are led to the conclusion that including an anisotropic conduction band will not change substantially our main conclusion, namely that interband tunneling seems to play a minor role in Si δ -doped diodes.

We have proposed a simple model to explain RT through δ -doped diodes grown by Si-molecular beam epitaxy. The conduction-band modulation is obtained by means of the TF approach and the corresponding electronic states are described by a scalar Hamiltonian. Our results show that NDR effects are due to conventional resonant tunneling process in vertical transport, whereas interband tunneling does not give rise to significant contributions. The obtained results are in excellent agreement with recent measurements by Sardela *et al.*² This success suggests that our approach, being very simple and computationally inexpensive, may be very useful in dealing with semiconductor nanostructures.

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