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Modelling of Current through n^+-GaAs / i-$Al_xGa_{1-x}As$ / n^+-GaAs Structures and Comparison with Measurements

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Introduction

Our purpose is to model current flow through n^+-GaAs / i-$Al_xGa_{1-x}As$ / n^+-GaAs single-barrier tunneling structures. We calculate current as a function of voltage, I(V), and conductivity at low voltage as a function of temperature, G(T), and compare the results with those measured in several such structures. We have treated structures with n-doped injection layers, where the current is mainly carried by electrons.

Description of the Physical Model

We assume that the current flowing from one side (z=0) of the structure to the other (z=L) is made up by a tunneling plus a thermionic emission current and thus[1] is given by:

$$j = q\frac{m^* k_B T}{2\pi^2\hbar^3}\int_{\max(E_c(0),E_c(L))}^{\infty} dE \quad T(E) \quad \ln\left(\frac{1+\exp\left(\frac{E_f(z=0)-E}{k_B T}\right)}{1+\exp\left(\frac{E_f(z=L)-E}{k_B T}\right)}\right) \quad (1)$$

where z is the space coordinate perpendicular to the layer interfaces. T(E) is the transmission coefficient through the structure for a plane wave with energy E. In order to calculate T(E), it is necessary to know the shape of the potential $E_c(z)$ seen by the electrons, which is governed by Poisson's equation. We solve this equation self-consistently for the following model of the charge distribution : The hole and ionized donor and acceptor densities are evaluated according to Fermi-Dirac statistics and assuming a continuous density of states for the hole density. The electron density (n) is calculated from the electronic wavefunctions. Using the envelope function model, and taking into account that our structures are homogeneous in the x-y plane, we have :

1 L. Esaki, R. Tsu, IBM J.Res.Dev. 14, 61 (1970)

$$n(z) = \frac{m^* k_B T}{2\pi^2 \hbar^3} \sqrt{\frac{m^*(z)}{2}} \int_{E_c(z)}^{\infty} \frac{dE}{\sqrt{E - E_c(z)}} |\psi(z,E)|^2 \ln\left(1 + \exp\left(\frac{E_f - E}{k_B T}\right)\right) \quad (2)$$

$\psi(z,E)$ are envelope functions and obey the following Schroedinger equation :

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m^*}\frac{d\psi}{dz}\right) + E_c(z)\psi(z) = E\psi(z) \quad (3)$$

Since we deal with a structure open at its boundaries, equation (3) is not an eigenvalue problem. Electrons flow into the structure with any energy E which they may have in the material adjacent to the structure. The wavefunctions $\psi(z,E)$ are assumed to be plane waves when entering the structure, and then evolve according to equation (3). We have normalized the wavefunctions such that the resulting total electron density in the structure exactly compensates the net positive charge. Once the solution has converged, the quantum mechanical electron density at the borders always ends up to be equal to the semiclassical value there, provided the borders are chosen sufficiently far away from the barrier. Yet, when normalizing such that the quantum mechanical electron density at the borders equals the semiclassical electron density at the borders, convergence cannot always be achieved.

In order to take into account inelastic scattering, one might still calculate the envelope functions from (3), but allow E to be a function of z which changes somewhat randomly over a mean-free-path distance by an amount typical for phonon or impurity scattering. Our way to treat scattering has been proposed by Rajakarunayake *et al.*[2] and consists in damping the Friedel oscillations appearing in the electron density in the electrode layers. When the oscillations are completely damped, then the so obtained electron density in the electrodes is identical to the semiclassical one.

When a bias is applied to the structure, then E_f becomes a function of z. From semiclassical calculations where we have solved self-consistently Poisson's equation together with the electron and hole density continuity equations, we know that the quasi-Fermi levels are almost constant in the n-doped layers and vary approximately linearly in the intrinsic layer. We therefore assume such a form for $E_f(z)$.

2 Y. Rajakarunanayake, T.L. McGill, J. Vac. Sci. Technol. B5, 1288 (1987)

Finally, we also have calculated the I(V) and G(T) characteristics using the semiclassical expression for the electron density. Results from such a calculation will be called "semiclassical (SC)" as opposed to those obtained with the above model for the electron density which we then shall call "quantum mechanical (QM)".

Calculation procedure

We start with the potential obtained by a semiclassical calculation at zero bias. Then we iterate the solution of Poisson's equation until the maximal variation of the potential between two successive iterations is less than 10^{-4} V. The iteration scheme is based on an undamped Newton method employing an approximate Jacobian matrix as proposed by Laux [3]. Schroedinger's equation is solved with a transfer matrix method [4].

When convergence has been attained, we impose a first step of applied bias by superimposing on the potential obtained at the last step a potential which is flat in the cladding layers and varies linearly by the applied bias in the barrier. The same is done for $E_f(z)$. Then we iterate until again convergence is achieved. When working with the semiclassical electron density, we solve Poisson's equation in the subsequent iterations with Dirichlet boundary conditions. When working with the quantum mechanical electron density, Neumann boundary conditions implying a zero electric field at the boundaries must be used. It turns out that with Neumann boundary conditions, the potential difference due to the applied bias is maintained, but the potential is shifted by a constant value throughout the structure. Compensating for this shift after each solution of Poisson's equation then leads to convergence.

Results

Some examples of calculated and measured results are shown in figures 1 to 6. The notations are the following : x is the AlAs mole fraction in the barrier layer, L_B the barrier width and N_D the donor doping density in the electrode layers.

Fig.1 : electron density in an n-i-n single barrier structure calculated semiclassically (solid line), according to (2) (dashed line), and according to (2) modified as proposed in reference 2 with λ =300 Å (dotted line)

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3 S. Laux, F. Stern, J. Appl. Phys. 49, 91 (1986)

4 Y. Ando, T. Itoh, J. Appl. Phys. 61, 1497 (1987)

Fig.2 : conduction band diagram under an applied bias of 16 mV, calculated with the SC electron density (solid line) and the QM electron density (dashed line) for a structure with a 500 Å wide barrier having an Al concentration of 4%, the doping density in the cladding layers being equal to 10^{17} cm^{-3}.

Fig.3 : tunneling current obtained for the structure of fig.2 when calculating the conduction band diagram with the SC electron density (solid line) or the QM electron density (dashed line)

Fig.4 : calculated and measured I(V) characteristics; the calculations having been performed with the parameters indicated in the figure and the SC electron density; the nominal parameter values of the structure are x=0.04, L_B=500 Å, N_D=8*10^{16} cm^{-3}.

Fig.5 : calculated and measured I(V) characteristics, and Fig.6 : calculated and measured G(T) characteristics; the calculations have been performed with the parameters indicated in the figure and the QM electron density; the nominal parameter values of the structure being the same as in Fig.4.

Conclusions

We have compared the calculated and measured I(V) and G(T) characteristics for single barrier structures where the doping level in the injection layers is higher than 5*10^{16} cm^{-3} and where the barrier height is varied between 30 and 100 meV and the barrier width varied between 150 and 600 Å. With both the quantum mechanical electron density and the semiclassical electron density, very good agreement between measured and calculated data has been obtained, with a choice of structural parameters whose values are within the uncertainty limits (i.e. 10%) of the nominal growth values. However, an uncertainty even smaller would be necessary in order to decide which model is closer to reality. Our numerical method has proven reliable also in the case of higher or lower and thicker or thinner barriers as well as many-barrier structures, but no experimental data have been available to us for comparison.

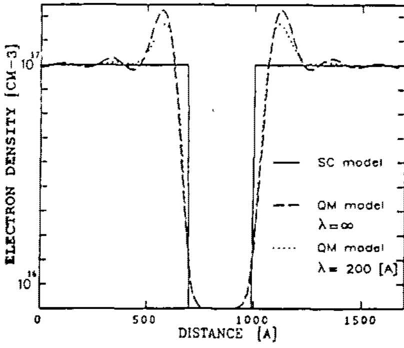

Figure 1

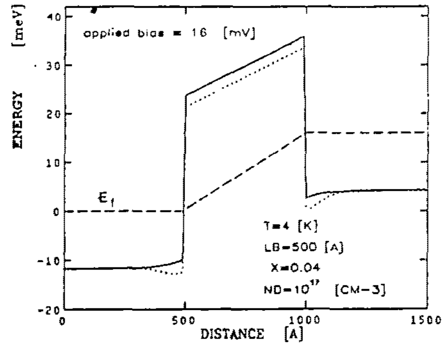

Figure 2

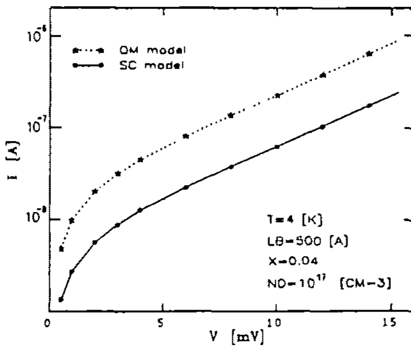

Figure 3

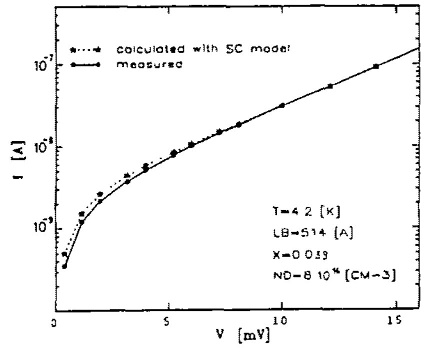

Figure 4

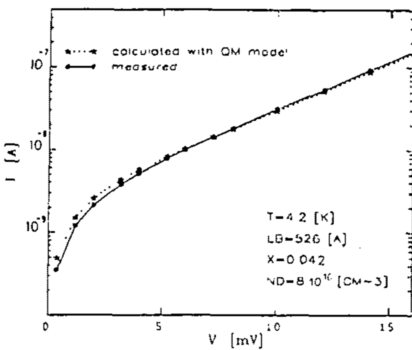

Figure 5

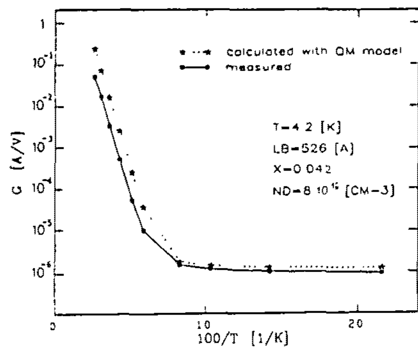

Figure 6