Analysis of Phase Breaking Effect in Triple-Barrier Resonant-Tunneling Diodes

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1. Introduction

Non-Equilibrium Green's Function (NEGF) formalism is widely used to describe electronic transport in quantum devices such as double-barrier resonant-tunneling diodes [1]. However, to our knowledge, there is no application to triple-barrier resonant-tunneling Diodes (TBRTDs) which have an important potential for estimating phase coherence of hot electrons at finite temperatures [2]. A theoretical treatment in Ref. [2] that described phase coherence as solely exponential decay led calculated current density to be small more than two orders in magnitude compared with measured one. Therefore, here, we apply NEGF formalism to TBRTD for the first time.

We use Datta's local scattering model to take phase breaking effects into account [1]. While the model is capable of describing the inelastic nature of scattering, we use more numerically manageable derivative, that is, the model with constant phase relaxation time (Ref. [1]) which ensure the current conservation.

As results, we show calculated values of current densities become same order in magnitude as experimental data.

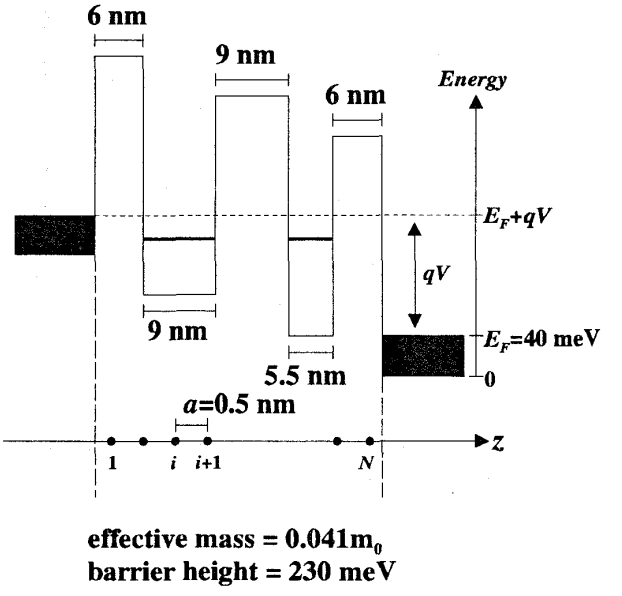

Figure 1: TBRTD model used in the analysis

2. Summary of Equations

In this section, we summaries equations to be used in present NEGF analysis. Figure 1 shows potential energy distribution of our TBRTD model where we assume rectangular shape and neglect any band bending due to space charge effects for the purpose of comparison with Ref. [2]. The whole system is divided into three regions, the left electrode, the device and the right electrode. Since we use the tight-binding model (Ref. [3]) to solve equations, the device region is composed of N lattice points with lattice constant a.

There are two main functions in the analysis, that is the retarded Green's function G^R and electron distribution function f. We assume RTD structure is uniform in the transverse direction and we treat the transverse degrees of freedom by averaging discussed later [1]. Therefore, G^R and f are dependent only on z direction and this fact leads G^R and f to be $N \times N$ matrix and N column vector respectively. When we write down equations for G^R and f at a particular energy E (not to be denoted explicitly) bellow, letters with underbar represent $N \times N$ matrices and letters with upperallow represents N column vectors.

Equation for $\underline{G}^R$

The matrix equation for the $\underline{G}^R$ is written as

$$\left[E\underline{I} - \underline{H}_0 - \underline{\Sigma}_\varphi^R - \underline{\Sigma}_E^R\right] \underline{G}^R = \underline{I}. \qquad (1)$$

Here, $\underline{I}$ is the identity matrix and $\underline{H}_0$ is the coherent part of Hamiltonian in the device region whose matrix elements are given with device potential V_D by

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$$\underline{H}_0(i,j) = \begin{cases} V_D(i) + 2t & i = j \\ -t & i = j \pm 1 \\ 0 & \text{otherwise} \end{cases}, \quad (2)$$

where $t = \hbar^2/2m^*a^2$.

$\underline{\Sigma}_\varphi^R$ in eq. (1) is the self-energy matrix due to the phase breaking effects and the matrix elements are

$$\underline{\Sigma}_\varphi^R = -i\frac{\hbar}{2\tau_\varphi}\delta_{i,j}, \quad (3)$$

where τ_φ is the phase relaxation time and has constant value.

$\underline{\Sigma}_E^R$ in eq. (1) describes effects of presence of electrodes. If we assume electron's motion is coherent in electrodes, we can write

$$\underline{\Sigma}_E^R(i,j) = \begin{cases} -te^{ik_L a} & i = j = 1 \\ -te^{ik_R a} & i = j = N \\ 0 & \text{otherwise} \end{cases}, \quad (4)$$

where $k_{L,R}$ are related to electron energy E through dispersion relation

$$E = V_{L,R} 2t(1 - \cos k_{L,R} a). \quad (5)$$

$V_{L,(R)}$ is the conduction bandedge in the left (right) electrode.

Equation for $\vec{f}$

The equation for the electron distribution function $\vec{f}$ is given by

$$\vec{f} = \underline{K}\vec{f} + \vec{K}_L f_L + \vec{K}_R f_R. \quad (6)$$

$\underline{K}$ represents net inscattering effects due to phase breaking within the device region and is written by

$$\underline{K}(i,j) = \frac{\hbar |G^R(i,j)|^2}{2\pi N_0(i)\tau_\varphi}. \quad (7)$$

Here, N_0 is the local density of state and

$$N_0(i) = -\frac{1}{\pi}\mathrm{Im}G^R(i,i). \quad (8)$$

$\vec{K}_{L,(R)}$ in eq. (6) represents the net supply from left (right) electrode and

$$\vec{K}_{L,(R)}(i) = \frac{\hbar v_{L,R} |G^R(i,1(N))|^2}{2\pi a N_0(i)}, \quad (9)$$

where $v_{L,(R)}$ is the electron velocity in the left (right) electrode and

$$v_{L,(R)} = 2at\sin(k_{L,(R)}a). \quad (10)$$

$f_{L,(R)}$ in eq. (6) is the distribution function in left (right) electrode and we assume electrodes are in thermal equilibrium, that is

$$f_{L,(R)} = \frac{1}{\exp[(E - \mu_{L,(R)})/k_B T] + 1}, \quad (11)$$

where $\mu_{L,(R)}$ is the electrochemical potential in the left (right) electrodes.

Current Density

Finally, we write down the expression for the current density J. In so doing, we treat the transverse degrees of freedom by averaging as it is in Ref. [1] and use eq. (8.5.4) in Ref. [3] for the expression of the current density per unit energy. These lead

$$J = \frac{2q}{a}\int_0^\infty dE\,[\langle f(N;E)\rangle - f_R(E)]\,\langle v_R(E) N_0(N;E)\rangle. \quad (12)$$

q is the elementary charge. Here, we write E dependence of each functions explicitly. The averaging operation for any function $A(E)$ is defined by

$$\langle A(E)\rangle = \frac{m^*}{2\pi\hbar^2}\int_{-\infty}^{E} dE_z A(E_z). \quad (13)$$

3. Results and Discussion

By using the above mentioned formalism, we calculate the current density through TBRTD for the first time and compare the result with experimental data and the result obtained by the method in Ref. [2]. The experiment was done in GaInAs/InP TBRTD at 4.2K whose structure is shown in Fig. 1 [4].

Figure 2 shows $J - V$ curves at 4.2K. The solid line is derived by NEGF. We also show an experimental data by dashed line and a simulation result using the method in Ref. [2] by dotted line. In the NEGF formalism, we set the phase relaxation time τ_φ 0.2 ps by which we can reproduce the same value of half width at half maximum measured experimentally in the simulation result. For the same reason, we set the phase coherence length 90 nm in the simulation using the method in Ref. [2].

From Fig. 2, we can recognize that the peak current density derived by NEGF has the same order of magnitude as measured one. On the other hand, the peak current density derived by the method in Ref. [2] is small more than two orders in magnitude compared with measured value. These facts indicate that NEGF formalism can be applied to TBRTD structures to produce realistic device features and we can do more improved estimations of hot electron's phase coherence by using NEGF formalism. From present result, we can say that the phase relaxation time is more than 0.2ps.

We also examined validity of an empirical model for phase breaking effects proposed in Ref. [5] by comparing with NEGF and could conclude the model was valid.

4. Conclusion

We have applied NEGF formalism to TBRTD structure for the first time in order to reproduce more realistic J-V curves measured experimentally than that derived by the conventional method [2]. It is shown that the peak current density derived by NEGF can be the same order

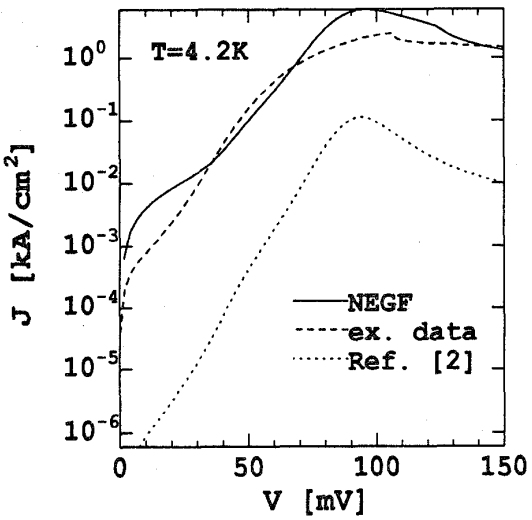

Figure 2: Comparison between calculated and measured TBRTD $J-V$ curves

of magnitude measured experimentally and we can perform more improved estimation for the coherence of hot electrons by using NEGF formalism than that based on the conventional method.

Acknowledgements

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