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Multiband Simulation of Quantum Electron Transport in Nano-Scale Devices Based on Non-Equilibrium Green's Function

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1 Introduction

Aggressive scaling of devices has reduced device dimensions into nanometer scale in which the single band effective mass model is insufficient to simulate quantum transport in such devices. This has stimulated the necessity of more realistic full band structures in quantum transport simulations [1]. In this study, we have performed the analysis of multiband quantum carrier transport in a nano-scale devices based on a non-equilibrium Green's function (NEGF) formalism [2] coupled self-consistently with the Poisson equation.

2 Simulation Method

The non-equilbirium Green's function within empirical tight binding approximation (TBA) is performed self consistently along with the Poisson equation. The empirical sp^3s^* TBA [3-4] is employed to obtain a realistic multiband structure along the transport direction. The simulation is performed using recursive Green function algorithm as in Ref. [5]. The retarded Green's function can be obtained from this equation

$$G_D = [(E + i0^+)I - H - \Sigma_L - \Sigma_R]^{-1} \tag{1}$$

The boundary self energy, $\Sigma_{L,R}$, which take into account the effect of semi-infinite left and right contact into the device can be calculated from

$$\Sigma_L = -t_{0,-1} X K X^{-1} \tag{2}$$

$$\Sigma_R = -t_{N,N+1} X K X^{-1} \tag{3}$$

Where the eigenvalues, K, and eigenvectors, X, to calulate these boundary self energy can be obtained by solving this eigenvalue equation

$$T_c T_a \begin{bmatrix} C_a \\ C_c \end{bmatrix} = \exp(-ik_x\Delta) \begin{bmatrix} C_a \\ C_c \end{bmatrix} \tag{4}$$

where T_c (for cation) and T_a (for anion) are transfer matrix, defined by

$$T_b = \begin{bmatrix} -\left[H^b_{l,l-1}\right]^{-1}\left[H^b_{l,l}\right] & -\left[H^b_{l,l-1}\right]^{-1}\left[H^b_{l,l+1}\right] \\ 1 & 0 \end{bmatrix} \tag{5}$$

Half of these states propagate or decay to the right, while the other half propagate or decay to the left. The complex band structure, solved from Eq. (4), is plotted in Fig. 1.

Once the Green's function obtained, one can calculate the carrier density from

$$n_L = \frac{-2i}{A\Delta} \sum_{\boldsymbol{k}} \int \frac{dE}{2\pi} \sum_{\alpha} G^{<}_{\alpha,L;\alpha,L}(\boldsymbol{k}, E) \tag{6}$$

and the current density from

$$J_L = \frac{2e}{\hbar A} \sum_{\boldsymbol{k}} \int \frac{dE}{2\pi} 2\mathrm{Re}\{\mathrm{tr}\{t_{L_1;L_2} G^{<}_{L_2,L_1}(\boldsymbol{k}, E)\}\} \tag{7}$$

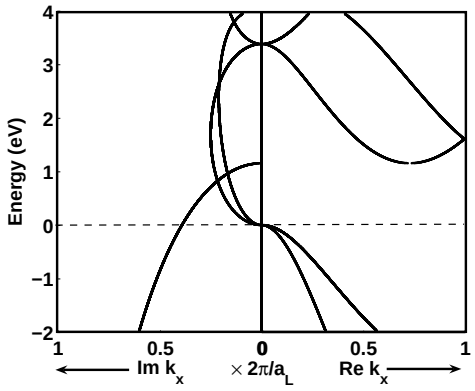

Fig. 1. Complex band structure of Si along the [100] direction. Re k_x shows the realistic bandstructure of Si with indirect bandgap

3 Results and Discussion

The simulated device structure is a Si nano-scale device with intrinsic channel of 6 nm length and source/drain doped at $N_D = 10^{26}$ m^{-3}. The device structure is equivalently considered as ref [2], although the channel length is shorter. The transport is assumed in [100] direction. The channel and both contacts are discretized with each layer is equal to half of the Si lattice constant, a_L = 0.5431 nm. In the simulation source-to-drain are biased at V_{bias} = 0 - 0.25 V.

Simulation results are presented in Fig. 2. for carrier density and Fig.3. for potential profiles, respectively, calculated under several applied bias voltage, V_{bias} = 0 -

0.25 V. Potential profile and I-V characteristic of multiband simulation (MB) are compared to those obtained by singleband simulation (SB) as shown in Fig. 4. and Fig. 5., respectively. For comparison, we also plot the density of spectral function obtained from MB simulation and SB simulation as shown in Fig. 6. and Fig. 7., respectively. In order to get a fair evaluation, characteristics in the SB calculation is assumed to be the same with those of MB calculation, i.e. lattice spacing, electron effective mass, etc. From the results, we have found that the MB features considerably change the results of EMA where only parabolic SB is considered in the simulation.

References

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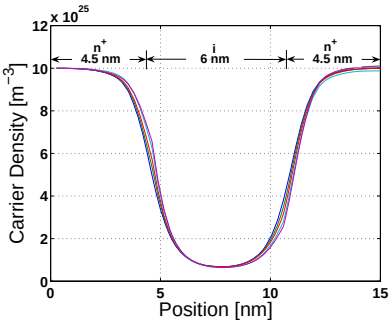

Fig. 2. Carrier densities calculated by multiband sp^3s^* NEGF for various applied voltage biases V_{bias} = 0 - 0.25 V

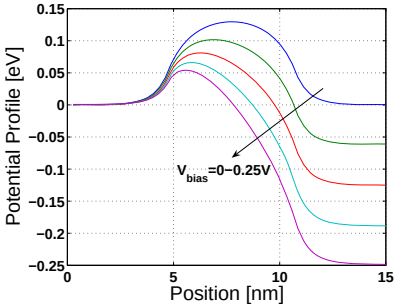

Fig. 3. Potential profiles calculated by multiband sp^3s^* NEGF for various applied voltage biases V_{bias} = 0 - 0.25 V

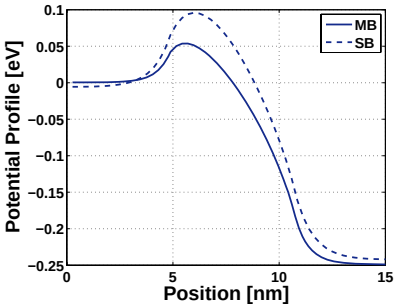

Fig. 4. Comparison of potential profile with applied bias V_{bias} = 0.25 V from singleband simulation (SB) and multiband simulation (MB).

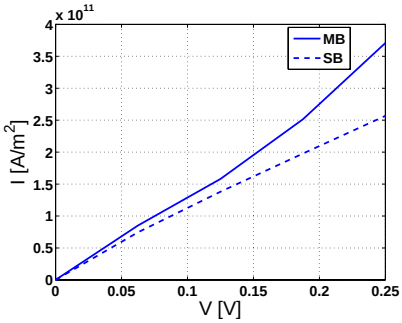

Fig. 5. Comparison of I-V characteristic, from singleband simulation (SB) and multiband simulation (MB).

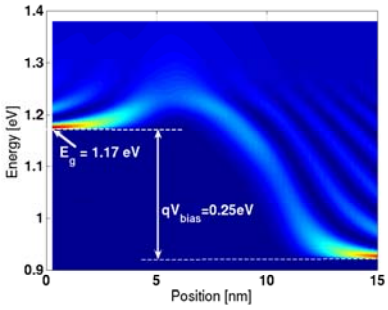

Fig. 6. Density plot of spectral function for (multiband simulation (MB) with applied bias V_{bias} = 0.25 V.

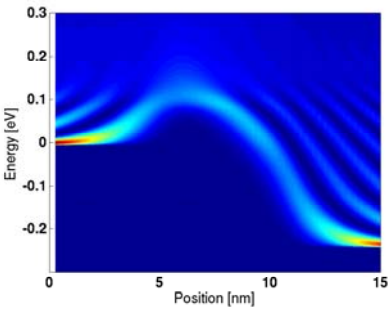

Fig. 7. Density plot of spectral function for singleband simulation (SB) with applied bias V_{bias} = 0.25 V.