Full Band Monte Carlo Simulation of Silicon Nanowires and Junctionless Nanowire MOSFETs

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INTRODUCTION

Junctionless nanowire MOSFETs have recently gained popularity since its debut fabrication at the Tyndall National Institute [1]. The device is simple to fabricate setting it as a strong future contender for the semiconductor industry. Simulations of such nanowire transistors have either involved the assumption of ballistic transport [2] or an effective mass approximation to the nanowire band structure in order to calculate the mobility [5]. In this work we implement a full band Monte Carlo simulation of such devices. The band structure is obtained from a semi-empirical $sp^3d^5s^*$ tight binding (TB) model including spin [3] and deformation potential scattering is included. Results are presented on the mobility of nanowires using k-space simulation, as well as I-V characteristics for device structures such as junctionless nanowire MOSFETs.

NUMERICAL PROCEDURE

The device structure considered is a gate all around junctionless transistor. The oxide thickness is 2nm. The source and drain are doped to $10^{20}cm^{-3}$ while the channel is doped to $10^{19}cm^{-3}$. The device is divided into slabs along the transport direction (axis of the nanowire). Each slab is considered as an individual material with its own band structure and scattering rates. The deformation potential scattering is calculated using the method outlined in [4] modified slightly to include full band optical phonon dispersion. In treating the acoustic modes we still assume a linear dispersion relation as well as the equipartition approximation. The 1D scattering rates are calculated from every k_x to k'_x (assuming the transport direction is the x-axis) and stored in lookup tables [6]. The Poisson equation is solved self-consistently with the Schrödinger equation (through the band structure and scattering rates). To couple 1D transport to a 3D Poisson's solver, we assume that the carrier has a smeared-like charge along the confined directions. The charge distribution at atom *m* along the confined direction of the wire (for each slab) is assumed to be the carrier charge weighted by $\Sigma|C^2_{lm}|$ over the *l* orbitals of the atom. This is shown in Fig. 1. The potential obtained from the Poisson solver is then entered back into the TB calculation and new band structures and scattering rates are recalculated for every slab. To make this computationally practical, the band structures and scattering rates are recalculated only every 0.5ps till convergence is reached.

RESULTS

The k-space simulations are run once the band structure and scattering rates for a slab is calculated and stored. The simulations are run till steady state is reached. Interesting physical insights such as particle position and/or valley occupancy in the band structure can be obtained from such a simulation as is shown in Fig. 3. Fig 4. shows the variation of mobility versus nanowire width considering just deformation potential scattering. A plot of the scattering rate versus energy for a 5nmx5nm silicon nanowire is shown in Fig. 2. The rates are lower than that of the bulk material due to the lower density of states of the 1D system. A plot of I_D versus V_G for a 3nmx3nm silicon nanowire junctionless MOSFET is shown in Fig. 5.

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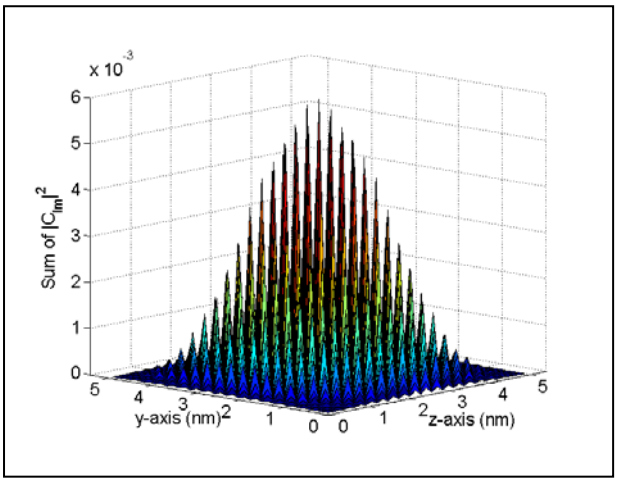

Fig. 1. The distribution of the carrier charge at the 1st CB at the gamma valley in a 5nmx5nm Si nanowire.

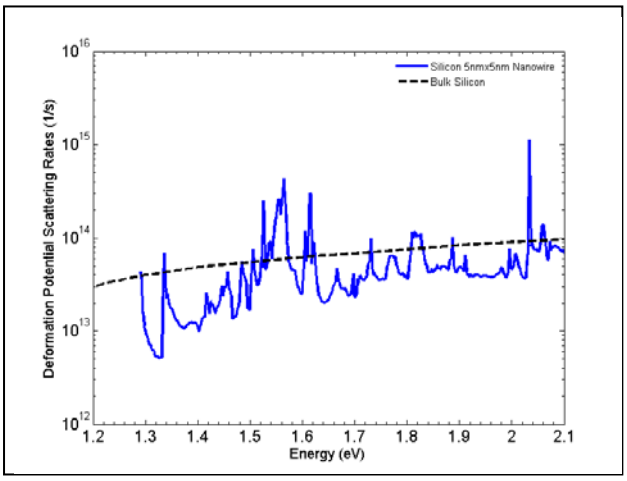

Fig. 2. Deformation potential scattering rates of a Si 5nmx5nm nanowire as compared to the bulk rates calculated by the EPM method.

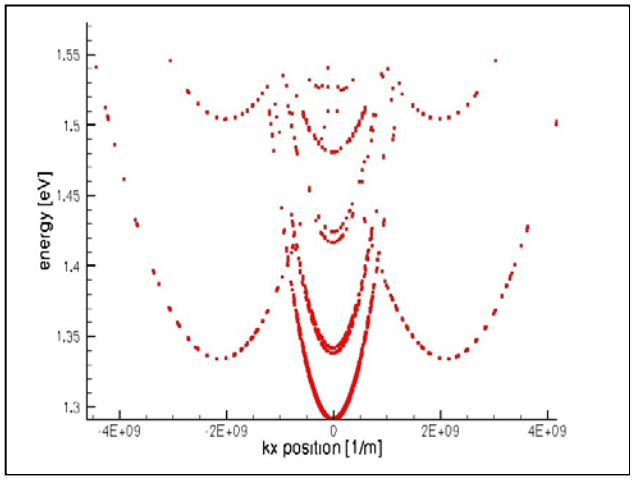

Fig. 3. Position, in k-space, of 20000 carriers taken at steady state in a 5nmx5nm Si nanowire under an applied electric field of 1kV/cm along the axis of the wire.

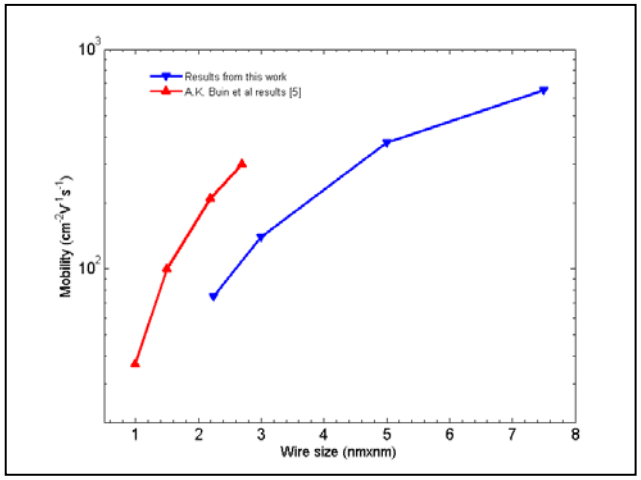

Fig. 4. Phonon limited mobility at steady state for different wire widths (inverted triangles) against the values calculated by [5] (triangle).

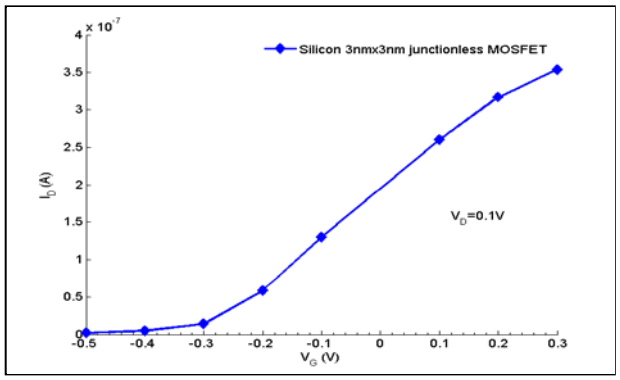

Fig. 5. I_D-V_G curve for 3nmx3nm Si nanowire junctionless MOSFET at V_D=0.1V.