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## P:34 Wigner modelling of surface roughness in quantum wires

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Aggressively scaled More Moore devices, such as FinFETs and nanowire transistors, are designed around the concept of spatial confinement, where electrons are not point-like particles with a continuous spectrum of the momentum: The finite electron size precludes - according to the Heisenberg principle - a well-determined momentum component. Physical processes are usually modelled by a decomposition of the problem into transport and eigenvalue tasks. In quantum wires, the transport is along the wire, where homogeneous conditions are assumed, while the eigenvalue problem in the transverse plane is posed in terms of eigenfunctions and energy subbands. Within this approach shape variations (e.g. roughness) are treated as perturbations which give rise to scattering. Scattering probability models based on the Fermi Golden Rule depend explicitly on the in-plane eigenfunctions, while the subband energies appear in the energy conserving delta function. The eigenvalue problem can be solved either for an ideal wire or with account for the rough interface [1]. A statistical averaging is performed, which gives rise to a roughness-aware, but homogeneous model as long as the probability is independent of the position along the wire. The electron dynamics is captured by the long-time limit of the electron-surface potential interaction process.

In this work, we use the Wigner function approach to simulate the time-dependent electron dynamics in the presence of surface potential variations. The generic process is tunnelling; no artificial borders are introduced. Identical, minimum uncertainty Wigner states [2] $f_w$=$N$exp {$(r-\ r_0)^2/s\sigma^2$}exp {$(k-\ k0)^2 2\sigma^2$} are periodically injected, with $r_0$ centered in the source contact of the wire and $\sigma_{x,y}$= $2nm$, corresponding to the equilibrium distribution around $k0$ with the effective mass $m*$ = 0.19 at $T$= $300K$. A signed particle method [3][4] with coherence length $L_x$= $L_y$= $45nm$is applied. The behavior of currents and densities in the time domain provides rich information about the involved physics. Figure 1 shows an initial penetration in the walls, until the potential modifies the initial distribution with the evolution of the electrons along the channel. The current, calculated with the Ramo-Shockley theorem, linearly increases due to the $5fs$periodic injection of electron states. After $400fs$, steady-state conditions are reached. Figure 2 compares densities of the ideal and the rough wire. The latter is obtained by superimposing variations of the potential with a correlation function $L_0$exp {$\Delta$x/$c_l$} [5] on the ideal geometry. The assumption for homogeneous conditions is challenged in both cases, in particular the source and drain regions are well identified in the ideal case. Figure 3 shows the current evolution in the time domain for three different values of $k_{o,y}$. States with a higher $k_{o,y}$travel faster, therefore a steady-state is reached earlier. Moreover, the

effect of the surface roughness is also less pronounced. The difference of the wave vector probability distributions (cf. Figure 4) shows both a reduction of the probability for high $k$values and the existence of negative $k$values due to the quantum reflection caused by the rough potential.

We conclude that the homogeneous conditions may be disturbed in considerable parts near the wire contacts, when the system is open. The effect of the non-ideal surfaces depends not only on the geometry of the wire, but also on the boundary conditions imposed on the electron system.

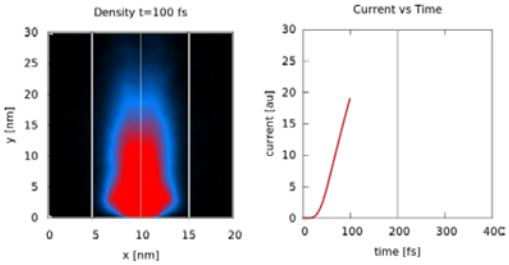


Figure 1. $100fs$ evolution of density and current. The 5nm wide $0.8eV$ potential walls smoothly drop to zero for a distance of $2nm$ towards the middle of the channel. The electron states are centered around $r_0$ given by $x = 10\text{nm}, y = 0\text{nm}$. Tunnelling is the only process which controls the penetration of the electrons into the walls.

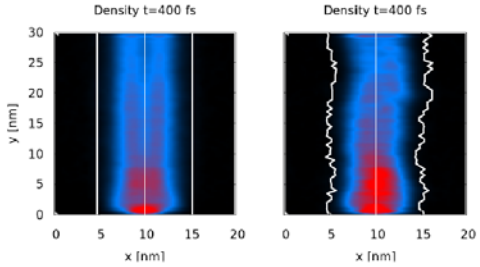


Figure 2. After $400fs$ evolution the system reaches steady-state. The potential variations are characterized by a mean offset of $0.5nm$ and a correlation length of $5nm$. The density is homogeneous in the middle half of the ideal wire.

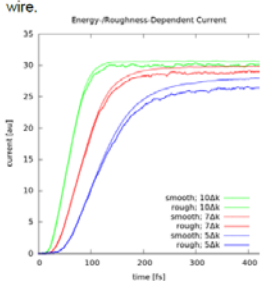


Figure 3. Current evolution for different values of $k_{0,y}$; $\Delta k$ corresponds to $1meV$.

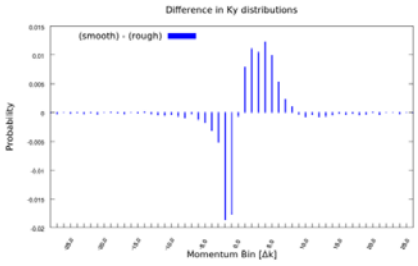


Figure 4. Difference of the ideal and rough wave vector distributions in transport direction.

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