Wigner Analysis of Surface Roughness in Quantum Wires

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Surface roughness (SR) is the low field electron mobility limiting mechanism in confined structures. Classical (Monte Carlo) transport models describe the effect of the electron interaction with the surface imperfections in terms of the Fermi Golden Rule, characterized by the stationary (long time) limit of the interaction process giving rise to the energy conserving delta function, and a statistical averaging which provides a position-independent scattering probability. An alternative approach, which allows a deep insight in the processes governing time-dependent, quantum electron dynamics in presence of SR, is based on the signed particle model [1], which provides an equivalent autonomous formulation of the Wigner theory [2]. The model retains many classical notions like phase space and point-like particles which drift and scatter like Boltzmann particles. The quantum information is carried by positive or negative sign [3] used to evaluate the physical averages. Particles generate - according to rules defined by the Wigner potential - couples of novel signed particles. Their inertial motion is not affected by the potential, in particular the electric field does not cause any acceleration. The signed particle model is utilized via *ViennaWD* [4] for a comparative study of quantum evolution in ideal and rough-surface wires. Identical Wigner states $f_w = Nexp\{-(r-r_o)^2/2\sigma^2\}\exp\{-(k-k_0)^2 2\sigma^2\}$, injected with a period of $5\,fs$, are centered in the source contact of the wire. The governing physical process is tunneling, there are no artificial walls which stop or reflect the particles: On the contrary, particles are removed after reaching the domain boundaries. Fig.1 shows that the electron density is not evenly distributed even in the ideal case. The initial penetration into the walls is followed by a reflection and further shrinking of the channel towards the drain ($y = y_{max}$). The SR pattern in Fig.2 (left) is generated by the function $L_0 \exp\{-\Delta x/c_l\}$ [5] with the mean offset L_0 and the correlation length c_l. The electron evolution is retarded by the roughness so that the density at the drain becomes stationary after $200\,fs$. It is well seen how the density is reshaped by the variations of the potential. Fig.3 presents the difference between the ideal and rough marginal distributions $fi_w(k_y,*) - fr_w(k_y,*)$ where $*$ denotes the integration over x, y and a sum over (the discrete values of) k_x. The fact that $fi_w(k_y,*)$ remains unaffected during the evolution (due to the y-independence of the potential) provides a reference for the analysis: The existence of negative wave vector values prompts for quantum reflection, where $fi_w(k_y,*)$ values dominate. The major conclusions are that far from equilibrium the conditions along the wire become inhomogeneous and that quantum reflections are caused by the SR. Another effect is the reduction of the speed in the transport direction as confinement keeps the density away from the interface thus reducing the SR effect.

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4. ViennaWD: http://viennawd.sourceforge.net/
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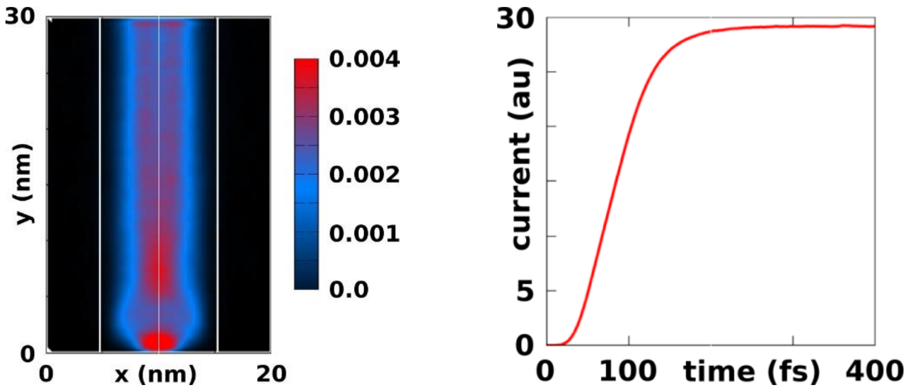

Fig. 1: The ideal wire walls are formed by $5\,nm$ wide $0.8\,eV$ potential strips which smoothly drops to 0 in the next $2\,nm$ towards $x = 10\,nm$. The injected states use $r_0 = (10, -4\sigma)\,nm$ and $\sigma_{x,y}$ of $2\,nm$ corresponds to the equilibrium at $300\,K$. A stationary picture of the density (in arbitrary unit) is reached after $175\,fs$ injection, when the current enters the $3\,\%$ limits around its mean value.

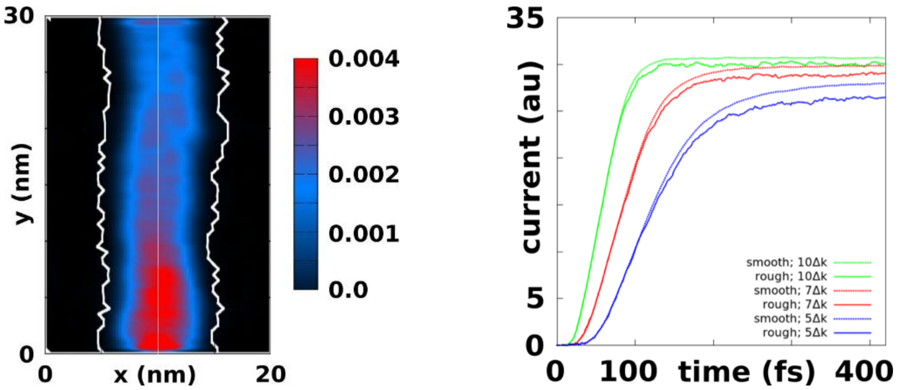

Fig. 2: The SR density (in arbitrary unit) pattern with $5\,nm$ correlation length and $0.5\,nm$ mean offset causes a reduction of the current, given on the right picture for three different values of $k_{0,y}$; Δk corresponds to $1\,meV$.

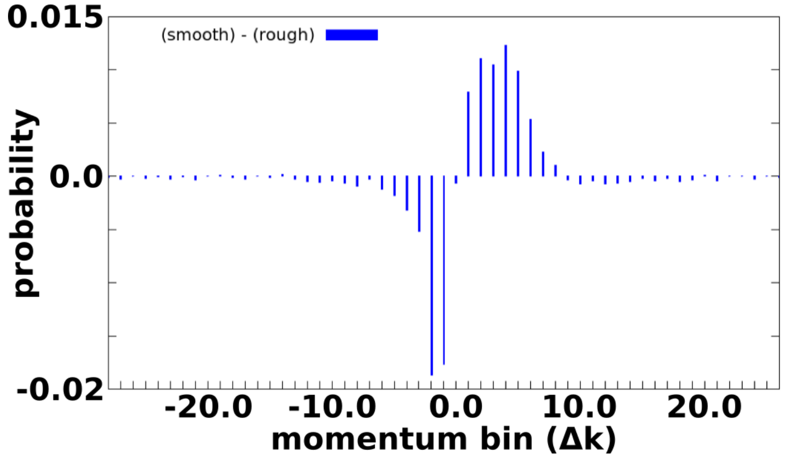

Fig. 3: The difference between the ideal and rough marginal ky-distributions shows a reduction of the speed in the transport direction and a reflection caused by the SR varying potential.

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