Green Function Treatment of Electronic Transport in Narrow Rough Semiconductor Conduction Channels

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Abstract. We explore the effect of geometrical fluctuations on the electronic transport in rough Si nanowire (NW) thermoelectric devices of diameter $D < 10$ nm. At this scale, the quantum nature of transport is accounted in the computation of energy dependent transmission coefficients through a recursive green function algorithm. The rough 3D NW geometry is used as a direct input to simulations through the roughness height $\Delta$ and autocovariance length $L$. Using a non parabolic band structure, the channel conductance above 0.1 eV is drastically reduced in such NW with high $D/\Delta$ ratio. In addition, the roughness induced resistivity is only increased by 6% on the first energy level of 10 nm Si channels with $\Delta = 7.7$ Å, showing possible application for high thermoelectric figures of merit $ZT$.

While semiconductor nanowires (NW) have found viable applications in field effect transistors [1], interconnects [2], and thermoelectrics [3], scattering of charge carriers with the surface nevertheless limits transport in these structures, owing to their high surface-to-volume aspect ratio. Recent experimental and theoretical work on such NW [3, 4] showed that, through careful nano-engineering of intentionally rough edges, it is possible to decouple thermal and electrical transport, making such devices extremely appealing for novel applications in thermoelectric energy conversion. In particular, it is believed than in thin NW of diameter $D < 15$ nm, where electrons are pushed away from the surface, phonons may be scattered more efficiently than electrons by asperities at the NW surface [5], leading to high thermoelectric figures of merit $ZT$. Conventional formalism which accounts for electron – surface roughness scattering is based on the derivation of a perturbed hamiltonian of the system due to geometrical fluctuations [6, 7] and is adapted to a 2D electron gas (2DEG) conducting near an interface. However, at low NW scales, this approach does not account for the quantum nature of electron transport, where charge carriers theoretically impinge on a series of potential barriers resulting from geometrical constrictions in the transport direction [8]. In this study we compute an energy dependent electrical quantum conductance in thin Si NW from a Recursive Green Function (RGF) approach [9], including evanescent modes, non-parabolic bands, a 3D description of NW, and a model for arbitrary rough surfaces through the root mean square (RMS) roughness height $\Delta$ and autocorrelation length $L$. In the absence of other scattering mechanisms, we show that surface roughness contributes to an increased resistivity for high energy carriers in Si NW of diameter $D < 10$ nm, while having little effect on the lower energy levels, thus building good hopes for application of rough thin NW in thermoelectrics.

The quality of thermoelectric devices is measured by the dimensionless figure of merit $ZT = (S^2\sigma/\kappa)T$, where $S$ is the Seebeck coefficient, $T$ the temperature, $\sigma$ the electrical...
conductivity and $\kappa$ the thermal conductivity. With this respect, a standard approach to achieve performance is to design a “phonon glass - electron crystal”, with high electron mobility and poor thermal conductivity. Recently, thermal conductivity in Si NW with etched rough edges was experimentally reduced by a factor of about 100 in comparison to bulk crystalline Si [3, 4], to nearly the value of amorphous Si. In order to provide supplementary information for the design of efficient thermoelectric devices, the present model relates the transmission of charge carriers in a rough Si NW conduction channels to the NW diameter, the experimental roughness parameters $\Delta$ and $L$, and the electron energy $E$. While considering geometrical fluctuations as the sole source of resistivity in the NW, the transmission probability $T(E)$ of carriers with energy $E$ is directly linked to the electrical current $I$ flowing between two Büttiker probes held at Fermi energies $E_{F,1}$, $E_{F,2}$ through Landauer’s formula $I = 2e/h \int_{E_{F,1}}^{E_{F,2}} T(E) dE$. Hence, in the ideally smooth case, the channel conductance varies in steps of integer multiples of the fundamental quantum conductance $e^2/h$.

The 3D conduction channel is modeled by a 1D tight binding (TB) chain where each site $q$ represents a cross section of the whole 3D TB domain (Fig. 1). The NW is assumed in contact with two semi-infinite leads of perfectly smooth NW of the same diameter. The quantum nature of NW transport is accounted by solving the tight binding Schrödinger equation (TBSE) in a series of 2D cross sections along the transport direction, and recursively computing the transmission between adjacent sections through the overlap of the wavefunctions $\langle m|G_{rl}|n\rangle$. The total transmission at energy $E$ is $T(E) = \sum_{m,n} |t_{mn}(E)|^2$. The NW resistivity due to geometrical constrictions is then obtained from $G_{rl}$. Since the propagator $G$ is known for a perfectly smooth semi-infinite lead, the algorithm functions in a recursive way. Once the right lead is attached, at the step $q$ of the recursion, the propagator $G_{r,q+1}^R$ between site $r$ and $q + 1$ is computed. The site $q$ is then

Figure 1. 2D Model of the RGF approach in a rough NW. Each transverse chain is represented by a single site in the 1D system, and the propagators $G$ are computed to connect the energy modes between neighbor sites.
Attached in order to determine the new propagators $G^{L+R}_{r,q}$ and $G^{L+R}_{q,q}$

\[
G^{L+R}_{r,q} = G^R_{r,q+1} V_{q+1,q} \left( I - G^L_{q,q} V_{q,q+1} G^R_{q+1,q+1} V_{q+1,q} \right)^{-1} G^L_{q,q}
\]

(2)

\[
G^{L+R}_{q,q} = \left( I - G^L_{q,q} V_{q,q+1} G^R_{q+1,q+1} V_{q+1,q} \right)^{-1} G^L_{q,q}
\]

(3)

Non-parabolicity is included in the computation of the longitudinal wavevectors $|10, 11|

\[
E_{y,z} [1 + 2\alpha(E_x + E_{y,z})] = E - E_x
\]

(4)

where $\alpha$ is the coefficient of non-parabolicity, $E_{y,z}$ is the TBSE cross section energy, and $E_x = \hbar^2 k_x^2 / (2m_x^*)$ is the effective energy available for longitudinal transport. As a result of non-parabolicity, transverse energy levels appear shifted down (Fig. reffig:Fig3). Conduction is assumed along the $\Gamma - X$ direction with $m_x^* = 0.19m_0$ and $\alpha = 0.5$. Non-parabolic bands allow better accuracy in the computation of roughness limited $T(E)$ at $E > 0.1$ eV.

We model transport in 100 nm long NW of average width $D < 10$ nm. Surface roughness alleviates the degeneracy of the cross section eigen-modes (Fig. 2). Subsequently, the computation of $T(E)$ is averaged over 500 randomly generated NW. The effect of RMS height $\Delta$ is compared at different diameters and varying energy (Fig. 3). Increasing $\Delta$ results in a series of higher potential steps encountered along the $x$-direction, thus reducing the average transmission on rough NW. The quantum features of conduction disappear at high $\Delta$ where the step-like behavior is smoothened as a consequence of carrier back-scattering from surface asperities. In addition, the resistivity incurred at similar RMS height is stronger in NW of smaller diameter.

Noticeably, surface roughness has limited impact on the transmission of the first energy level, particularly at $D = 10$ nm, in accordance with Wang et al. [8]. Thus, geometrical fluctuations are expected to have only a minimal influence on the low field NW mobility. In this regime of operation, where thermal conductivity varies as $(D/\Delta)^2$ [4], it is expected to achieve high $ZT > 1$. The RMS height $\Delta$ measures the average height of roughness peaks or constrictions. This statistical picture is consistent with the case of chemically grown NW, where one may control the amplitude of geometrical variations rather than the actual shape of the edge. In

![Figure 2. (a) Energy levels in a perfectly smooth NW. (b), (c) Examples of cross-section wavefunctions in a perfectly smooth NW. (d) Energy levels in a rough NW. (e), (f) Cross-section wavefunctions in a rough NW. D = 10 nm, $\Delta = 5$ Å and $L = 22$ Å throughout.](image-url)
10 nm NW with $\Delta = 7.7 \, \text{Å}$, we observed constrictions of effective diameter down to 6 nm. Hence, for high $\Delta / D$ ratio, transmission does not occur until sufficiently high energy is reached to tunnel through constriction barriers. Nevertheless, the surface is generally comparable to a random noise around the average diameter. As a result, higher variance of NW behavior is observed when $E$ is near the transition between energy levels. The standard deviation of NW transmission is also increased at high $\Delta / D$ ratio, but remains small at the center of energy steps.

As a conclusion, we explored the effect of surface roughness on electronic transport in thin Si NW of diameter $D < 10$ nm based on a recursive green function algorithm. This approach allows a 3D representation of the NW geometry through the statistical parameters $\Delta$ and $L$, and further includes the effect of non-parabolicity of the Si band structure. As the quantum nature of charge carriers is accounted for, an energy dependent transmission is computed for such devices. With geometrical fluctuations as the sole electronic decay process, conductance at energies $E > 0.1 \, \text{eV}$ is drastically decreased in such NW with high $\Delta / D$ ratio. Nevertheless, surface asperities have little effect on low energy transport, leading to possibly high thermoelectric figure of merit $ZT$ in this regime of operation. To test such assumption, it is necessary to additionally model thermal transport in channels with dimensions below the average phonon mean free path.

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