Extracting thermoelectric properties of nanostructures using the atomistic $sp^3d^5s^*$-SO tight-binding model

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Introduction

Low dimensional materials can provide the possibility of improved thermoelectric performance due to the additional length scale degree of freedom on engineering the electronic and thermal conductance of nanostructures. Recently, large improvements on the thermoelectric figure of merit ($ZT=\sigma S^2/(k_e+k_l)$) have been reported in silicon nanowires compared to the raw material's bulk ZT value [1, 2]. Most of this improvement was a result of suppressed phonon conduction (k_l). Low dimensionality can also be beneficial in increasing the power factor (σS^2) of the device [3, 4]. This work investigates the magnitude of this potential improvement.

Approach

The atomistic $sp^3d^5s^*$-spin-orbit-coupled tight-binding model is used to calculate the electronic structure of ultra thin cylindrical silicon nanowires (NWs) [5, 6]. The Landauer formalism is then used to calculate an upper limit for the electrical conductivity, Seebeck coefficient and power factor [7]. The effects of orientation and diameter in NWs are examined. The atomistic model can provide an accurate estimate of the electronic structure and carrier velocities and inherently includes the effects of quantization and different orientations. We consider n-type and p-type nanowires of diameters from D=3nm to 12nm, in [100], [110] and [111] transport orientations and at different doping concentrations.

Results-Discussion

Figure 1 and 2 show the electrical conductivity and Seebeck coefficient of the [111] n-type NW versus the 1D carrier density. A comparison between the wires of different diameters (from D=3nm to D=12nm) shows that both quantities shift to the right as the wire diameter increases. This is because at the same 1D doping, the Fermi level is at a lower position in the thicker NWs that have more subbands.

The power factor for the n-type [111] NWs is shown in Fig. 3. Large benefits in the peak value of the power factor can be achieved for diameters below ~7nm. Above that, the peak saturates and no more benefits are observed. These benefits might be overestimated in our calculation due to the existence of scattering and non-idealities that we do not consider, and due to the fact that surface roughness scattering might be more severe for the narrower NWs. Our purpose, is to provide an upper limit of the performance, and a design length scale up to which dimensionality can potentially provide benefits.

Figure 4a and 4b show the Seebeck coefficient of the n-type and p-type NW families respectively. At smaller diameters, (D=3nm) differences in the Seebeck coefficients of the devices appear. At higher diameters (D=12nm), however, those differences are less distinguishable.

Figure 5a and 5b show the power factor of the n-type and p-type NWs respectively. Similarly, the strong dependence on orientation smears out at larger diameters, where all wires have a relatively similar power factor. At smaller diameters, however, benefits to the power factor vary from 0-100% depending on the orientation, and in some cases there is not benefit at all ([110], [111] p-type cases).

Summary

Thermoelectric properties of n-type and p-type nanowires in different transport orientations and for diameters varying from D=3nm to D=12nm are examined. The atomistic $sp^3d^5s^*$-SO TB model is used for the electronic structure calculation, and the Landauer formalism for the calculation of the upper limit of the conductivity and the Seebeck coefficient. We find that at room temperature, relative power factor improvements can be found for NWs of diameters smaller than ~7nm. The magnitude of these potential improvements is at most ~100%, and differs from case to case.

References

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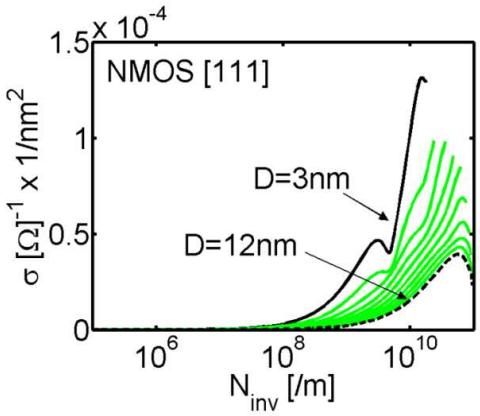

Fig. 1: The conductivity of the n-type NWs in the [111] direction as a function of the 1D carrier concentration. Conductivities for wires with diameters from D=3nm (solid-black) to D=12nm (dash-black) are shown. The green lines indicate wires with diameters of 1nm increment.

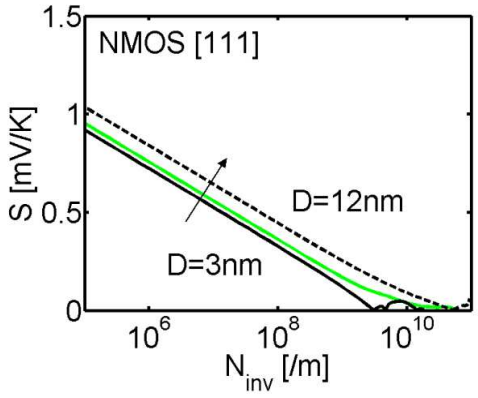

Fig. 2: The Seebeck coefficient of the n-type NW in the [111] direction as a function of the 1D carrier concentration. Seebeck coefficients for wires with diameters D=3nm (solid-black), D=7nm (green) and D=12nm (dashed-black) are shown. The arrow indicates the direction of diameter increase.

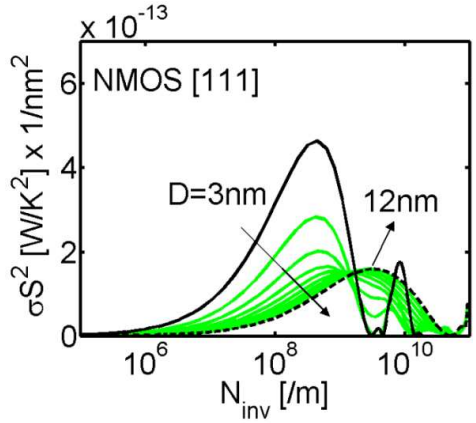

Fig. 3: The power factor of the n-type NWs in the [111] direction as a function of the 1D carrier concentration. Power factors for wires with diameters from D=3nm (solid-black) to D=12nm (dash-black) are shown. The green lines indicate wires with diameters of 1nm increments.

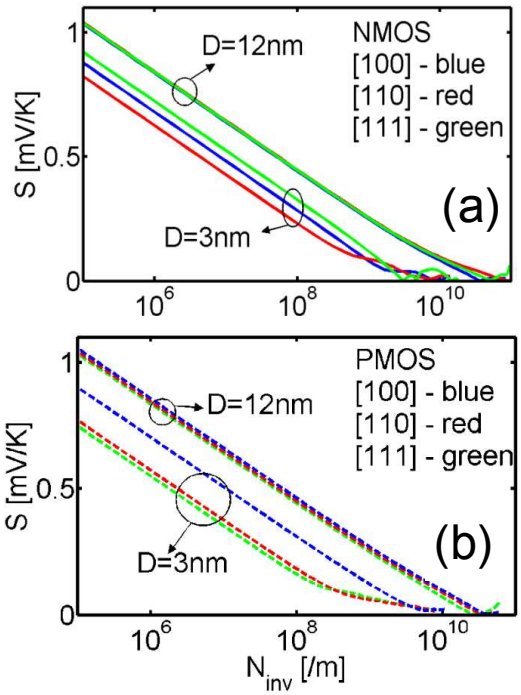

Fig. 4: The Seebeck coefficient of the NWs in the [100] (blue), [110] (red) and [111] (green) orientations as a function of the 1D carrier concentration. Results for wires with D=3nm and D=12nm are shown. (a) n-type. (b) p-type.

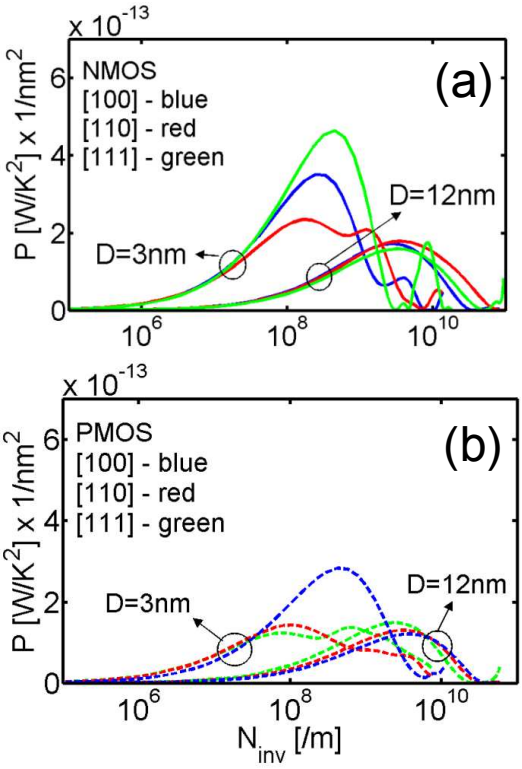

Fig. 5: The power factor of the NWs in the [100] (blue), [110] (red) and [111] (green) orientations as a function of the 1D carrier concentration. Results for wires with D=3nm and D=12nm are shown. (a) n-type. (b) p-type.