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Designing width-modulated Si nanowires for enhanced thermoelectric efficiency

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ABSTRACT

Efficient thermoelectric energy conversion requires good electronic properties and low thermal conductivity. Width-modulated nanowires have been proposed for thermoelectric efficiency enhancement. We have used the Monte Carlo simulation technique to study the effect of width modulation on the thermoelectric transport properties of Si nanowires. We have found that it is possible to achieve significant decrease of the thermal conductivity without deteriorating the electrical transport properties. Our simulations predict enhanced thermoelectric efficiency in Si nanowires modulated by a single constriction compared to the corresponding non-modulated nanowires.

1. Introduction

The thermoelectric efficiency (TE) of a material can be estimated by the figure of merit $ZT = \sigma S^2 T / \kappa$, where σ, S, and κ are the electrical conductivity, the Seebeck coefficient and the thermal conductivity respectively. High thermoelectric efficiency requires good electronic properties to ensure significant TE power factor σS^2 and low thermal conductivity. High thermal conductivity prohibits the use of traditional semiconductors such as silicon from TE applications because it keeps ZT small [1]. Nanowires have smaller thermal conductivity than the corresponding bulk materials and they have been considered promising for enhanced TE efficiency [2,3]. The thermal conductivity of Si nanowires of width below 50 nm was found considerably decreased compared to bulk [3]. Very thin wires are, however, not easy to fabricate and their electrical conductivity is poor. As an alternative, it has been proposed to use diameter-modulated nanowires [4]. It has been theoretically predicted a big decrease of the thermal conductivity of modulated nanowires [5–9]. Current state of the art of the fabrication technology allows for the realization of modulated nanowires with control on the modulation morphology [10].

In previous works [8,9], we showed that modulated Si nanowires with thickness above 50 nm, can have thermal conductivity significantly decreased compared to non-modulated nanowires. However, this effect itself would not ensure TE efficiency enhancement because constrictions would result in simultaneous decrease of the electrical conductivity. For ZT enhancement, a bigger decrease of the TE power factor in the modulated nanowire than the corresponding enhancement of the thermal conductivity would be needed. To deal with this issue we have explored the effect of constrictions on the electron transport properties of Si nanowires using the Monte Carlo (MC) simulation technique. The MC technique directly accounts for the geometry details of the nanostructure. We have explored the effects of one and of multiple constrictions. We have used our MC simulations on electrons and phonons to estimate the TE efficiency. We found that ZT enhancement is possible in Si nanowires in the presence of one constriction. The simulation technique is briefly presented in Section 2. In Section 3, we present and discuss our MC results on the TE transport properties of Si nanowires modulated by a constriction. Conclusions are drawn in Section 4.

2. MC simulation method

We have performed ensemble Monte Carlo (MC) simulations on the electron transport properties. The MC technique is described in detail in Refs. [11–15]. The mobile charge of the nanowire is represented by a number of "super-particles". The charge on each super-particle is $Q = eN / N_{sim}$, where e is the elementary charge, N is the total number of mobile charges in the nanowire and N_{sim} is the number of super-particles used in the simulation. We selected the number of super-particles in the range 10^4–10^5 ensuring a good statistics for the simulation time typically of the order of hundreds of picoseconds. The particles are initialized assuming thermal energy distributions with randomly oriented momenta. They are let to drift for periods of time τ shorter than the average time between collisions. The free flight time τ is directly related to the total scattering rate Γ: $\tau = -\ln(r) / \Gamma$, where r is a random number between 0 and 1. A fictive "self-scattering" rate is chosen so that the sum

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of all scattering rates is constant and independent of the carrier energy. The carrier drifts under the influence of the electric fields during the free flight time. Then, a random number between 0 and 1 is drawn and it is compared with cumulative probabilities of scattering which have been computed at the beginning of the simulation as a function of energy. A scattering mechanism is selected proportionally to the scattering probability of each process. For self-scattering, the particle continues its free flight with no change of its state. For real scattering process is selected the particle's state after scattering is stochastically chosen taking into account both energy and momentum conservation. This procedure is repeated for all particles. Ensemble averages are updated every time step. The super-particles are sampled at regular time-intervals until the required statistical accuracy is reached or the total simulation time ends.

The electron energy bands are modeled analytically including non-parabolicity. The six ellipsoidal, energetically equivalent conduction band valleys of silicon are explicitly included. The phonon dispersion branches, acoustic and optical, are treated with the isotropic approximation. The parameters have been chosen to fit the bulk Si phonon dispersion curves for all phonon modes. The scattering rates have been calculated within Born approximation. Intravalley and intervalley electron transitions are included. The carrier transitions are induced by scattering by phonons, impurities, and other electrons. Electron–phonon interaction by deformation potential is assumed for both acoustic and optical phonons. Ionized impurities scattering is included. The effect of the electron–electron interactions has been taken into account in the determination of the electron distribution function. The Pauli exclusion principle has been implemented using the rejection technique [16].

The phonon MC simulation technique that has been used for the calculation of the thermal conductivity data [9] is extensively described in [17–19]. The method is equivalent to solving the Boltzmann transport equation. Bulk Si dispersion properties have been used for the sampling of phonon frequency and group velocity, as well as for the calculation of the scattering relaxation times following the model proposed by Holland [20].

3. Results and discussion

We performed MC simulations on nanowires modulated by constrictions as shown in the schematics of Fig. 1.

The width d of the nanowire is modulated by a constriction of width b. We present here representative results for Si nanowires of width $d =$ 100 nm and constriction widths b in the range 100–10 nm. The constriction length has been assumed 20 nm. In this dimensions range, the electron band structure can be safely considered the same as in bulk Si.

We first discuss the effect of the number of constrictions on the transport properties. Our previous systematic MC simulations on nanowires modulated by constrictions [9] concluded that the decrease of the thermal conductivity of the modulated nanowires is maximized in the presence of multiple constrictions. This is shown in Fig. 2 where the thermal conductivities of a nanowire modulated by a single constriction and one modulated by a periodic sequence of constrictions are plotted together. The electron MC simulations showed, though, that the addition of multiple constrictions results in suppression of the electrical conductivity. The electrical conductivities of nanowires modulated by a single and by two constrictions are shown in Fig. 3. It is shown that the addition of a second constriction causes already an important decrease of the conductivity. For this reason, we restrict our study to the effect of one constriction.

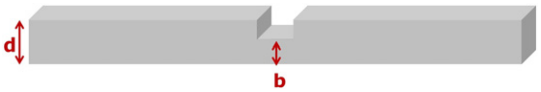

Fig. 1. Schematics of a nanowire of width d modulated by a constriction of width b.

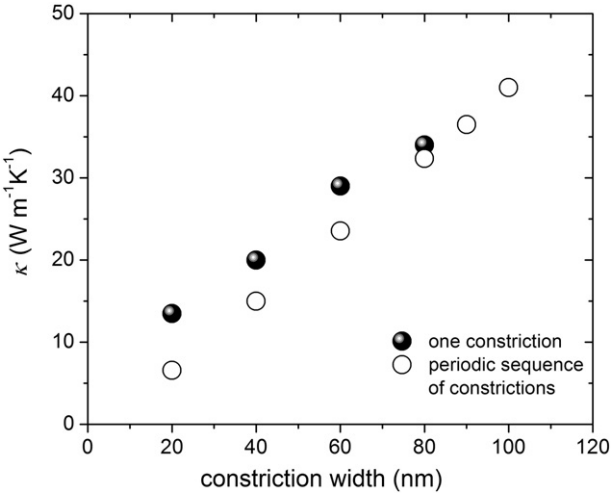

Fig. 2. The thermal conductivity of Si nanowires with width 100 nm modulated by one constriction (solid dots) and by a periodic sequence of constrictions (open dots) versus the constriction width at $T = 300$ K. After Ref. [9].

The conductivity and Seebeck coefficient for electron concentration $n = 10^{19}$ cm^{-3} are plotted in Fig. 4 versus the constriction width b for three nanowire lengths $L = 500$, 200 and 100 nm. The conductivity decreases with decreasing constriction width in all nanowires. The decrease is more significant in shorter nanowires. The Seebeck coefficient is much less sensitive to the constriction width. It remains nearly constant for the 500 nm nanowire and shows a weak decrease for the 200 nm and 100 nm nanowires with decreasing b. The obtained behavior is analyzed in what follows.

In Fig. 4 electron MC results for the 500 nm nanowire results are shown. For $b = d = 100$ nm the data correspond to the straight, non-modulated nanowire. The simulated values for σ and S are in agreement with available experimental data, standard reference data [21] as well as more recent ones [1] for bulk Si. The MC estimated resistivity is 6.8×10^{-3} Ω cm for $n = 10^{19}$ cm^{-3} at 300 K and agrees with the data given in [21]. Reported measurements on S [1] are in the range 0.35–0.45 mV/K for $n = 1.0$–1.4×10^{19} cm^{-3} at T = 300 K. The MC estimated S is 0.41 mV/K for $n = 1.0 \times 10^{19}$ cm^{-3} at T = 300 K (Fig. 4).

The conductivity decreases with decreasing constriction width b. The decrease can be interpreted by the increasing constriction resistance with decreasing b. Electron scattering is enhanced at the

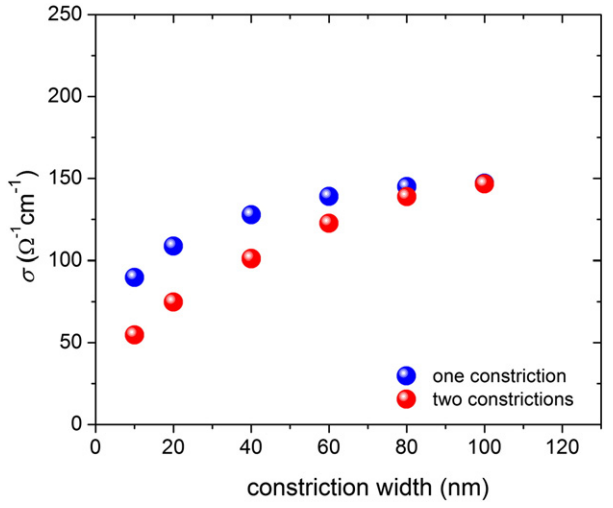

Fig. 3. The electron conductivity of modulated Si nanowires versus the constriction width at $T = 300$ K and for $n = 10^{19}$ cm^{-3}.