Thermoelectric Transports in Geometry- and Doping-Controlled Nanostructures

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ABSTRACT SUBMISSION

This work investigates electron and phonon transports in semiconductor nanowires and nanoribbons with geometrical fluctuation and non-uniform carrier doping concentration, expecting an efficient phonon blockade with a minimal impact on electronic transport, so that enhancement of thermoelectric efficiency is expected. This comprehensive study examines trade-offs to find an optimal design for thermoelectric applications.

INTRODUCTION

Nanostructured semiconductors have attracted considerable attention due to their potential applications in thermoelectric devices [1]. Utilizing their large phonon mean-free-path (MFP) compared to electron MFP, nano-structures have achieved improved thermoelectric efficiency dictated by the dimensionless thermoelectric figure of merit ($ZT = S^2\sigma T/\kappa$) [2]. In such nanowires, the phonon confinement starts developing ahead of the electron confinement and reduces thermal transport with hardly affecting electronic transport [3]. In this study, we investigate thermoelectric properties of silicon nanowires and nanoribbons with their geometry- and doping-modulation, expecting an enhancement of the figure of merit ZT.

MODEL

We will consider sinusoidally undulated nanowires and non-uniformly doped nanoribbons with rough edges, as schematically depicted in Fig. 1 and 2, respectively. It is expected to possibly realize an efficient phonon blockade through the structural barriers, without degrading appreciably the electronic current. The high doping concentration along the center region of the nanoribbon is anticipated to confine electrons adequately, so that the rough edges have a minimal impact on electron transport while phonon transport which is free from carrier concentration gets interfered by the structural variation

METHODS

Change in the electronic transport due to the geometry variation and non-uniform doping is examined by computing an energy dependent electrical quantum conductance of the structures under consideration employing a Recursive Green Function approach [4]. The 3D conduction channel is modeled by a 1D tight binding chain, and the quantum nature is accounted by solving the Schrödinger equation in a series of 2D cross sections in the transverse direction. The quantum transmissions of the sinusoidal nanowires are compared with those of straight uniform nanowires in Fig. 3. The nanowire undulations directly affect the resistivity particularly at higher carrier energy but have little effect on low energy transport, leading this structure be potentially good for use of thermoelectric applications. Quantum transmissions of the nanoribbons can be also investigated using the same method with the highly doped region brought into the calculation by solving the Schrödinger equation of the cross sections. The Seebeck coefficient and electrical conductivity of the structures will be computed through Landauer formula as a function of quantum transmission.

The lattice thermal conductivity of those non-uniform structures can be computed with molecular dynamics at a constant temperature. We adopt the reverse non-equilibrium MD method, which imposes a heat flux first and measures the resulting temperature gradient, performed with the Stillinger-Weber interatomic potential. The MD simulation should reveal a decrease in thermal conductivity as structural barriers are imposed to the system. In Fig. 4, it is shown that the lattice thermal conductivity of the sinusoidal nanowire is lower than that of the straight nanowire.

ISBN 978-0-692-50554-0

CONCLUSION

We will show comprehensive results illustrating possible trade-offs to optimize the thermoelectric figure of merits of uniform and non-uniform nano-structures. As we consider geometrical fluctuation and non-uniform doping as the sole perturbation to our system, the ratio of the figure of merits should provide an insight of an optimum design for thermoelectric applications.

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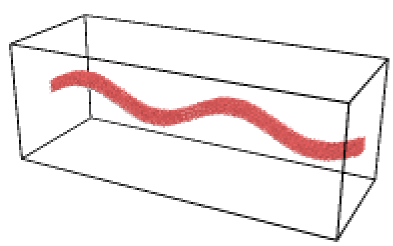

Fig. **1**. A schematic of a semiconductor nanowire with sinusoidal undulations

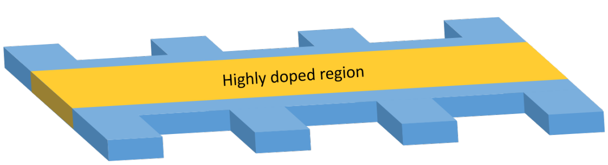

Fig. 2. A schematic of a non-uniformly doped semiconductor nanoribbon with edge-variation

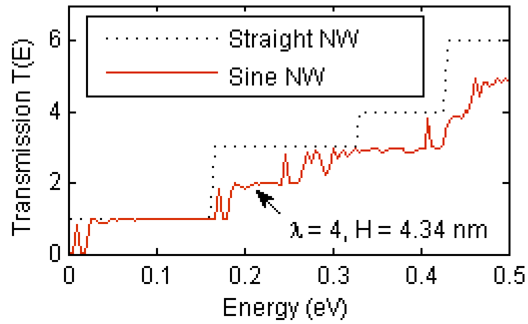

Fig. 3. Comparison of quantum transmissions of a sinusoidal nanowire and a straight uniform nanowire (w = 4.34 nm, L = 108.6 nm)

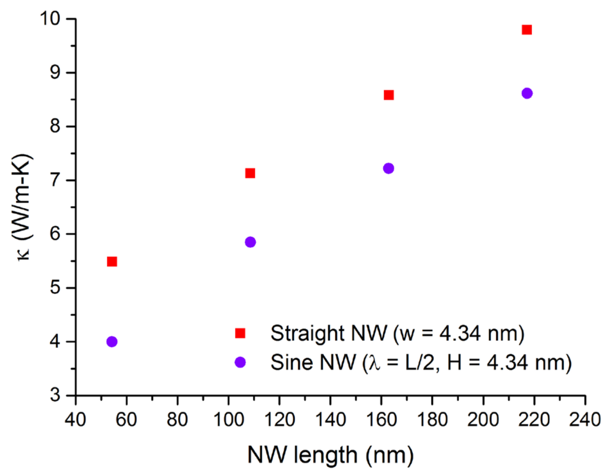

Fig. 4. Comparison of lattice thermal conductivity of a sinusoidal nanowire and a straight nanowire