Thermal conductivity of Si/Ge and Ge/Si core–shell nanowires: molecular dynamics study

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Introduction

1D materials have unique properties, different from bulk materials. This gives them vast applications in the fields of electronic, optoelectronic, and energy conversion devices [1]. Among them, crystalline semiconductor NWs are very promising materials in the present miniaturization of devices towards the nanoscale. Since thermal conductivity of nanoscale materials is also quite different from that of bulk materials, understanding and predicting the thermal conductivity of NWs play an important role in thermal management.

The efficiency of a thermoelectric material is characterized by the figure of merit $ZT = \frac{S^2\sigma}{k}$ where T is the absolute temperature, S is the Seebeck coefficient, σ is the electrical conductivity, and k is the total thermal conductivity, respectively. Semiconductor nanowires have an increased ZT value due to them having very low thermal conductance due to surface scattering by the phonons [2,3].

To further improve ZT value, a number of methods are proposed, among which effects of core-shell structure and strain effects come to spotlight of research. This work's main focus is on investigation of thermal conductivity of core-shell structured NWs. The advantage of core-shell structure is that the electronic and phonon transports in such NWs are decoupled, which is very favorable for thermoelectric purposes. Core-shell structure can further decrease thermal conductivity thanks to suppression and localization of longwavelength phonon modes at the core–shell interface and high frequency, non-propagating, diffusive modes [4].

Method

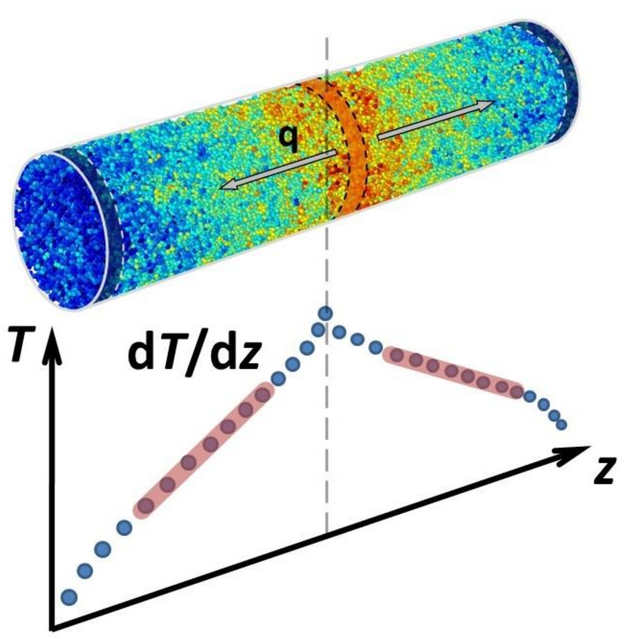

Fig. 1. Simulation set-up for computing the thermal conductivity, which illustrates the subdivision of the nanowire into separate slices, hot in the middle and cool at the edges. The resulting time-averaged temperature profile inside the nanowire (along the z-axis) is illustrated at the bottom.

Using molecular dynamics simulations there were generated different types of NWs, where their thermal conductivity was calculated using the Muller-Plathe algorithm, which schematically illustrated on **Fig.1.**

The idea of this algorithm is in that the slowly converging heat flux is imposed through velocity rescaling, so that the temperature T and its gradient dT/dz are calculated by averaging the atomic kinetic energy over time and over a large number of atoms.

The thermal conductivity along the direction of heat propagation z is defined by Fourier's law

$$k = -\frac{q}{dT/dz}$$

Results

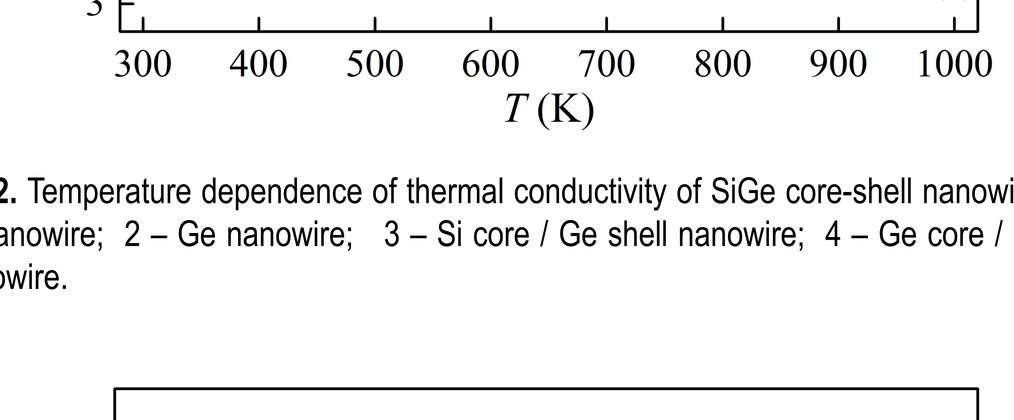

Fig.2. Temperature dependence of thermal conductivity of SiGe core-shell nanowires: 1 - Si nanowire; 2 – Ge nanowire; 3 – Si core / Ge shell nanowire; 4 – Ge core / Si shell nanowire.

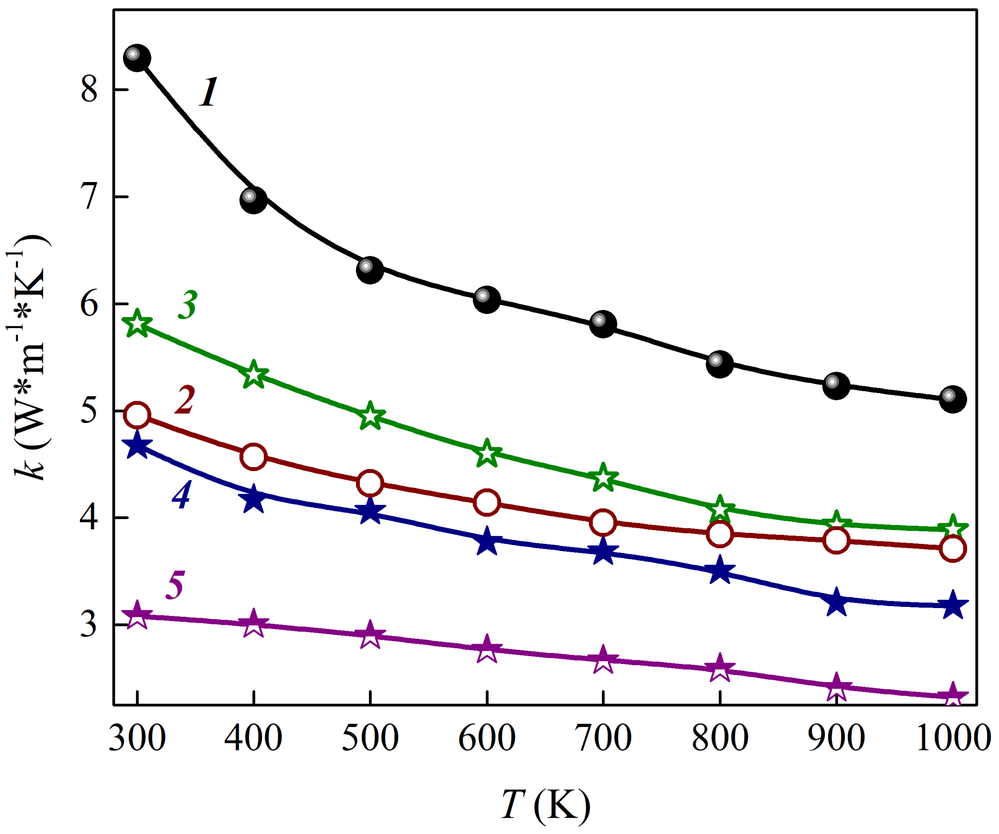

Fig.3. Temperature dependence of thermal conductivity of Si core / Ge shell nanowires with various volumetric ratio η=VSi/VGe : 1 - Si nanowire; 2 – Ge nanowire; 3 – Si core / Ge shell nanowire with η=0.5; 4 – Si core / Ge shell nanowire with η=1; Si core / Ge shell nanowire with η=2.

Conclusions

Non-equilibrium molecular dynamics simulation is performed to investigate thermal conductivities of two kinds of SiGe nanowires (core(Si)/shell(Ge) and core(Ge)/(Si)). The influence of the volumetric ratio $\eta = V_{Si}/V_{Ge}$ on the thermal conductivity of nanowires is studied as well. We have demonstrated that SiGe core-shell nanowires are promising low thermal conductivity materials.

References

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