PHONON ENGINEERED SUPPRESSION OF LATTICE THERMAL CONDUCTIVITY IN SEGMENTED AND CROSS-SECTION MODULATED SILICON NANOWIRES

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Abstract. *The strong suppression of lattice (phonon) thermal conductivity in segmented nanowires, consisting of acoustically-mismatched materials, as well as in cross-section modulated Si nanowires is theoretically demonstrated using the Born-von Karman and Face-centered Cubic Cell models of lattice vibrations. This effect is explained by the exclusion of the phonon modes trapped in nanowire segments from the heat flow. As a result 3- to 30-fold drop of the phonon heat flux in the 50 – 400 K temperature range is predicted for segmented or cross-section modulated nanowires under consideration.*

Keywords: *nanowire, phonon, lattice thermal conductivity*

I. Introduction

Phonons, i.e. quanta of lattice vibrations, manifest themselves in all electrical, thermal, and optical phenomena in semiconductors. Reduction of the size of electronic devices below the acoustic phonon mean free path creates a new situation for the phonons propagation and interaction. From one side, it may complicate heat removal from the downscaled devices. From the other side, it opens up an opportunity for engineering phonon energy spectrum in nanostructured materials, referred as phonon engineering [1-2], and achieving enhanced operation of nanoscale devices.

In spite of the fact that bulk Si is a poor thermoelectric with room-temperature figure of merit ZT ~ 0.01, thin Si nanowires (NWs) and rough Si nanowires are considered very promising for thermoelectric applications [3-4] due to low values of the RT lattice thermal conductivity k_{ph} <1 W m^{-1} K^{-1}. The reduction of the RT lattice thermal conductivity up to 75% was also theoretically demonstrated in Si/Ge core-shell NWs with Ge thicknesses of several monoatomic layers [5].

In this report I will theoretically demonstrate a three- to sevenfold reduction of the room-temperature (RT) lattice thermal conductivity in periodically cross-section modulated Si and Si/SiO_2 nanowires (MNWs) and up to to 30-fold drop of the RT lattice thermal conductivity in Si-based segmented nanowires (SNWs) consisting of acoustically-mismatched materials due to a strong re-distribution of their phonon energy spectra in comparison with generic Si NWs [6-7]. The phonon energy spectra in the MNWs, SNWs and NWs under analysis were calculated using both five-parametric Born–von Karman and Face-Centered Cubic Cell models of lattice dynamics [6-7].

II. Theoretical results

Figure 1 illustrates the drop of the thermal conductivity in a SNW consisting of segments made of Si, Ge and model materials, in comparison with the Si nanowire with the same cross-section 4.88 nm × 4.88 nm. In the Si/plastic SNW the average phonon group velocity strongly decreases due to the decelerating effect of the plastic material and dispersionless phonon modes trapped in the superlattice segments. An interplay between these two effects leads to a decrease of the thermal conductivity by a factor of 25 – 35 in comparison with the Si nanowire. The thermal conductivity of the Si/SiC and Si/SiO_2 SNWs is smaller than that in the Si nanowire by the factors of 5 – 10 and of 8 – 15, respectively, depending on the temperature. Redistribution of the phonon energy spectra in the cross-section modulated Si nanowiers also leads to a strong decrease of the average phonon group velocities, exclusion of the phonon modes, trapped in MNWs segments, from the heat flow and a corresponding suppression of the phonon thermal flux in these nanowires as compared to the generic nanowires. As a result, three- to sevenfold drop of the phonon heat flux in the 50 – 400 K temperature range is predicted for the Si and Si/SiO_2 MNWs under consideration.

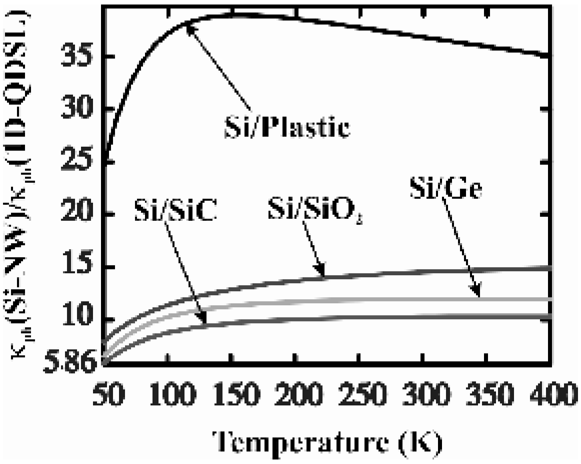

Figure 1. Temperature dependence of the ratio between lattice thermal conductivity in an Si NW and that in different segmented NWs with six atomic layers of Si and two atomic layers of an acoustically-mismatched material (Ge, plastic, SiC, or SiO2) per superlattice period. Figure is reproduced from Ref. [6] with permission from the American Physical Society.

III. Conclusions

The strong 3- to 30-fold drop of the phonon heat flux in the 50 – 400 K temperature range is predicted for the segmented and cross-section modulated nanowires under consideration. This effect is explained by the strong redistribution of phonon energies and group velocities in segmented and cross-section modulated nanowires in comparison with generic nanowires. The obtained results show that many phonon modes trapped in segments of segmented and cross-section modulated nanowires is excluded from the heat flux.

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IV. References

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