Acoustic phonon engineering of thermal properties of silicon-based nanostructures

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Abstract. We have theoretically studied the influence of the nanostructure cladding materials on the phonon thermal conduction in the Si-based planar heterostructures and rectangular hetero-nanowires. The phonon energy spectra were obtained in the framework of the face-centered cell-dynamic lattice model. Using this model we have shown that the nanostructure claddings with the low sound velocity decrease the phonon group velocities and thermal conductivity in the nanostructures, while the claddings with high sound velocities have the opposite effect. The described modification of the thermal conductivity of the semiconductor nano- and heterostructures may have important consequences for electronic industry in a view of continuing miniaturization.

1. Introduction

As the feature size of the devices continues to decrease and the amount of dissipated power increases, the problem of heat removal and thermal management becomes extremely important for further progress in the electronic industry. It is well known that the thermal conductivity of the generic semiconductor nanostructures is smaller than that of constituent bulk materials [1]. In the technologically important semiconductors and dielectrics heat is mostly carried by the acoustic phonons and the decrease of thermal conductivity happens due to the increased phonon – boundary scattering and, in the very small structures, due to the modification of acoustic phonon energy spectra and decrease in the phonon group velocity [2-4]. Modification of the acoustic phonon dispersion is particularly strong in the freestanding thin films or in nanostructures embedded into the elastically dissimilar materials [4-6]. Such modification may turn out to be desirable for some applications while detrimental for others. Thus, nanostructures offer a new way of controlling phonon transport via tuning its dispersion relation, i.e. *phonon engineering* [2, 7].

The reduction of the thermal conductivity, being a bad news for the thermal management of downscaled electronic devices, is good news for the thermoelectric devices, which require materials with the high electrical conductivity and low thermal conductivity [7]. It has been shown theoretically that the decrease of the thermal conductivity of free-standing Si thin films [2] and Si nanowires [3, 6] can be as large as two orders of magnitude in the in-plane direction or along the length of the nanowire. The measurements of the thermal conductivity of the individual Si nanowires with the diameter from 115 nm down to 22 nm revealed a two orders of magnitude decrease of the thermal conductivity due to the size effects [8], which is in excellent agreement with the theoretical predictions

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[3]. Using the elastic continuum approach, we have previously shown [4, 9-10] that by a proper selection of the cladding material parameters and their thicknesses one can tune the phonon group velocity in nanostructures, embedded into the elastically dissimilar materials.

In this paper we investigate the influence of the cladding materials on the phonon thermal conductivity in Si-based planar heterostructures and rectangular hetero-nanowires using the dynamic lattice face-centered cubic cell (FCC) model for the acoustic phonons. The thermal conductivity calculations were performed taking into account the major mechanisms of phonon scattering [1-3] such as scattering on the point defects and impurities, boundary scattering and three-phonon Umklapp processes.

2. Theoretical model

We considered Si-based planar three-layered heterostructures and rectangular heterowires with the layer thickness of few nanometers to ensure the confinement of acoustic phonons. Applying the FCC dynamic-lattice model to the specific nanostructures, we obtain the acoustic phonon energy spectra. The crystal lattice of silicon can be represented by two face-centered cubic cells, which are shifted along the diagonal by 1/4 of its length. In our model calculations we assume two shifted FCC-cells and consider them as a common FCC cell with the doubled mass at each lattice point. This simplification neglects the relative motion of the FCC sublattices and leads to the acoustic phonon solution only. Since we are primarily interested in the lattice thermal conduction, the focus on the acoustic phonons is justified.

The important feature of the dynamic approach is the use of the force constants, which describe the interaction between the atoms. Our model is based on three independent force constants expressed through three elastic modulus c_{11}, c_{12} and c_{44}. In order to obtain the phonon energy spectra in the planar heterostructures and hetero-nanowires we derived and solved the system of the equations of motion written as

$$m(n)\omega^2 w_i(n,q) = \sum_{n'} D_{il}(n',n,q) w_l(n',q), \quad i = 1,2,3. \tag{1}$$

Here n is the index for counting the atomic monolayers of the considered nanostructure, q is the phonon wave vector, ω is the phonon frequency, $w_i(n,q)$ are the amplitudes of the displacement vector components, $m(n)$ is the mass of the lattice point and $D_{il}(n,n',q)$ are the elements of the dynamic matrix describing the interaction between atoms of n and n' monolayers. The thermal conductivity of the planar heterostructures (HS) and hetero-nanowires (HW) was calculated using the following formulas [6]

$$\kappa_{\mathrm{ph}}^{\mathrm{HS}} = \frac{1}{4\pi k_{\mathrm{B}} T^2 d} \sum_{\alpha,s} \int_0^{q_{\max}} (\mathrm{h}\omega_s^{\alpha}(q))^2 \left(\frac{\partial \omega_s^{\alpha}(q)}{\partial q}\right)^2 \tau_{tot}(\omega_s^{\alpha}) \frac{\exp\left(\frac{\mathrm{h}\omega_s^{\alpha}(q)}{k_{\mathrm{B}}T}\right)}{\left(\exp\left(\frac{\mathrm{h}\omega_s^{\alpha}(q)}{k_{\mathrm{B}}T}\right)-1\right)^2} q\,\mathrm{d}q, \tag{2}$$

$$\kappa_{\mathrm{ph}}^{\mathrm{HW}} = \frac{1}{2\pi \mathrm{h} k_B T^2 d_1 d_2} \sum_{\alpha,s} \int_0^{E_{\max}} (E_s^{\alpha}(q))^2 \left\langle v(\omega) \right\rangle N_b(\omega) \tau_{tot}(\omega_s^{\alpha}) \frac{\exp\left(\frac{\mathrm{h}\omega_s^{\alpha}(q)}{k_B T}\right)}{\left(\exp\left(\frac{\mathrm{h}\omega_s^{\alpha}(q)}{k_B T}\right)-1\right)^2} \mathrm{d}E, \tag{3}$$

where $\tau_{tot}(\omega_s^{\alpha})$ is the total phonon relaxation time, α is the phonon polarization and $N_b(\omega)$ is the number of phonon branches crossing the frequency ω and $\langle v(\omega) \rangle$ is the average phonon group velocity. While calculating the thermal conductivity using equations (2-3), we determined the maximum value of phonon frequency (cut-off frequency) directly from the phonon energy dispersions.

3. Results and discussion

To study the influence of the nanostructure claddings on the thermal conductivity we considered the Si-slab (5nm) and two types of heterostructures: plastic/Si/plastic with the dimensions 3nm/5nm/3nm and diamond/Si/diamond with the dimensions 3nm/5nm/3nm. Plastic (Pl) was chosen as an example of material with a low sound velocity, while diamond (C) as an "acoustically fast" material. The longitudinal and transverse velocities in Pl are equal to 2 km/s and 1 km/s, and in C are 17.5 km/s and 12.8 km/s, correspondingly. For simplicity, we assumed that the plastic material has the cubic crystal lattice and that the lattice constants of both model materials are the same. The lattice constant of Si was taken to be a=0.543072 nm. The dependence of the phonon group velocities $v_s^\alpha = \mathrm{d}\,\omega_s^\alpha / \mathrm{d}\,q$ on the phonon wave vector is presented in figure 1 (a-c) for Si slab (a), Pl/Si/Pl (b) and C/Si/C (c) hetero-structures. The results are shown for SA phonon polarization. The negative values of phonon group velocities reflect the quasi-optical behavior of the acoustic phonon branches at some values of q in heterostructures [4-5, 9]. As one can see, the plastic claddings significantly reduce the phonon group velocities in comparison with Si slab, while the diamond claddings increase them. These results are similar for other phonon polarizations.

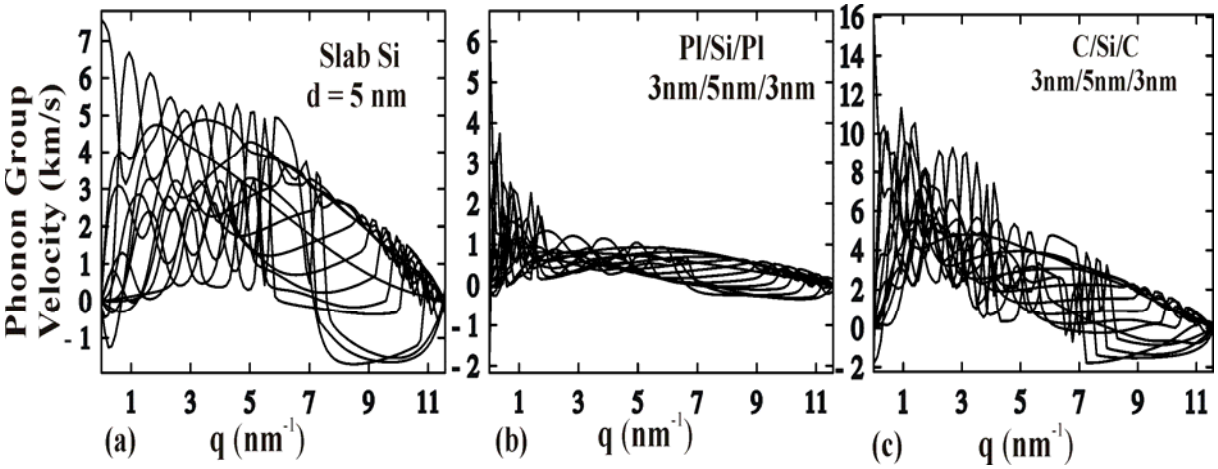

Figure 1. Phonon group velocities in (a) Si-slab with thickness of 5 nm, (b) heterostructures Pl/Si/Pl (3nm/5nm/3nm), (c) heterostructures C/Si/C (3nm/5nm/3nm) as a function of q. The lowest 15 phonon branches of the SA polarized phonons are depicted.

The influence of different cladding materials on the phonon thermal conductivity is illustrated in figure 2 (a). One can see from this figure that the "acoustically fast" diamond claddings increase the thermal conductivity in heterostructure over a wide temperature range. At low temperature the thermal conductivity of C/Si/C heterostructure is about two times larger than that in Si-slab. The "acoustically slow" claddings have an opposite effect. The thermal conductivity of Pl/Si/Pl heterostructure is lower than in the 5-nm Si slab by a factor of 1.3 at low temperature. Similar ratios are found for the room temperature thermal conductivities.

The dependence of the thermal conductivity on temperature in Si nanowires with Ge_xSi_{1-x} shell is shown in figure 2 (b) for different Ge content. One should note here that Ge is "acoustically slower" material than Si. The thermal conductivity of Si nanowire decreases with increasing Ge content x. The thermal conductivity of Si/Ge hetero-nanowire is by a factor of 1.5 lower than that in Si nanowire. The main reason for the decrease of the thermal conductivity is the modification of the acoustic phonon energy spectra and reduction of the group velocities in Si/Ge_xSi_{1-x} hetero-nanowires in comparison with the generic free-standing Si nanowire.

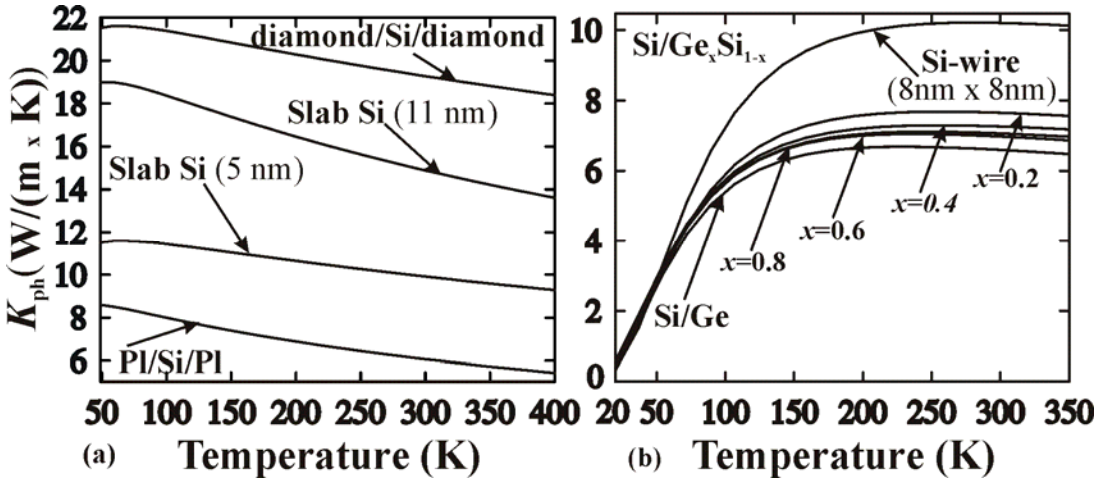

Figure 2. Lattice thermal conductivity as a function of the temperature for different Si-based nanostructures: (a) planar heterostructures with dimensions 3nm/5nm/3nm and (b) hetero-nanowires of the 8nm × 8nm and 5nm × 5nm Si-nanowire cross-sections.

4. Conclusions

We have theoretically investigated the phonon thermal conductivity in Si-based nanostructures using the face-centered cubic-cell dynamic lattice model. We have found that the cladding materials in such nanostructures influence on the lattice thermal conductivity, i.e., the claddings with the higher (lower) sound velocities increase (decrease) the phonon thermal conductivity in comparison with the generic nanostructure without claddings. This effect is explained by the change in the phonon energy spectra and group velocities in the nanostructures with the acoustically dissimilar layers. The obtained results may lead to a new method for tuning the phonon thermal conductivity in nanostructures by a proper selection of the elastic parameters of the cladding layers and their thicknesses.

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