Phonon scattering at the interface between elastically dissimilar materials

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In recent years there have been growing interests in Si and Ge nanowires as promising structures for future electronics. Among these, the application to thermoelectric devices has attracted particular attention because it is found experimentally that the thermal conductivity of Si nanowires becomes largely suppressed as the cross-section decreases.[1] Low thermal conductivity is beneficial for maintaining temperature difference of thermoelectric devices and thus enhances the thermoelectric efficiency when associated with high electrical conductivity and large Seebeck coefficients. The underlying principle to reduce thermal conductivity is the introduction of phonon scattering centers because major heat transport in semiconductors is carried by phonon. The schemes include surface roughness, void defects, nanoparticles, alternate stacking of two different layers, and coated nanowires into devices.

In this work, we examine another structural defect that may be easily realized in experiments; several elastically-dissimilar layers are inserted into Si nanowires as shown in Fig. 1-(a). Silicides such as PtSi and W_2Ni_3Si are good candidates because they have different acoustic impedance from Si as well as give good electrical conductivity. The theoretical formalism is based on a continuum elastic wave equation, which provides relatively smaller computational burdens than atomistic calculations. From the isotropic elasticity theory the Lagrangian is given by,

$$\mathcal{L} = \int dV \left[\rho\omega^2 u^{(i)}u^{(i)} - (\partial_j u^{(i)})C_{ijkl}(\partial_k u^{(l)})\right] \quad (1)$$

where ρ is the mass density, C_{ijkl} is the elasticity tensor, and $u^{(i)}$ is the ith coordinate of the displacement. Since our system contains structural defects, the elasticity tensor and the mass density are position-dependent. In order to study the phonon propagation, we calculate phonon transmission using a Green's function method derived from the Lagrangian of Eq. (1).[2]

The calculated transmission for a single layer is shown in Fig. 2. Due to the different elasticity of a host material Si and the dissimilar layer, the overall transmission becomes smaller. For the case of a PtSi silicide layer, the phonon transmission is suppressed by approximately 20% at $E = 10$ meV. It is found that the suppression depends on detailed crystal parameters rather than a simple acoustic impedance ratio between host and dissimilar layers; a SiC layer with a acoustic impedance ratio $\alpha_{SiC}/\alpha_{Si} = 1.77$ results in more suppressed behavior than for a PtSi layer $\alpha_{PtSi}/\alpha_{Si} = 2.66$. As the number of layers increases, the transmission function is more reduced as plotted in Fig. 3. We find that the transmission exhibits Ohm's behavior with the number of the dissimilar layer even though elastic scattering at the interfaces is assumed. In this case the inverse of the transmission function increases linearly with the number of layers as shown in Fig. 4.

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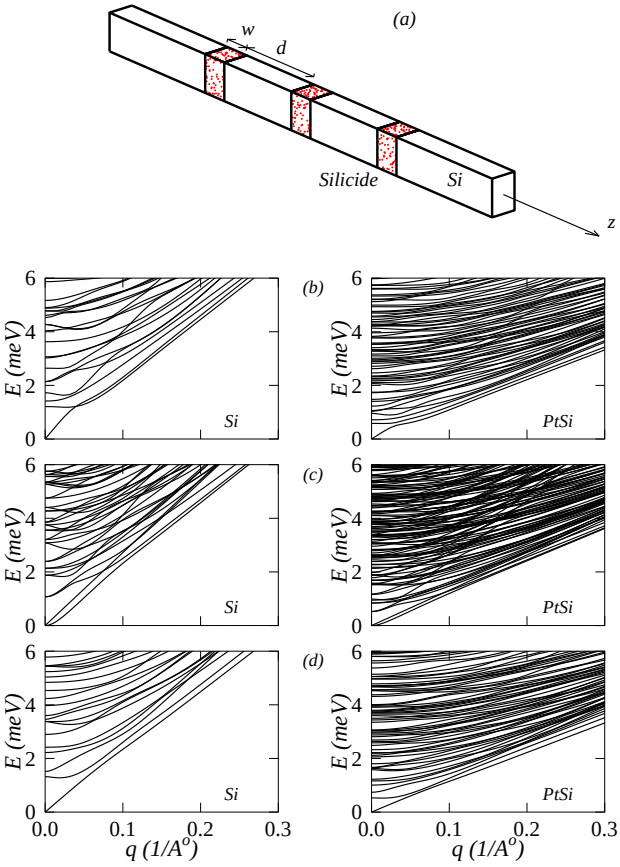

Fig. 1. (a) Schematic representation of a Si nanowire with three elastically dissimilar layers. The nanowire is assumed to have a rectangular cross-section and extends infinitely. Energy dispersions of dilatational(b), flexural(c), and shear/torsional(d) modes are shown for infinitely long Si (left) and PtSi (right) nanowires with a 8 nm $\times$ 8 nm cross-section.

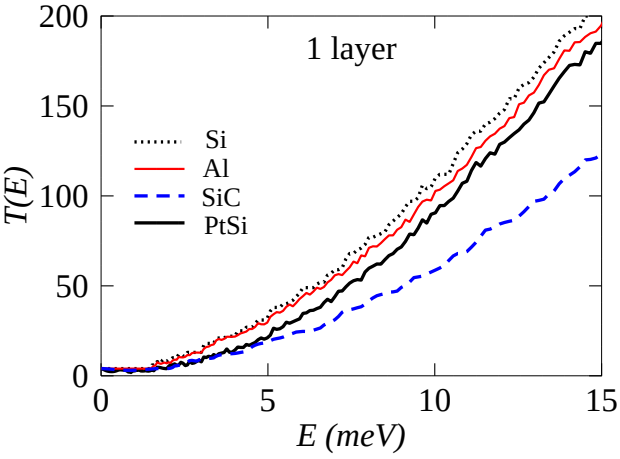

Fig. 2. Calculated transmissions of elastic waves are plotted as a function of incident energy for the case of a single dissimilar layer; PtSi (thick solid), SiC (dashed), Al (thin solid), and Si (dotted, corresponds to the no-layer case). We assume that nanowire cross-sections are a 8 nm $\times$ 8 nm and a layer thickness is $w = 10$nm.

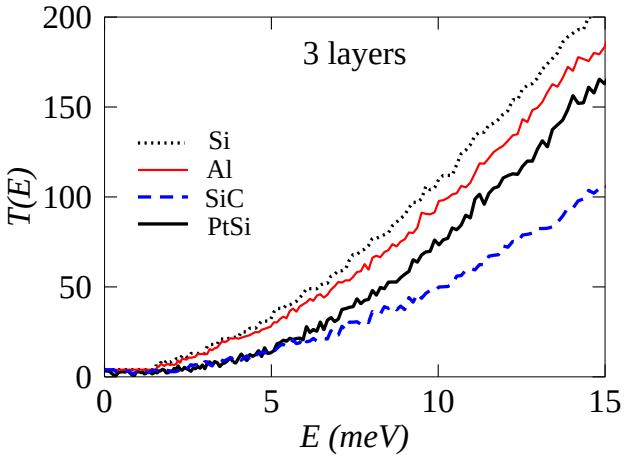

Fig. 3. Calculated transmissions of elastic waves are plotted as a function of incident energy for the case of three dissimilar layers; PtSi (thick solid), SiC (dashed), Al (thin solid), and Si (dotted, corresponds to the no-layer case). A 8 nm $\times$ 8 nm nanowire cross-section is used with a layer thickness, $w =$ 10nm, and a distance between layers, $d = 20$ nm.

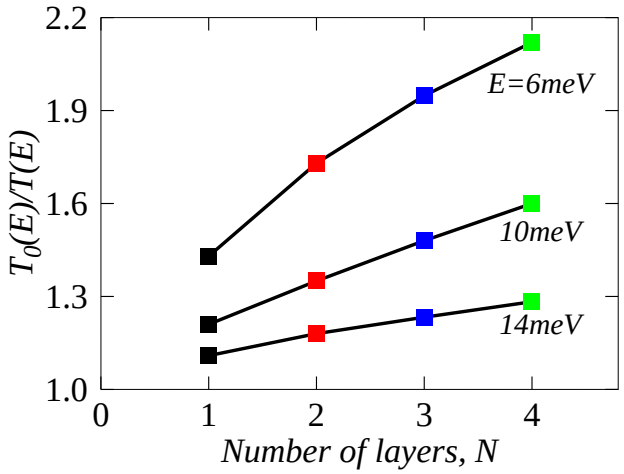

Fig. 4. The suppression of the transmission function relative to the result $T_0(E)$ of a pristine Si nanowire is emphasized as the number of layers increases for three different energies. The layer is assumed to be PtSi with a cross-section 8 nm$\times$ 8 nm, $w = 10$ nm, and $d = 20$ nm.