Calculation of phonon transmission in Si/PtSi heterostructures

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INTRODUCTION

In thermoelectric devices, the thermal conductance of materials is an important factor to enhance the figure of merit because it is responsible for maintaining the temperature difference between the hot and cold sides. The thermal conductance of materials was suppressed using a underlying principle to prohibit phonon propagation through devices as much as possible. This is because most thermal energy is carried by phonons in semiconductors. There have been efforts to suppress thermal conductance in a variety of ways in nanowires(1D), phononic-crystals(2D), and three-dimensional heterojunctions (3D).[1], [2]

In this work we examine the suppression of phonon transport in another example, Si and SiPt heterostructures (3D). This heterostrucure is believed to have the benefit that the electrical conductance can be kept high while the phonon propagation is suppressed due to the large acoustic impedance mismatch between Si and PtSi.[3]

METHOD AND DISCUSSION

In order to obtain a quantitative value for the phonon suppression, we use a method based on atomic vibrations. To do this, we first perform DFT calculations for phonon dispersion of Si and PtSi and find Harrison's potential parameters of Si and PtSi by fitting to them (Fig. 1). To generate atomic positions around the interfaces between Si and PtSi, we resort a molecular dynamic method based on the Stillinger-Weber potential while atoms in PtSi layers are fixed. An example of a unit block for heterostructures is illustrated in Fig. 2 after several hundred simulations with different initial conditions. It is found that the redistribution of atoms in the Si layer occurs roughly within one unit cell ($a_{\mathrm{Si}} = 0.546$ nm). We also find that most atoms in the Si layer near the interface deviate from the 4-bond geometry as shown in the two lower panels of Fig. 2. A phonon transmission function $T(E)$ is calculated using a Green's function method and the results are shown in Fig. 3. It is found that the transmission function is reduced by one order of magnitude, compared to the Si bulk value (dotted line), when a PtSi silicide layer is incorporated. Since there is a lack of acoustic modes at $20 \sim 30$ meV and of optical modes above 50 meV in a PtSi layer, phonons in this energy range are completely blocked. As we increase the number of PtSi layers, the calculated thermal conductance becomes smaller. In Fig. 4, we show the suppression of the thermal conduction. It is found that thermal conductance is rapidly suppressed by the insertion of a PtSi layer, however, eventually saturated over about 3 layers. In the case of $\mathrm{T} = 300$ K with three PtSi layers, the thermal conductance is suppressed by about 30-times, compared to the value for Si bulk.

ACKNOWLEDGMENT

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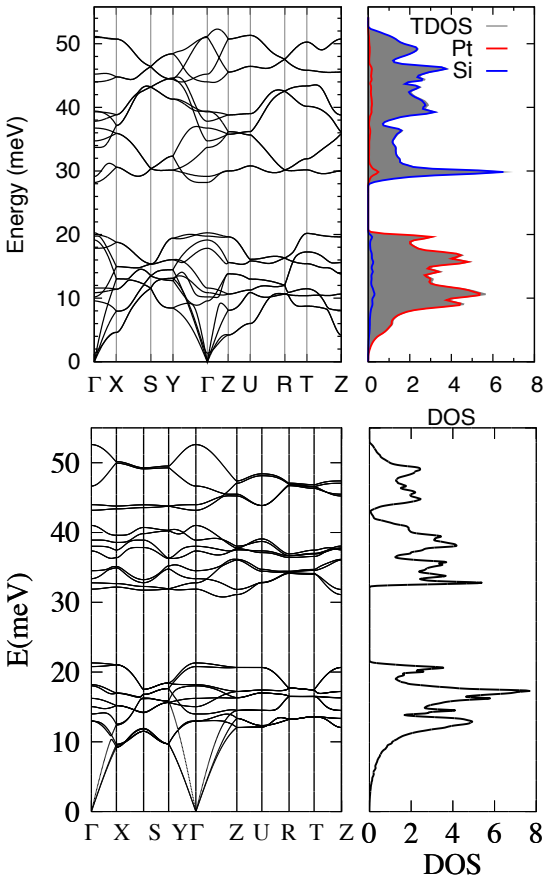

Fig. 1. Phonon dispersion calculated with an *ab initio* method (upper panel) and a Harrison-type potential (lower panel). An orthorhombic unit cell of size $0.592\text{nm}\times0.560\text{nm}\times0.385\text{nm}$ is used and there are four Si and four Pt atoms within it.

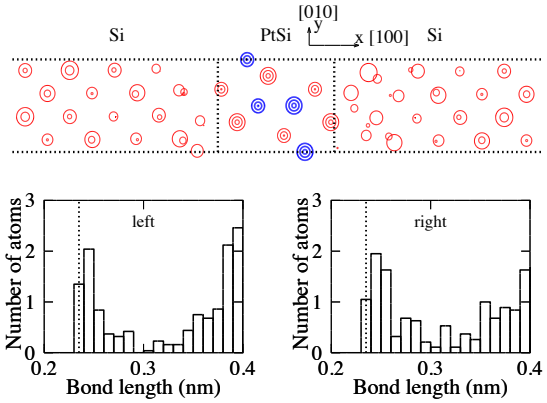

Fig. 2. (upper panel)Schematic representation of a Si/PtSi heterostructure. Thin (thick) circles are Si (Pt) atoms where the size of circles denotes their positions on the z-axis. The x-axis ([100]) is a phonon propagation direction and the cross-sectional area normal to that is $a_{\text{Si}}\times2a_{\text{Si}}$. (two lower panels) In a unit cell just left (right) to the PtSi layer, the average number of neighboring atoms for each Si is plotted as a function of bond length. The dotted line denotes the Si bond length in bulk ($\sqrt{3}/4a_{\text{Si}}$).

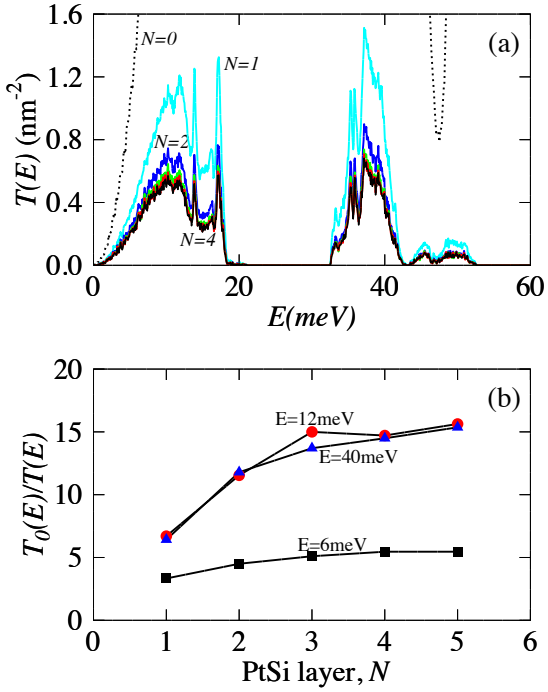

Fig. 3. (a) Calculated transmissions as a function of energy for different numbers of PtSi layers. (b) Normalized transmission functions for three different energies plotted against the number of PtSi layers. The thickness of the PtSi layer is 8.89nm (15 cells) and their intervals are 8.18nm (15 Si cells), with a cross-sectional area of $0.546\text{nm}\times1.092\text{nm}$.

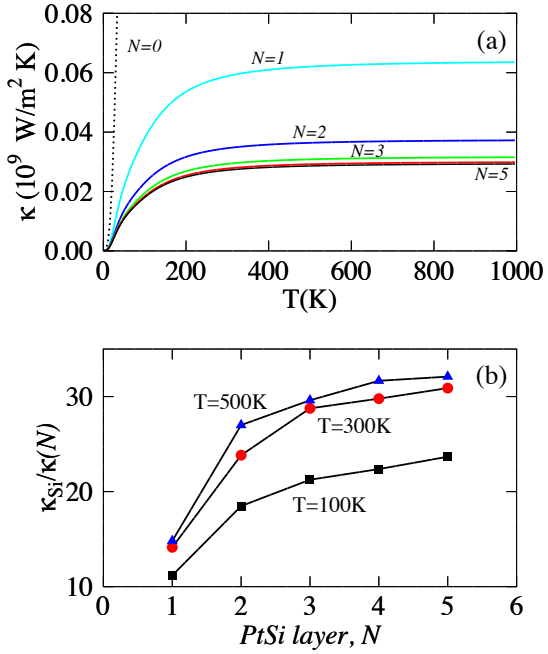

Fig. 4. (a) Calculated thermal conductance is plotted as a function of temperature with the transmission function in Fig. 3. (b) Ratios of thermal conductance between bulk Si and PtSi/Si heterostructures are compared as we increase the number of PtSi layers for three different temperatures.