Thermal Transport in Silicon Nanowires

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Abstract

The thermal conductance of small diameter silicon (Si) nanowires was determined using a Density Functional approach. Nanowires were isolated from a bulk clathrate system with a unit cell of 30 Si atoms. The equilibrium coordinates of the atoms in the unit cell were determined through structural relaxation based on Hellmann-Feynman forces. Additionally, coordinate relaxations of a clathrate nanowire with terminating hydrogen atoms were also done. The force constant matrix was evaluated for a SiH nanowire with three unit cells. Phonon bands were obtained from the force constant matrix, and the transmission function was used to calculate thermal conductances for 20 temperature values. The high temperature conductance limit was 4.75×10^{-10} W/K.

Introduction

Heat dissipation is a critical variable in the design and analysis of electronic systems. As device sizes approach the nanoscale order, constructing effective, thermally conductive fins becomes increasingly difficult. Transport of phonons and heat is ballistic in thermal conduits with length scales on the order of a nanometer. As a result, the analysis of the thermal conductance of nanowires requires a different approach from macroscopic systems. In this research, the thermal conductance was calculated by predicting how phonons would transmit through the system.

Phonons are the primary carriers of thermal energy in semiconductors. Phonons are waves created by the vibration of atoms in crystalline structures. The propagation of phonons through a lattice is responsible for thermal transport. In order to quantify the propagation of the phonons through the system, the force constant matrix of the nanowire system has to be determined. The phonon band diagram can be produced from the force constant matrix, and using this information, the transmission function of the system can be calculated as a function of frequency.

The transmission function T(ω) can then be used to calculate the thermal conductance, σ, with the following equation [1]:

$$\sigma = \frac{1}{k_B T^2} \int_0^\infty (\hbar\omega)^2 \frac{e^{\hbar\omega / k_B T}}{(1+e^{\hbar\omega / k_B T})^2} \mathrm{T}(\omega) d\omega / 2\pi$$

where T is the temperature, ω is the phonon frequency, k_B is the Boltzmann constant, and ħ is the reduced Planck constant.

Coordinate Relaxation

The first step in calculating the thermal conductance was to determine the atomic coordinates of the silicon nanowire taken directly from the bulk system. Figure 1 shows a top view of an isolated clathrate nanowire [2] with a unit cell composed of 30 Si atoms (dark grey) and 20 hydrogen (H) atoms (light grey).

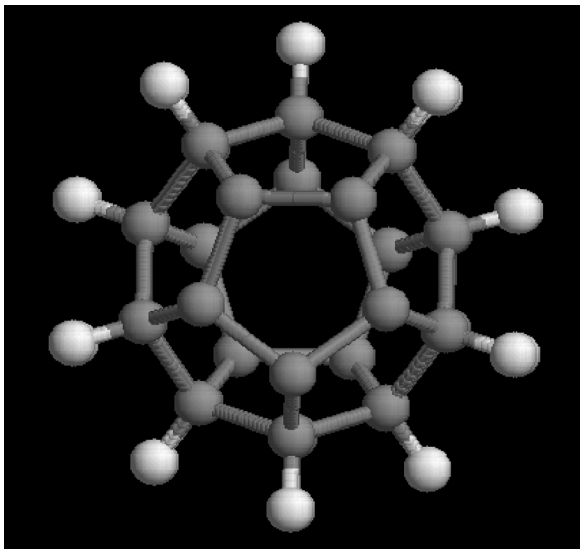


Figure 1: Isolated clathrate silicon nanowire with terminating hydrogens. Diameter (d) = 9.66 Å.

Figure 1 was created using Si-Si bond lengths of 2.38 Å and Si-H bond lengths of 1.50 Å [3]. The structure contains only regular pentagons. Structural relaxations were done using SIESTA, a self consistent density functional code with a atomic orbital basis set [4]. For the relaxation analysis, a cutoff energy of 200 Ry and a double-ζ basis set were used. A force tolerance of 0.0025 eV/ Å was taken for the calculation. Pseudopotentials were generated using Troullier and Martins' method [5]. 16 k-points in the z direction were used for the calculation.

The calculation of the relaxed coordinates produced a structure that looked very similar to the isolated structure shown in Figure 1. The relaxed nanowire had a diameter of 9.60 Å, as compared to the isolated nanowire which had a diameter of 9.66 Å. The lattice constant of the relaxed system was 10.31 Å, as opposed to a lattice constant of 10.59 Å.

Force Constant Matrix Generation

A force constant matrix for the relaxed Si nanowire was generated by linking three unit cells together and disturbing atoms in the middle unit cell. The forces induced on neighboring atoms by the disturbance were used to generate the force constant matrix. The force constant matrix was used to create a phonon band diagram, and the transmission of phonons was calculated as a function of frequency. The phonon band diagram is shown in Figure 2, and the transmission function is shown in Figure 3.

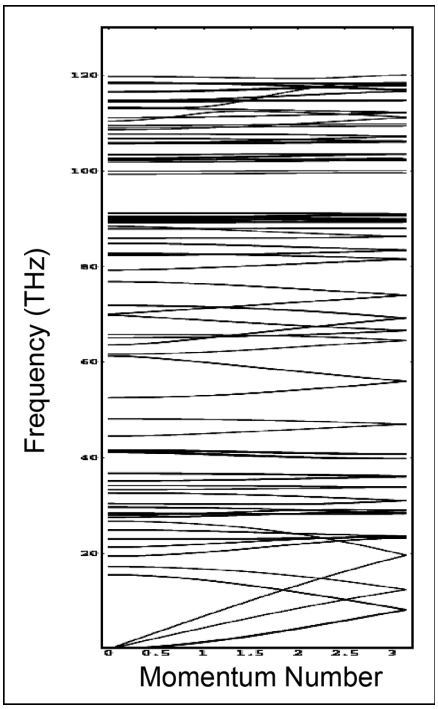
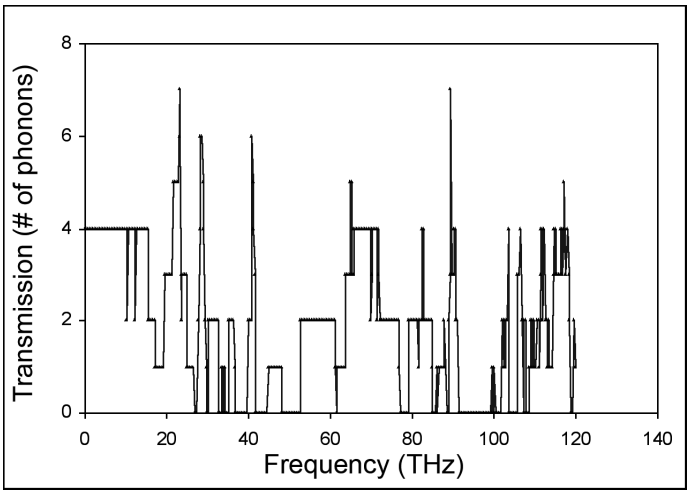


Figure 2, left: Phonon band diagram for terminated clathrate system.

Figure 3, below: Transmission function for terminated clathrate system.



The transmission function was generated from the phonon band diagram by observing the density of phonon bands at each frequency. The transmission function has sharp peaks at frequencies where the bands are flat and dense, and is zero for frequency ranges with no bands.

Thermal Conductance Calculation

Using the transmission function shown in Figure 3, the thermal conductance of the silicon clathrate nanowire with terminating hydrogens was calculated as a function of temperature, by numerically solving the conductance equation for temperatures ranging from 0 to 500 K, in increments of 20 K. The resulting graph is shown below in Figure 4, and the high temperature conductance limit of this system was determined to be approximately 0.475 nW/K. In comparison, a (7,0) carbon nanotube was determined to have a greater high temperature conductance limit of 4.50 nW/K [1].

Acknowledgments

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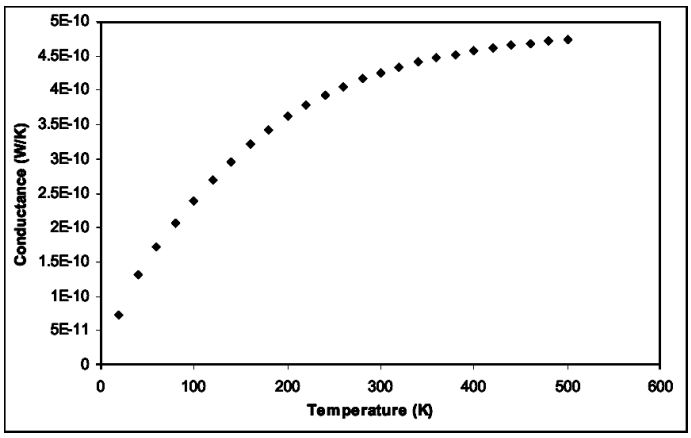

Figure 4: Thermal Conductance as a function of Temperature.