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Probing thermal phonon mean free path using phononic crystal nanostructures

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Abstract. We demonstrate an experimental method to obtain information of thermal phonon mean free path (MFP) spectra in thin films using hole based two dimensional phononic crystal nanostructures. The characteristic length of the system can be swept by changing the radius of circular holes of the phononic crystals. Then, thermal conductivities of single-crystalline Si, amorphous SiGe, and poly-SiGe thin films (150 nm thick) were measured for phononic crystals with different characteristic length between 20 nm and 200 nm. We observed different characteristic length dependence of the thermal conductivity among these three systems and the trend can be explained by the thermal phonon MFP spectra of the materials.

1. Introduction

Nanoscale heat transfer has been investigated because of its importance in both fundamental physics and other applications, such as thermoelectrics.¹ The thermal phonon MFP is an important physical parameter and determines the thermophysical property of a system. Some characteristic phonon transport phenomena have been reported in a variety of nanostructures.²⁻⁹ Recent theoretical and experimental works have simulated or measured thermal conductivity accumulation distribution as a function of thermal phonon MFP.¹⁰⁻¹⁴ It is known that the thermal phonon distributions span very broad frequencies and thus lead to broad thermal phonon MFP spectra. As thermal phonon MFP is directly connected to thermal conductivity, the impact of nanostructuring on thermal conductivity seems strongly dependent on the relation between the thermal phonon MFP spectrum and the characteristic length of the nanostructures. In this contribution, we report a method to obtain the information of thermal phonon MFP in solid by measuring in-plane thermal conductivity in 2D phononic crystal (PnC) nanostructures. In-plane thermal conductivity measurement was performed for a series of PnC nanostructures, which have different characteristic lengths, namely the shortest distance between two circular holes. The PnC nanostructures were fabricated in different materials; single-crystalline Si, amorphous and poly-SiGe, which have completely different MFP spectra. The observed different characteristic length dependence of the thermal conductivity among these three systems gives us some useful information on thermal phonon MFP spectrum in the thin film.

2. Sample and fabrication of phononic crystal nanostructures

Single-crystalline Si, amorphous SiGe, and poly-SiGe membranes were used for this study. For Si samples, we used a commercially available (100) nominally boron-doped silicon-on-insulator wafer



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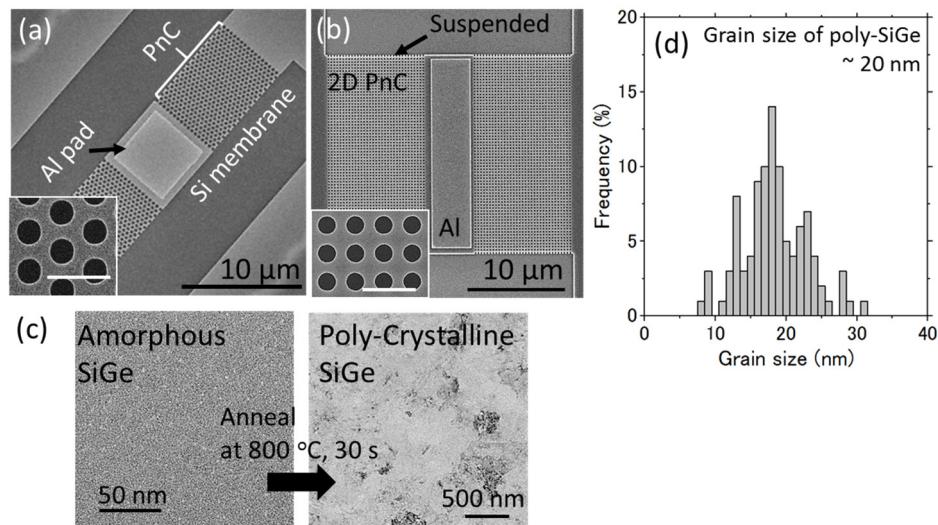


Figure 1. SEM images of the whole suspended structures: (a) hexagonal lattice Si PnC and (b) square lattice SiGe PnC structures. (c) TEM images of the surfaces of amorphous SiGe and poly-SiGe layers. (d) Histogram of the measured grain sizes of poly-SiGe on the surface.

with a 145 nm-thick upper Si layer and a 1 μm-thick buried SiO₂ layer. For SiGe samples, an amorphous Si_{0.5}Ge_{0.5} layer with a thickness of 150 nm was deposited on the SiO₂/Si(001) substrate using solid-source molecular-beam-epitaxy at room temperature. A poly-SiGe sample was fabricated by annealing the amorphous SiGe sample at 800°C for 30 s in a N₂ atmosphere. Figures 1(a) and 1(b) shows scanning electron microscopy (SEM) images of the whole suspended Si and SiGe structures with two-dimensional PnC structures. An Al pad in the center enables microscale thermoreflectance (TDTR) measurements. The PnC structures were formed using circular holes aligned in periodic square or hexagonal lattice formations, as shown as the inset in Figs. 1(a) and 1(b). The PnC structures were fabricated with a fixed period, $a = 300$ nm, and a variety of radii. Figure 1(c) shows surface images, taken by transmission electron microscopy (TEM), of the amorphous and poly-SiGe membranes. The polycrystallization process formed crystal grains, which are expected to have changed the thermal phonon MFP spectrum. We analysed the TEM image to obtain a histogram of the grain size of the poly-SiGe [Fig. 1(d)]. It was found that the grain size is distributed between 10 and 30 nm in diameter. PnC nanostructures were fabricated with either single-crystalline Si, amorphous SiGe, or poly-SiGe thin films to change the characteristic length of the system. We can obtain some useful information about thermal phonon MFP spectra by measuring the sensitivity of thermal conductivity to the characteristic length. For example,

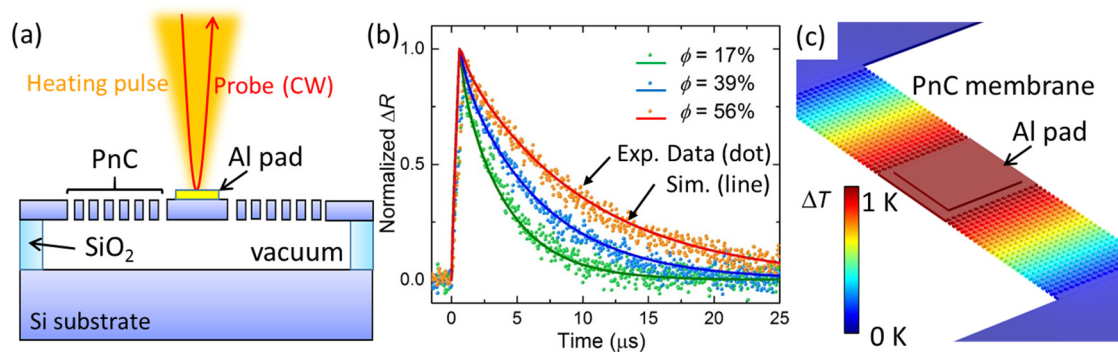


Figure 2. (a) Schematic of the μ-TDTR technique and cross section of the structure. (b) Measured (dot) and simulated (line) TDTR signal for a square-lattice PnC structure with various porosities. (c) Simulated temperature distribution 15 μs after heating for a SiGe PnC structure with $r = 100$ nm.

most of the thermal phonon in Si at room temperature have MFPs between 100 nm and 10 μm , resulting in Si showing a high sensitivity to PnC nanostructures with a characteristic size of around 100 nm.¹⁵ The characteristic length was swept between 20 nm and 220 nm by changing the radius of the circular holes of PnC nanostructures. Here, the periodicity of the holes does not affect the thermal conductivity through the band-folding effect,¹⁶ because phonon coherence is mostly lost at room temperature.

3. Simulation and experiment

To measure the in-plane thermal conductivities of the PnC nanostructures, a method using micro TDTR was developed. The Al pad was heated by a pulsed laser beam (wavelength $\lambda = 642$ nm) for 500 ns and the temporal evolution of the temperature of the Al pad was monitored using a continuous-wave laser beam ($\lambda = 785$ nm) as shown in Fig. 2(a). All the measurements were performed at room temperature. This well-defined system made it possible to obtain a highly reliable value for the thermal conductivity by analysing the temporal evolution of the TDTR signal. Figure 2(b) shows the measured TDTR signal (dots) and a simulated curve (solid line). The temperature evolution in the whole structure was simulated via the finite element method using exactly the same structural parameters as the experiment. Figure 2(c) shows the simulated temperature distribution, 15 μs after pulse heating, for a PnC structure with $r = 100$ nm. The value of thermal conductivity was obtained via the least squares method.

The thermal phonon MFP spectrum was investigated for the three thin films by comparing the thermal conductivities. The membranes have different thermal phonon MFP spectra owing to differences in their structures at atomic and nanometer scales. Therefore, the characteristic length dependence of thermal conductivity is also expected to be different owing to the different MFP spectra. The neck size is the characteristic length of the PnC nanostructure and is defined as the distance between two adjacent holes. Figure 3 shows the neck size dependences of the thermal conductivities of PnC nanostructures fabricated in the thin films. The thermal conductivities (dots) for the square-lattice PnC (κ_s) and hexagonal-lattice PnC (κ_h) nanostructures are plotted for a variety of radii. The orange and blue lines are the polynomial fits to the measured data to calculate the difference in thermal conductivity $D(\Phi)$, as defined by:

$$D(\Phi) = \frac{\kappa_s(\Phi) - \kappa_h(\Phi)}{[\kappa_s(\Phi) + \kappa_h(\Phi)]/2}. \quad (1)$$

The PnC patterning reduces the thermal conductivity from the unpatterned membrane value (neck = 300 nm). We note that the thermal conductivity itself is reduced as a result of surface scattering at the sidewalls of the holes. For all the materials, the hexagonal-lattice PnC nanostructures showed lower thermal conductivity than the square-lattice PnC nanostructures. This indicates that the placement of the holes influences heat transfer with ballistic phonon transport properties. The reductions from the

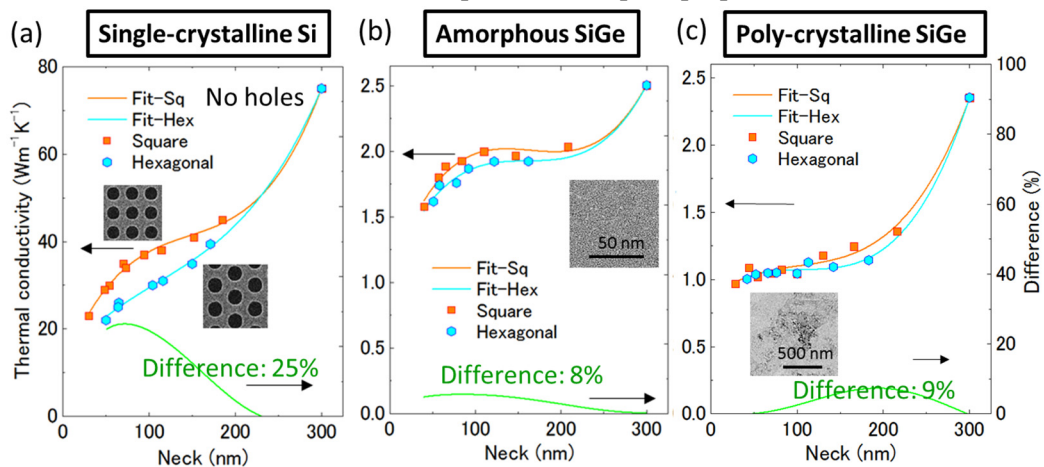


Figure 3. Measured in-plane thermal conductivity for PnC nanostructures with a variety of neck size at room temperature: (a) single-crystalline Si, (b) amorphous SiGe, and (c) poly-SiGe. The difference $D(\Phi)$ is shown by green lines (right vertical axis) at the bottom of figures.

membrane values are about 20% and 50% at the neck size of 200 nm for the amorphous and poly-SiGe, respectively. It is considered that the poly-SiGe has thermal phonons are distributed in very short (< 20 nm) and long (> 200 nm) MFP ranges. In amorphous SiGe, thermal conductivity sharply drops below the neck size of 70 nm. This can be explained by the fact that amorphous SiGe has a large thermal phonon MFP distribution in the range of tens of nanometers. In poly-SiGe, relatively weak dependence is observed between neck sizes of 20 nm and 200 nm, as shown in Fig. 3(c). It is considered that the transport of phonons with MFPs around tens of nanometers is impeded in poly-SiGe, owing to strong grain boundary scattering, which results in a poor contribution of these phonons to thermal conduction. This agrees with the grain size distribution shown in Fig. 1(d). This result suggests that nanostructures with dimensions comparable to the grain size do not reduce thermal conductivity effectively. Therefore, the characteristic length of the nanostructures should be chosen to avoid the overlap with other characteristic length. This series of experimental results indicates that the impact of nanostructuring on the thermal conductivity change is qualitatively explained by thermal phonon MFP spectra. Although the discussion is qualitative, the reported characteristic length dependences of the thermal conductivity with different MFP spectra may be useful to determine some parameters in the simulations for nanoscale heat transport.

4. Summary

The relation between thermal phonon MFP spectra and the impact of nanostructuring on thermal conductivity using Si, amorphous SiGe, and poly-SiGe membranes have been investigated. The experimentally obtained characteristic length dependences of thermal conductivity were qualitatively explained by thermal phonon MFP spectra. This thermal conductivity measurement, sweeping the characteristic length, can be used as thermal phonon MFP spectrum proving and gives useful information for designing nanostructures for highly efficient thermoelectric materials.

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