# Thermal conductivity of ultrathin Si films with a periodic pore pattern

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## INTRODUCTION

The design of new semiconducting materials with an ultra-low thermal conductivity $\kappa$ is currently one of the most active areas of research in solid-state physics. The 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 phonon transport of an infinite Si thin-film with periodic pores[1] whose unit cell is shown in Fig. 1. The structure may be easily realized in experiments and it is expected to provide phononic gaps in its dispersion to reduce the thermal conductivity.

## METHOD AND DISCUSSION

In most theoretical investigations of thermal transport through a patterned Si film, the continuum approach were employed because it can treat a large unit cell up to several $\mu m$. However, the continuum approach is believed to be valid in the low energy range below 20 meV, namely, suitable for describing acoustic phonon propagation. In order to take a full energy range of phonon into account, we use an atomistic method adopting the Stillinger-Weber potential. Via the Stillinger-Weber potential, we search for the relaxed atomic configuration of a Si thin-film when there is a pore at its center and calculate the transmission function with non-equilibrium Green's function method. Then, the thermal conductivity is calculated with the relation of,

$$\kappa = \frac{\hbar^2}{k_B T^2} \sum_m \frac{1}{2\pi} \int_0^\infty \mathcal{T}_m(\omega) \frac{\omega^2 e^{\hbar\omega\beta}}{(e^{\hbar\omega\beta}-1)^2} d\omega \quad (1)$$

where the integration is over the frequency $\omega$ of the modes $m$ and $\beta = 1/k_B T$. $\mathcal{T}_m(\omega)$ is the transmission function and, in the ballistic case, is equal to the number of the modes. Fig. 2 shows the phonon dispersion for a 2nm×2nm unit cell and the corresponding transmission function. One can see that a phonon gap is formed around energy of 20 meV. Fig. 3 shows the formation of the gap as we increase the pore size. Apparently, the larger pore size gives rise to enlarged gaps. In Fig. 4, with calculated transmission functions, we plot the thermal conductivity as a function of temperature for several pore sizes. As the pore size increases, the thermal conductivity decreases in the whole range of temperature. This is because the number of atoms in unit cells is reduced and corresponding phonon modes become smaller with the increase of the pore size. By considering the large unit cell up to several tens of nanometers, we discuss the gap formation and the optimal pore shape to reduce the thermal conductivity.

## ACKNOWLEDGMENT

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## REFERENCES

[1] J.-H. Lee, J. C. Grossman, J. Reed, and G. Galli, *Lattice thermal conductivity of nanoporous Si: Molecular dynamics study*, Appl. Phys. Lett. **91**, 223110 (2007).

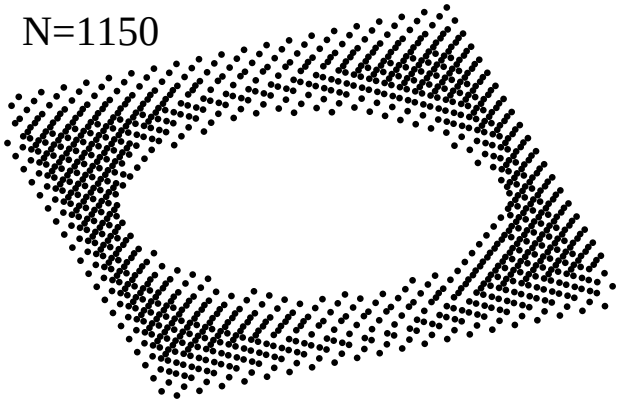


Fig. 1. A typical unit cell used for phonon transport calculations is shown. The size of the cell is 10.5nm×10.5nm and its thickness is 0.35nm along the [001] direction. The pore is assumed to be 52% of the cell area with a circular shape.

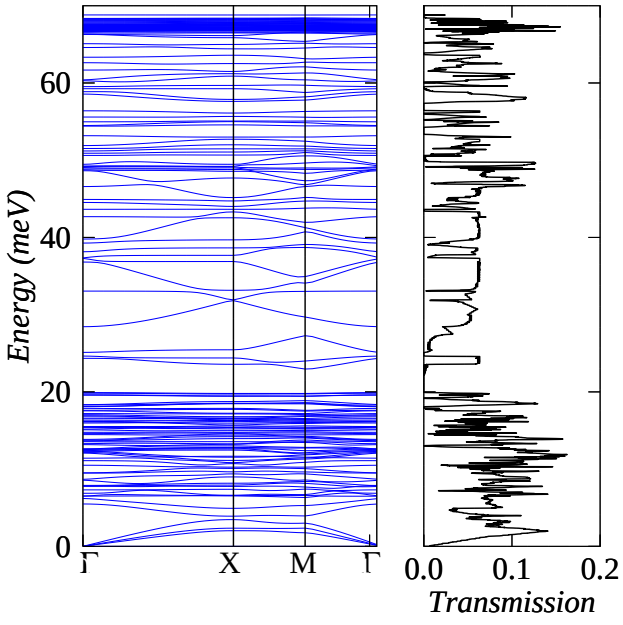


Fig. 2. Band structure and calculated transmission function are plotted for a Si thin-film. The unit cell size is 2nm×2nm with a 0.5nm thickness. The pore fraction is 32% of the unit cell area. It is found that a phonon gap is formed above 20meV.

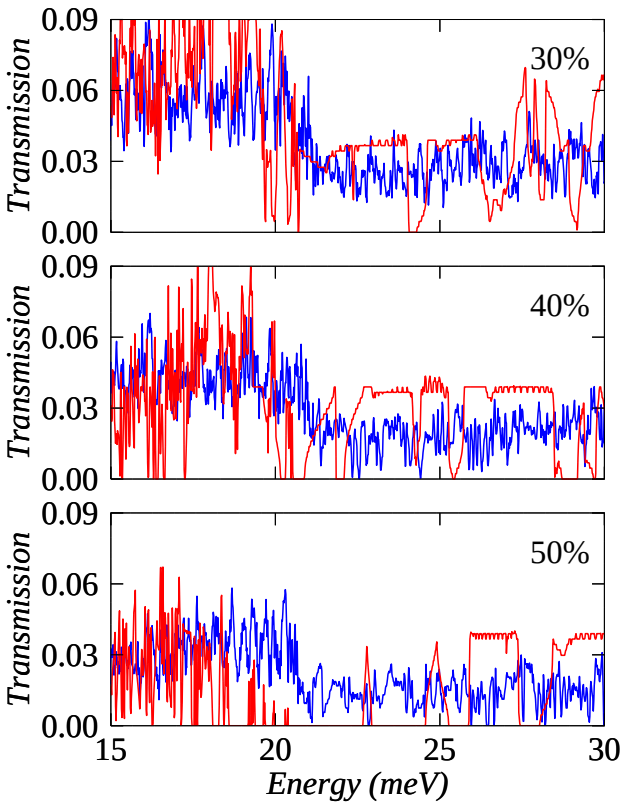


Fig. 3. For different pore sizes, the transmission functions are compared to show the formation of a phonon band gap. The unit cell sizes are 6.5nm×6.5nm (blue) and 2.7nm×2.7nm (red) with a 0.5nm thickness.

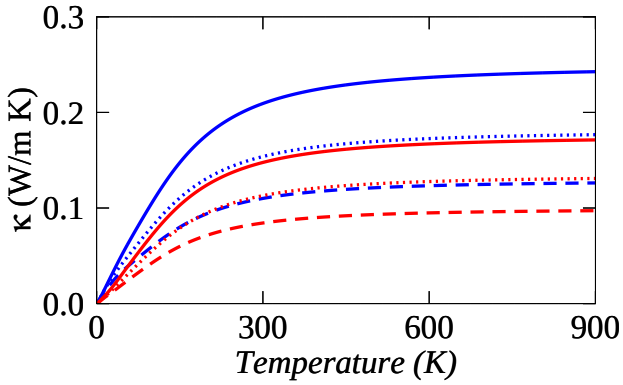


Fig. 4. Calculated thermal conductivities are compared for different pore sizes; 30% (solid), 40% (dotted), and 50% (dashed lines) relative to the unit cell area. The unit cell sizes are 6.5nm×6.5nm (blue) and 2.7nm×2.7nm (red) with a 0.5nm thickness. Without a pore, the thermal conductivity is saturated to 1.42 W/m K at 1000K.