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シリコン一次元周期ナノ構造における熱伝導率低減の起源に関する考察

Origin of the reduced thermal conductivity of a periodic 1D Si nanostructure

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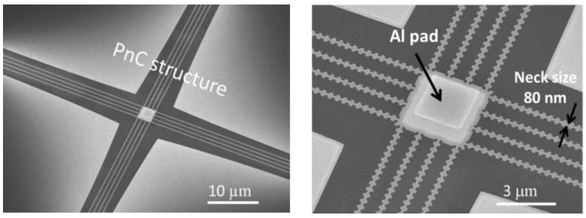
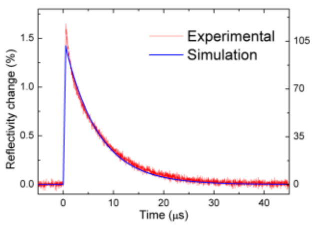
Improving thermoelectric efficiency by reducing the thermal conductivity in the otherwise poor thermoelectric material such as silicon would help the technology to spread further. At the nanoscale, the size effect due to phonon ballisticity and boundary scattering reduces the thermal conductivity [1]. In periodic structures, coherent effects [2] are expected to reduce the thermal conductivity even further. In this contribution, we report the fabrication and measurement of 1D periodic nanostructures. The mechanism of lower thermal conductivity compared to a similarly sized nanowire is investigated using Monte-Carlo simulations.

After determining the frequency range of phonons to target, namely the ones contributing the most to the thermal conductivity, we design the structures that effectively inhibit phonon transport in the range by performing FEM simulations with COMSOL Multiphysics. Then these structures are fabricated from an SOI wafer using a classical top-down approach, including Electron-Beam lithography (Fig. 1).

We developed a time domain thermoreflectance system to measure the reflectivity of these structures. We obtain the thermal conductivity by comparing the time history of the reflectivity with a heat conduction model solved by COMSOL Multiphysics for the same structure (Fig. 2).[3] The thermal conductivity of the same structures was also simulated using Monte-Carlo simulations solving the phonon Boltzmann transport equation. The variable in the simulation is the specularity parameter (p), where the phonons are reflected at the adiabatic surfaces either specularly (p=1) or diffusively (p=0). The experimental and the simulated thermal conductivity of the nanostructures (Fig. 3) exhibit a similar trend. The reduction in the thermal conductivity compared to that of the nanowire seems to arise mainly from backscattering of phonons at the surfaces with particular contribution from the walls perpendicular to the heat conduction direction since they reflects phonons against the heat flow most effectively. It can clearly be seen from Fig. 3 that a combination of both specular and diffusive scattering is needed to properly describe the thermal conductivity of the nanostructures, with the value of p slightly above 0.5 seemingly fitting best for larger wires. The steeper decrease in thermal conductivity observed in the experiments for thinner structures may be the result of a rougher surface caused during the fabrication.





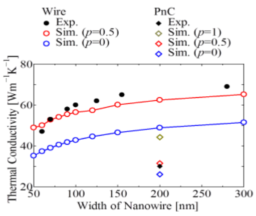


Fig. 1(left). SEM images of air-suspended 1D Si periodic nanostructures. Fig. 2(middle). Measured (red) and simulated results (blue) of heat dissipation through a Si 1D periodic nanostructure. Fig. 3(right). Monte Carlo simulated thermal conductivity compared to the measured ones.

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