Thermal Conductance Calculations of Silicon Nanowires

Kohei Yamamoto[1], Hiroyuki Ishii[1], Nobuhiko Kobayashi[1], and Kenji Hirose[2]

[1]Institute of Applied Physics, University of Tsukuba, Tsukuba, Ibaraki, 305-8573, Japan
[2]Green Innovation Research Laboratory, NEC Corporation, Tsukuba, Ibaraki, 305-8501, Japan

bk201130108@s.bk.tsukuba.ac.jp

Abstract

Phonon thermal transport properties of silicon nanowires (SiNWs) have attracted much attention recently. As silicon electron devices with nanowire structures become small to nanometer-scale, we need to reduce the thermal heating problem. Also, SiNWs are good candidates for efficient thermoelectric devices. Here, we present the phonon thermal conductance calculations for SiNWs with diameters ranging from 1 to 5 nm by using the nonequilibrium Green's function (NEGF) technique.

Experimentally, the thermal conductivities of SiNWs with diameters ranging from 15 to 115 nm have recently been measured and showed unusually low thermal transport properties. To understand the thermal transport properties of SiNWs less than 100 nm in diameter, we need to consider the phonon problems from an atomistic point of view. Thermal conductance calculations with the Boltzmann transport formula or molecular dynamics calculations are effective at high temperature in diffusive regime. Recent calculations with transmission model using the phonon dispersion relation with the data from "bulk" silicon showed good agreement with experiments for SiNWs which have diameters larger than 35 nm. However, for phonon transport at low temperature or with diameters less than 30 nm, the effects of nanometer-scale structures such as confinement and low speed modes on the phonon transport become significant. For such regimes, we need the computational approach taking the quantum effects explicitly into account. Here we use the NEGF technique with empirical Tersoff interatomic potential for the atomistic calculation of thermal conductance of SiNWs.

We present thermal conductance calculations of SiNWs with diameters from 1 to 5 nm with vacancy defects based on the NEGF approach, focusing especially on the difference of the position of the vacancies. We introduce two types of vacancies in the SiNWs, "surface-defect" with atoms at the surface missing and "center-defect" with atoms at the center of cross section of wires missing, for both of which we consider single and double vacancies. Then we compute how the thermal conductance of SiNW changes its behavior as the temperature decreases, changing the thickness of wires.

Fig. 1 shows the thermal conductance of SiNWs as a function of the diameter D at various temperatures from 5 to 300 K. Overall, it looks that thermal conductance shows the quadratic behavior for the diameter D. To see the diameter dependence on the conductance G more precisely, we extrapolate the curves of G to the power law of $G=AD^n$ where A is the constant. The obtained exponent n is shown in the inset. At high temperature above 100 K, we see $n = 2$, which shows that the thermal conductance increases in proportion to its cross-sectional area S, proportional to the square of diameter D as a usual Ohmic-type behavior. However, as the temperature decreases below 100 K, the diameter dependence on the conductance is seen to change. At low temperature below 5 K, we see $n = 0$ which shows that the thermal conductance does not depend on the thickness of the nanowire structure at all. This means that the thermal conductance changes its behavior from the usual Ohmic-type at room temperature, proportional to its cross-sectional area, to the unusual quantum-type at low temperature, not dependent on the cross-sectional area [1]. In the presentation, we show how we can understand these exponents behaviors. Also we found that introduction of the defects reduces the thermal conductance significantly and that "center-defect" reduces thermal conductance much more than "surface-defect". We also show the comparison of the results using the empirical interatomic potentials with those from the ab-initio calculations.

References

[1] K. Yamamoto, H. Ishii, N. Kobayashi, and K. Hirose, App. Phys. Express, **4** (2011) 085001.

Figures

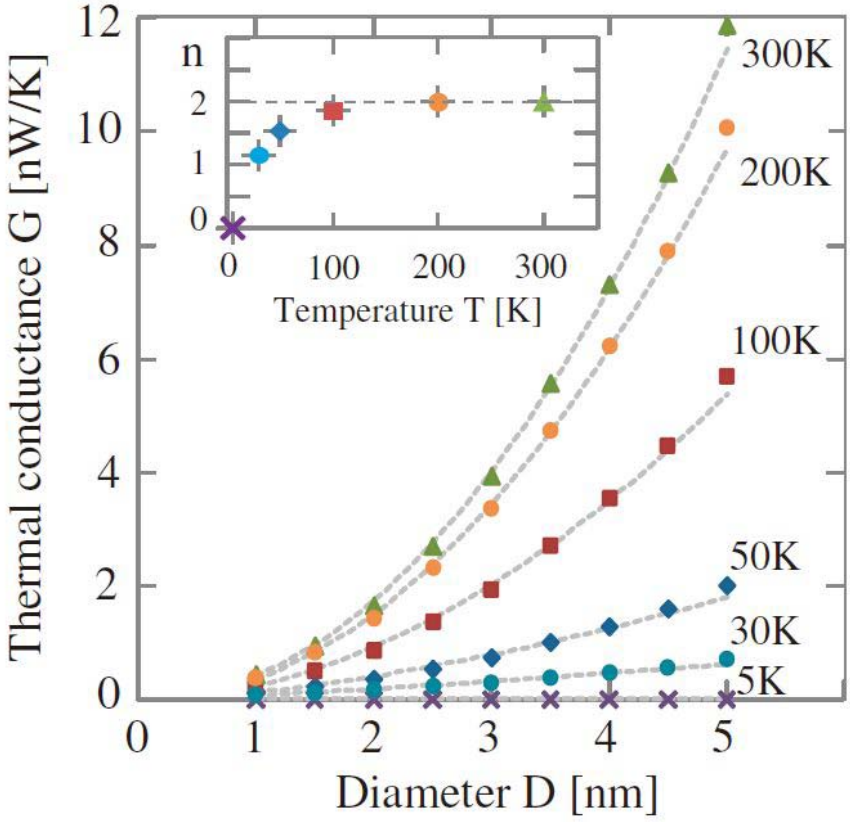

Fig. 1. Thermal conductance as a function of the diameter of SiNW without vacancy defects for several temperatures. (Inset) Exponent *n* for several temperatures extrapolated for the thermal conductance as $G = AD^n$ where *D* is a diameter of SiNW.