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Temperature dependence of thermal conductivity in quantum wires due to interaction between two-level systems and phonons

２準位系－フォノン相互作用が及ぼす量子細線における熱伝導率の温度依存性

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1. Introduction

Recent development of nanofabrication technology enables to make novel kinds of devices at the nanometer scale such as remarkably sensitive detectors. For example, membranes and/or quantum wires made of silicon nitride (SiN) are used for detecting far-infrared waves, X-rays, and elementary particles, and for calorimeters [1-4]. Since electronic and optical energies are localized in the nanoscale region, the specific heat and thermal conductance of the device become the key parameters to cap the device performance because of increase in the device temperature. The thermal transport in the nanostructures has therefore attracted much attention

The thermal conductivities κ of membranes and wires at sub-Kelvin temperatures are found to be proportional to T^p, where p takes a value roughly between 1 and 2 [3,4], while p=3 for a bulk material. One of the possible factors for the disagreement in p with the bulk material is the reduced dimensionality of phonon modes. However, the temperature dependences are observed even in the temperature region that the dominant wavelength of thermal phonons becomes smaller than the thickness of the systems, evidencing that the temperature dependence has no relation with the low dimensionality of phonon modes.

It is known that an amorphous solid has a thermal conductivity with p<3, which is originated from phonon scattering by the defects that the amorphous solid contains. Although the nanostructures are fabricated with top-down methods from a bulk crystalline solid, defects will be possibly formed in the system when fabricated. We expect that the defects hinder phonon transport in the nanostructure, resulting in the thermal conductivity with p<2 like the amorphous solids.

In this work, we theoretically investigate phonon scattering due to defects in a rectangular quantum wire of SiN [5,6], and declare that the defects affect significantly the thermal conductivity of the system, resulting in the thermal conductivity with p<2.

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2. Model and Methodology

We consider a rectangular quantum wire made of SiN of a wurtzite crystal structure [7]. The wire is assumed to contain dynamic defects, which are modeled by an ensemble of TLSs [8,9]. Supposing a uniform distribution for the defects, we take account of the interaction between phonons and TLSs. The mean free path of phonons is estimated using the Fermi golden rule, and the dependence of the power p regarding the thermal conductivity on the aspect ratio of the wire cross-section is declared.

In order to obtain precise acoustic phonon modes of the quantum wires, we use the *xyz*-algorithm [10], where the displacement vector is given by a power series of the Cartesian coordinates. The method can treat free vibrations of an object of an elastically anisotropic material with arbitrary shape. One of the present authors obtained precise acoustic phonon modes in a rectangular wire of cubic crystalline materials using the method, and classified the phonon modes into the dilatational, flexural, torsional, and shear modes, according to the symmetries of the modes. Applying the method to our system, we derive the normal phonon modes peculiar to the system, which are exploited in the evaluation of the thermal conductivity.

3. Numerical Results

Figure 1 shows the temperature dependence of thermal conductivity in the wire with cross-sectional dimensions 20 nm × 5 nm. In the temperature range below 1 K, κ is plotted linearly in a log-log plot, and the power of the *total* $\kappa \propto T^p$, denoted by solid triangles, is estimated to be 1.17 using the least-square method. Each normal phonon mode, numbered 1-4 for convenience, corresponds to the dilatational (1), two flexural (2 and 3) and

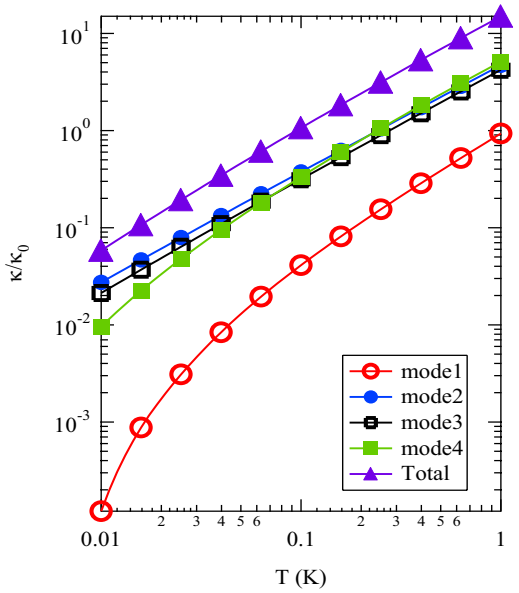

Fig. 1 Temperature dependence of thermal conductivity κ in SiN wire with cross-sectional dimensions 20 nm × 5 nm. The solid circles denote the contributions to κ from each normal phonon mode in the wire. Each mode numbered 1-4 corresponds to dilatational (1), flexural (2 and 3) and torsional (4) modes, respectively, according to their spatial symmetries. The open boxes denote the *total* κ, the sum of all modes.

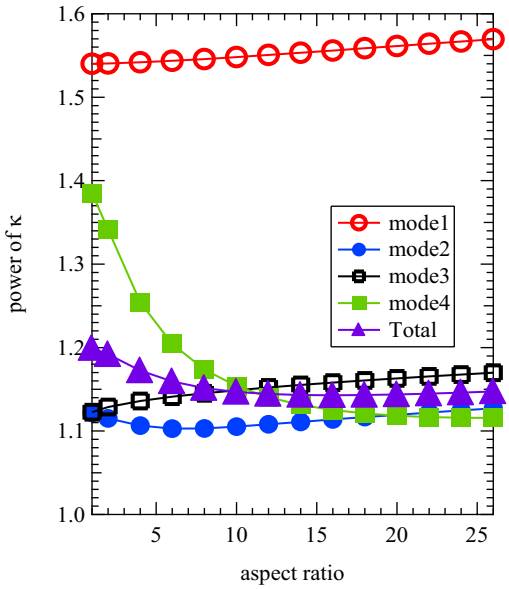

Fig. 2 The power of the temperature dependence of κ versus aspect ratio of the wire cross-section. The solid and open circles and boxes denote the power of each normal phonon mode, dilatational (1), flexural (2 and 3) and torsional (4) modes. The solid triangles denote the power of the *total* κ.

torsional (4) modes, respectively, according to their spatial symmetries. The power p for each mode is found to be 1.54, 1.10, 1.13, and 1.25, respectively. We find that the modes except for mode 1 equally contribute to the thermal conductivity at low temperatures.

Figure 2 shows the dependence of the power p on the aspect ratio of the wire cross-section, fixing the area. The solid and open circles and boxes correspond to the power p of each normal phonon mode in the wire. And the solid triangles denote the power of the total κ. From **Fig. 2**, we find that the *total* p, taking value between 1.1 and 1.2, becomes minimum at around the aspect ratio=15. In addition, we find that only mode 4 depends strongly on the aspect ratio. The reason is under consideration. Since the velocity of mode 1 is faster than the others, the power for mode 1 is the largest among them, but the contribution of mode 1 to κ is small.

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