1P1-8

Analysis and Estimation of Thermal Conductivity of Si Nanopillar/SiGe Composite Film by Using Photo-Thermal Spectroscopy Measurement with a Multi-layer Model Calculation

光熱変換分光測定と多層膜計算によるSiナノピラー/SiGe複合膜の熱伝導率の解析

Tomoki Harada[1†], Tsubasa Aki[1], Daisuke Ohori[2], Seiji Samukawa[2], Tetsuo Ikari[1] and Atsuhiko Fukuyama[1] ([1]Univ. of Miyazaki; [2]Tohoku Univ.)

原田知季 [1†], 安藝翼 [1], 大堀大介 [2], 寒川誠二 [2], 碇哲雄 [1], 福山敦彦 [1] ([1]宮崎大, [2]東北大)

1. Introduction

Thermoelectric (TE) materials have been attracting attention for solid state power generation devices because of importance by converting waste heat into electrical energy[1)]. The performance of TE device depends on the figure of merit, ZT, which is inversely proportional to thermal conductivity, κ. To realize a high performance of TE device, a reduction of κ is necessary. This is expected by using nanostructures because of an appearance of phonon boundary scattering. Bio-nanotemplate and neutral beam etching technique enable us to fabricate nanostructure arrays with diameters less than 20 nm. We have succeeded to fabricate a highly periodic Si nanopillar (Si-NP) with 10 nm diameter embedded in $Si_{0.7}Ge_{0.3}$[2), 3)], and reported that κ was estimated to be 3.5 ± 0.3 W/m·K from the 2ω method[2)]. This was about 40 times smaller than that of bulk Si. In addition, it was confirmed that there was an anisotropic nature of κ from the extended 3ω method[4)]. However, its analysis technique is not yet enough. In this study, in order to confirm the reduction of κ in more detail, we carried out the piezoelectric photo-thermal (PPT) measurements and estimated κ by adopting the multi-layer theoretical analysis.

2. Experimental Procedure

Figure 1 shows the schematic of the samples. Firstly, Si-NP array was fabricated on the silicon-on-insulator (SOI) substrate by using a bio-nanotemplate and a neutral beam etching technique[2)]. The height and diameter of Si-NP were 90 and 12 nm, respectively, and density was 1.6×10^{11} cm^{-2}. After that, $Si_{0.7}Ge_{0.3}$ was grown by thermal chemical vapor deposition (Si-NP sample). We also prepared a sample with 100-nm Si epitaxial layer grown on the SOI substrate for comparison (Si-epi sample).

For PPT measurements, a probing light was

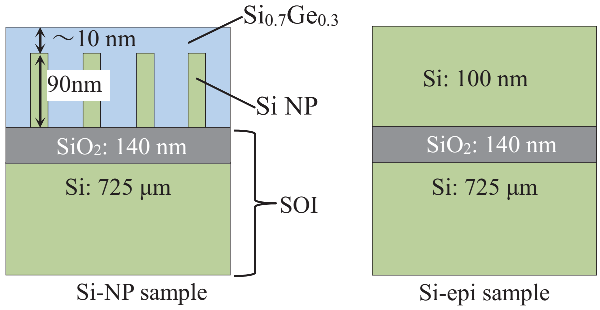

Fig. 1 Schematic structure of the sample

illuminated on the rear surface of the sample. A $LiNbO_3$ transducer was attached to the Si-NP/$Si_{0.7}Ge_{0.3}$ side for Si-NP sample and to the Si epitaxial layer side for Si-epi sample. If the propagation of heat and elastic waves were hindered by the presence of Si-NP before reaching the detector, the PPT signal may decrease. A spectral and a frequency-dependent PPT measurements were carried out. For the former, frequency was fixed at 108 Hz and the photon energy of the probing light was changed from 0.8 to 1.8 eV. For the latter, frequency was changed from 40 to 3500 Hz and probing light was fixed at 1120 or 1090 nm. All measurements were carried out at room temperature.

Theoretical analysis based on a multi-layer one-dimension heat propagation model was adopted for simplification[5)]. Since this model did not consider a depth profile of the light absorption, we modified by taking into account for the exponential light decay in position as a sub-surface heating. We assumed four layers for solving the heat diffusion equation. They are Si and SiO_2 layers in SOI substrate, Si-NP/$Si_{0.7}Ge_{0.3}$ composite layer, and transparent transducer. We further assumed that optical absorption coefficients of SiO_2 and detector were negligibly small. Then, we estimated κ of the composite layer by fitting the observed frequency dependence of the PPT signal to the model calculation.

hk15035@student.miyazaki-u.ac.jp

3. Results and discussion

Figure 2 shows experimental results of PPT spectra. Signal increases around the band gap of Si (1.12 eV at room temperature) were due to the non-radiative recombination of photo-excited carriers in the Si layer of SOI substrate. The PPT signal intensity of Si-NP sample was remarkably lower than that of Si-epi sample. This result indicates κ of composite layer was significantly lower than that of Si. By comparing a difference in PPT signal intensity between samples, and supposing that the thermal resistances of layers are placed in series, we calculated κ to be 0.58 mW/m·K. However, this was too small and was not a reasonable value. To reproduce the difference of signal intensity, extremely small κ were needed because the thickness of a composite layer was extremely thin. Therefore, another technique for evaluating κ should be considered.

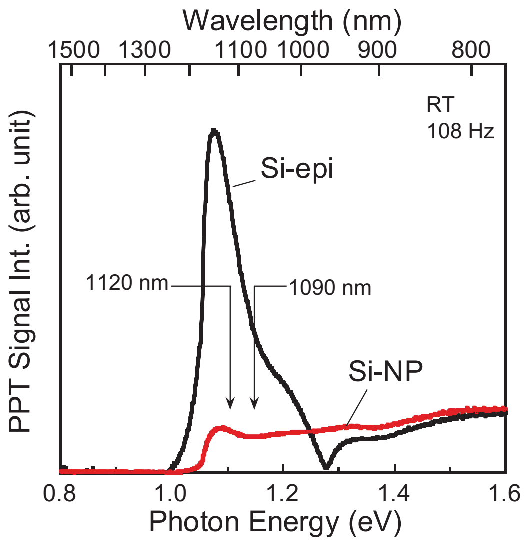

Fig. 2 PPT spectra of Si-NP and Si-epi samples.

Figure 3 shows experimental results of frequency dependence of PPT signal intensities. As the frequency increased, thermal diffusion length shortened and PPT signal decreased[5]. The PPT signal intensity for Si-epi sample almost linearly decreased as frequency increased. In contrast, a distinct signal dip was observed around 700 Hz for Si-NP sample. Since dip was reproduced by changing both κ and the optical absorption coefficient, α, this result indicates that the relation between the light penetration length and thermal diffusion length play an important role for the appearance of the observed signal dip. Then, we tried to estimate κ of composite layer by focusing on the signal dip. We have changed the fitting parameters, κ and α, to reproduce the signal dip. The results are shown in Fig. 3 by solid curves for 1120 and 1090 nm as an excitation wavelength. Although the dips may be well reproduced, a significantly large value for α in an order of 10^5 cm^{-1} was inevitable. Such large value of α near the band gap energy is not a realistic for Si. More detailed model calculation is necessary for explaining the role of very thin Si-NP/SiGe composite layer on the PPT signal generation.

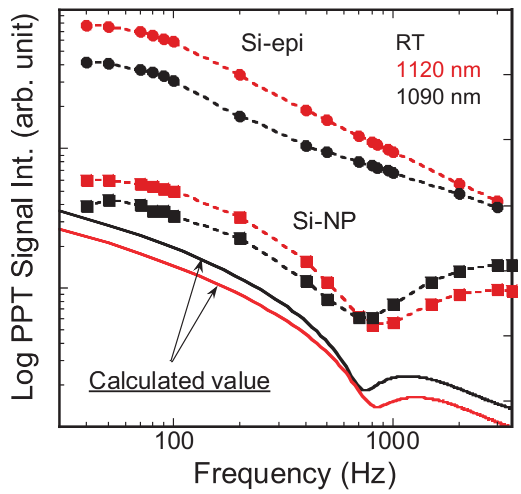

Fig. 3 PPT signal amplitudes of Si-NP and Si-epi samples as a function of frequency. Solid curves are for the theoretical calculation results.

4. Conclusions

We calculated κ of Si/SiGe composite layer by comparing the PPT signal intensities between Si-epi and Si-NP samples. Calculated κ of composite layer was remarkably lower than that of bulk Si. For frequency dependence of PPT, signal dip was only observed for Si-NP sample. Although the dip was reproduced by our theoretical model, the estimated α was remarkably large. We then concluded that κ and α of Si-NP/SiGe composite layer were significantly different from that of bulk Si. However, more elaborated models such as three dimensional analyses should be considered for explaining the observed dip.

Acknowledgment

Part of the work was carried out under the Collaborative Research Project of the Institute of Fluid Science, Tohoku University.

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