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Effect of Ion Irradiation on Thermal Conductivity along SiO_2/Si Interface Evaluated by Molecular Dynamics

Junya Takizawa[1], Sylvia Yuk Yee Chung[1], Motohiro Tomita[1, 3], Ryo Yokogawa[2, 3], Atsushi Ogura[2, 3], and Takanobu Watanabe[1]

[1] Faculty of Science and Engineering, Waseda University,
3-4-1, Okubo, Shinjuku-ku, Tokyo 169-8555, Japan
E-mail: junya.t1008@suou.waseda.jp
[2]School of Science and Technology, Meiji University,
[3]MREL,
1-1-1, Higashimita Tama-ku Kawasaki-shi 214-8571, Japan

Abstract

We investigate how the thermal conductivity of Si passivated with a SiO_2 film is modulated by Ar^+ ion irradiation using molecular dynamics (MD) simulation. The change in the thermal conductivity was quite slight, in spite of structural changes around the SiO_2/Si interface induced by the ion irradiation. The result is explained by that two opposing effects cancel each other: increase in the defect density causes the reduction of thermal conductivity, and the stress reduction in the Si lattice enhances the thermal conductivity. The result suggests that both the defects and stress are the essential factors to determine the thermal conductivity.

1. Introduction

Si nanowire is attracting considerable attention as a thermoelectric material which has a low environmental load for use in IoT systems. Decreasing thermal conductivity whilst maintaining electrical conductivity is a requirement for efficient thermoelectric performance. Our research group reported that interface stress between Si and SiO_2 film induced by oxidation causes a decrease in thermal conductivity [1]. A previous experiment using Raman spectroscopy [2] suggested that the thermal conductivity of Ar^+ ion implanted SiO_2/Si structure is higher than that of the SiO_2/Si structure. Resultantly, we anticipated that the oxide induced stress in the Si lattice is responsible for the decrease in the thermal conductivity, and the effect is accommodated by the ion irradiation.

In this study, we tried to confirm the effect via MD calculation. An SiO_2/Si interface model was created by oxidizing a part of Si crystal, and then we performed MD simulation of the Ar^+ ion implantation. We will discuss the change of stress, defect, and thermal conductivity before and after the Ar^+ ion implantation.

2. Simulation method

Fig. 1 shows the SiO_2/Si model and the Ar^+ ion implanted SiO_2/Si model created by MD calculation, with 2D periodic boundary conditions imposed in the x and y directions. Oxide film of the SiO_2/Si model was added onto the bare Si model using a layer-by-layer oxidation method, which inserts O atoms into the midpoint of the Si-Si bonds at the interface along the z-axis. Ar^+ ions, comprising 250V of the accelerating voltage, were introduced as defects via irradiation. 5 ions, which are equivalent to a $1.0\times10^{14}cm^{-2}$ dose, enters the SiO_2/Si model at an angle of 7 degrees from the z direction. The temperature of an Ar^+ ion implanted SiO_2/Si structure rises just after ion irradiation occurs, but a subsequent temperature reduction follows due to thermal diffusion. Calculation parameters control the mean temperature at 300K by reducing the velocity of model atoms at regular intervals. Finally, thermal conductivities were estimated via Fourier's law using both the heat flux and the temperature gradient, which were obtained by setting a temperature difference, in bare Si, SiO_2/Si structure, and Ar^+ ion implanted SiO_2/Si structure. We also calculated the stress distribution, phonon dispersion, and coordination number of these models to evaluate the change in thermal conductivity.

3. Results and Discussion

The thermal conductivity of bare Si is estimated to be 3 W/m·K, and that of SiO_2/Si structure and Ar^+ ion implanted SiO_2/Si structure are both estimated to be 2 W/m·K (Fig. 2). Decreasing thermal conductivity by forming an oxide film is in good agreement with previous research [1]. On the other hand, the change in thermal conductivity by ion irradiation has yet to be confirmed. Fig. 2 also shows an average stress before and after ion irradiation near the SiO_2/Si interface. The tensile stress relaxed conspicuously after irradiation. This result shows that ion irradiation reduces interfacial stress between Si and oxidation induced SiO_2 film. However, although a relaxation on the stress was observed, the thermal conductivity did not increase.

Fig. 3 shows the phonon dispersions of SiO_2/Si structure, and Ar^+ ion implanted SiO_2/Si structure, calculated to evaluate the effect of implementing a defect. The phonon dispersion of Ar^+ ion implanted SiO_2/Si structure is disturbed in the low-frequency region. This result shows that lattice disorder appears in Ar^+ ion implanted SiO_2/Si. Fig. 5 shows the coordination numbers of Si-Si bonds near the SiO_2/Si interface (sectioned area in

Fig. 4) to investigate the effect of lattice disorder, which is also an indication of the effect of ion irradiation. Before ion irradiation, coordination numbers of the atoms were confirmed to be 4, 2 and 0. A coordination number of 4 shows that the atoms have four Si-Si bonds in the Si region. In addition, a coordination number of 0 means that the atoms will only have Si-O bonds in the SiO_2 region. A coordination number of 2 will include two Si-Si bonds and some Si-O bonds on SiO_2/Si interface. After ion irradiation occurs, the coordination numbers have increased from 4, 2 and 0, to 0, 1, 2, 3 and 4. The change in coordination number showed that local defects are induced by ion irradiation in SiO_2/Si interface.

In literature, local defects in Si nanowire are known to decrease thermal conductivity [3]. Therefore, the stress reduction and defects appearance have opposing effects on the thermal conductivity. This is considered as why the thermal conductivity in the present simulation remains unchanged. Our calculation shows that ion irradiation not only induces defects, but also break bonds at the SiO_2/Si interface. The stress relaxation causes the bonds to break and negates the decreasing thermal conductivity induced by defects.

As mentioned in above, a previous experiment using Raman spectroscopy [2] suggested that the thermal conductivity of Ar^+ ion implanted SiO_2/Si structure becomes higher than that of the SiO_2/Si structure. There is a discrepancy between the previous experiment and the results reported in this current study. In the present simulation, quick cooling by reducing the velocity of the model atoms after ion irradiation, is different from the procedures utilized in experiment. Future work would entail increasing the reproducibility of an Ar^+ ion irradiation experiment.

4. Conclusion

We studied the effect of the ion implantation on the lattice thermal conductivity by means of classical MD calculation. The results show that the thermal conductivity does not change when stress relaxation occurs, as well as for the production of local defects. The result does not agree with the previous experiment using Raman spectroscopy. In the present MD simulation, the damage induced by the ion implantation is not fully recovered, and thus it canceled the increase in the thermal conductivity due to the stress reduction.

References

[1] T. Zushi et al., Phys. Rev. B **91** 115308 (2015). [2] R. Yokogawa et al., Jpn. J. Appl. Phys. **58** SDDF04(2019). [3] F. Murphy et al., Nano Lett. **14**, 7, 3785(2014).

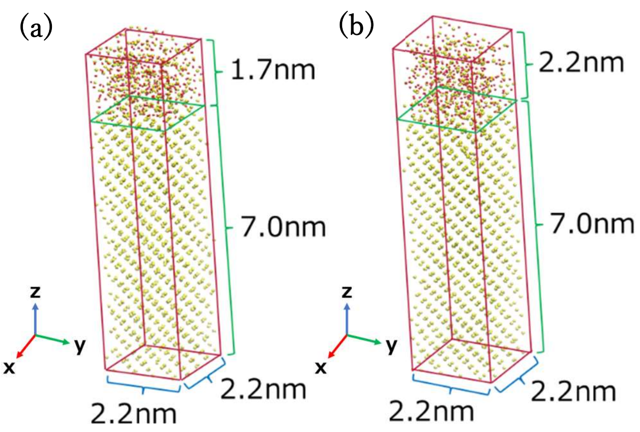

Fig. 1 Schematic of calculated (a)SiO_2/Si model, and (b)ion implanted SiO_2/Si model.

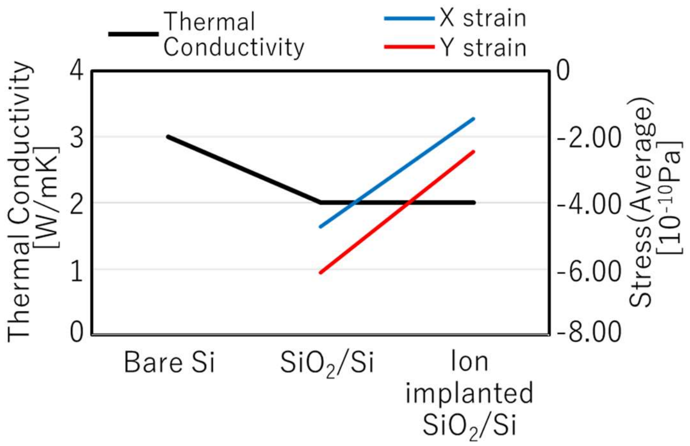

Fig. 2 Thermal conductivity and average stress of bare Si, SiO_2/Si film, and ion implanted SiO_2/Si film.

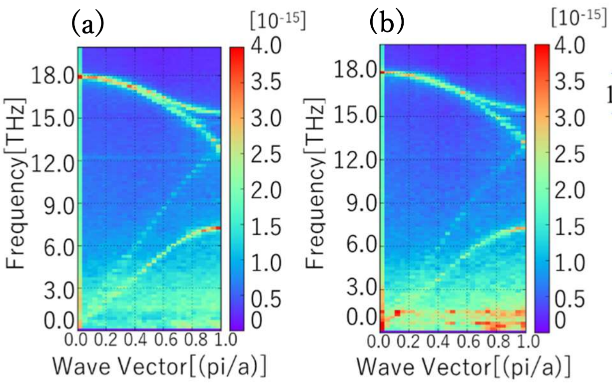

Fig. 3 Phonon dispersion (a)before, and (b)after ion irradiation.

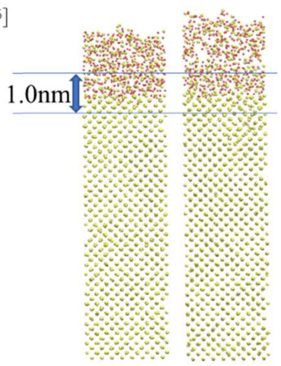

Fig. 4 Area of SiO_2/Si interface.

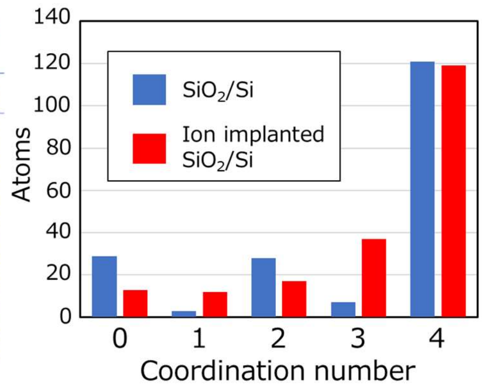

Fig. 5 Atom distribution of Coordination number.