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Thermal Transport Properties of Si Nanowire Covered with SiO₂ Layer: A Molecular Dynamics Study

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Abstract

We demonstrate the impact of SiO₂ layer on thermal conductivity of Si nanowire by nonequilibrium molecular dynamics simulation. Our results indicate that the presence of the oxide layer is influential to the significant decrease in the thermal conductivity. By analyzing the vibrational density of states, we show the reduction of the thermal conductivity stems from the attenuation of the low-frequency phonon modes. This work suggests that the disorders near the SiO₂/Si surface is crucial to characterize the thermal properties of practical SiNW.

1. Introduction

Understanding of thermal transport properties of Si nanowire (SiNW) is of particular importance for technological application such as FET and thermoelectric devices. This is because thermal conductivity κ of SiNW is 100-fold lower than that of bulk Si, and this κ would be the factor determining the device performance. For example, it is experimentally demonstrated that the low κ results in a great enhancement of the figure of merit as thermoelectric material[1]. Meanwhile, SiNW MOSFET requires a rapid heat dissipation rate to prevent the degradation due to Joule heating. Therefore, in order to design the best performance of the nanoscale devices, an accurate prediction of the thermal properties is essential.

Recent atomistic simulation studies[2,3] have made a point that the amorphous layer, which inevitably covers the practical NW, is influential to the κ reduction observed experimentally. Donadio and Galli[2] calculated the κ of SiNW covered with amorphous Si by molecular dynamics (MD) technique and revealed that the presence of amorphous layer reduces the κ considerably. Saegusa et al.[3] performed MD simulation to estimate the κ of SiO_x-coated SiNW and showed that the surface SiO_x decreases the κ. However, despite of theses progresses about thermal transport properties, mechanism of the reduction of κ in realistic SiNW is not fully understood.

In this work, in order to obtain a microscopic picture of heat transport in the realistic nanostructured Si, we compute the κ of SiNWs covered with the oxide layer using nonequilibrium MD simulation, and investigate the impacts of the SiO₂ layer on the reduction of κ by analyzing the vibrational density of states (VDOS).

2. Simulation Method

The <100> SiNW model covered with an oxide film was built from a cylindrical SiNW with a 5.0 nm diameter and 16.3 nm long, as shown in Fig. 1(a). The oxide film was formed in a layer-by-layer manner from the surface, and two models with different oxide thickness, two and three mono layers (ML) oxide, were prepared (Fig. 1).

We conduct the nonequilibrium MD simulation[4] to compute the κ of the NWs. To establish a temperature gradient ∇T along the NW axis, left (right) end region of the NW was placed into cold (hot) bath with temperature of 275 (325) K. Figure 2 illustrates an typical ∇T used to estimate the κ. The κ is calculated from the Fourier's law, $\kappa = -J/\nabla T$, where the heat flux J is defined as the removed (added) energy from cold (hot) bath region in unit time through the unit cross section area.

All MD simulations in this work are carried out using an interatomic potential function for Si, O mixed systems[5].

3. Results and discussion

In Fig. 3, we plot the calculated κ of three SiNW models as a function of the oxide layer thickness. Clearly, the covering the NW by SiO₂ layer lowers the κ drastically. The reduction in the κ of 41 % occurs when coating the bare NW by 2 ML oxide layer, while the drop is only about 3 % as the oxide film thickens from 2 ML to 3 ML. This means that the presence of SiO₂ layer is crucial to determine the κ.

To investigate the mechanism of the κ degradation for the SiNWs with oxide layer, phonon dispersions of the NWs are calculated in Fig. 4. For the oxidized NWs, it is observed that the low energy branches spread into broad spectra, agreeing with our previous MD study[6]. This is due to the presence of SiO₂ layer including the SiO₂/Si interface[6], and these low frequency mode must impact on the κ.

In order to clarify the role of SiO₂ layer on the reduction of κ, we analyze the partial VDOS for the SiNWs. Figure 5(a) and 5(b) show the VDOS of Si atoms on the Si core region (from 11th to 13th atomic layer from the surface)

and Si surface region (from 2nd to 4th layer), respectively. In the Fig. 5(a) the VDOS for the oxidized NW is almost identical with that of bare NW. In contrast in Fig. 5(b), the VDOS near the SiO₂/Si interface is depressed in the ranges 4-8 THz and 10-20 THz as the oxide film covers. This attenuation is attributed to the disorders of Si atoms at the SiO₂/Si interface caused by the presence of the oxide layer, and the depression of the low-frequency phonon mode leads to the dramatic reduction of κ. It is worth to note that these random configurations near the SiO₂/Si interface also deteriorate the drive current of narrow SiNW transistor[7], indicating that the atomic disorder at the interface is key to obtain the best performance of the SiNW devices.

4. Conclusion

The κ of SiNWs covered with the oxide layer is calculated by means of nonequilibrium MD simulation. Our results show that κ of oxide-coated SiNW is about 40 % of the bare SiNW, meaning that the SiO₂ layer is influential to the significant decrease in κ in practical SiNW. The reduction is originated from the depression of the low-frequency phonon mode due to the disorders of Si atoms near the SiO₂/Si interface.

Acknowledgements

References

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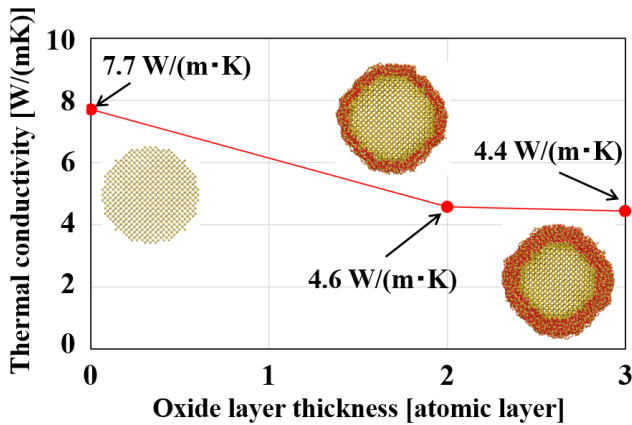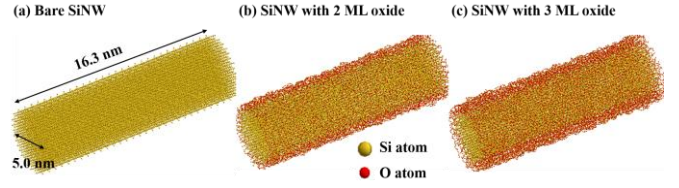
Fig. 1 SiNW models for MD simulations. (a) Bare SiNW, (b) SiNW covered with 2ML, and (c) SiNW covered with 3 ML of oxide layer.
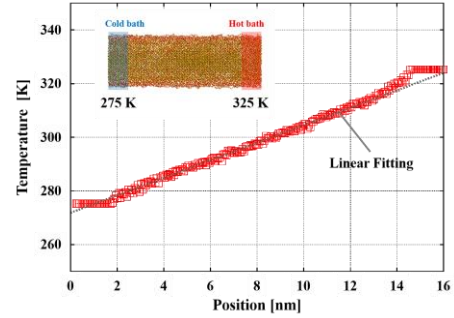

Fig. 2 The temperature gradient along the wire axis direction. The gray dashed line is a linear fit to the temperature gradient.
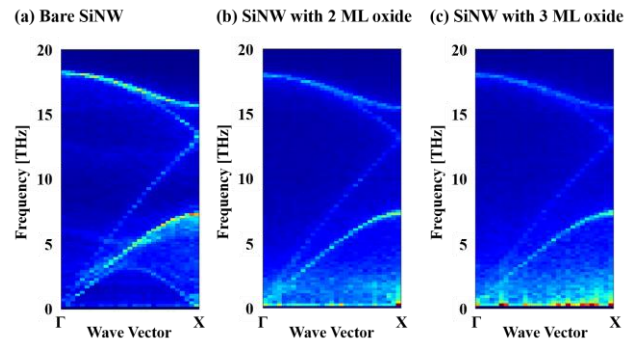

Fig. 4 Phonon dispersion of (a) bare SiNW, (b) SiNW covered with 2ML, and (c) SiNW covered with 3 ML oxide layer.
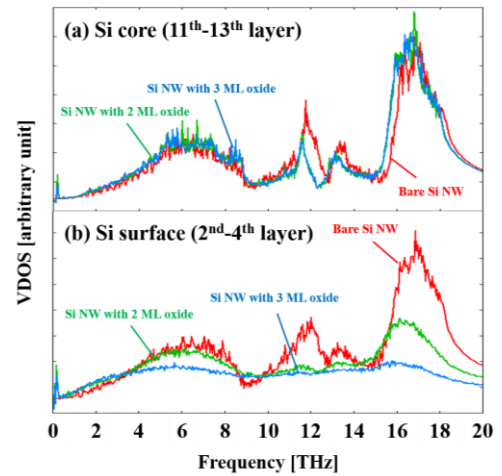

Fig. 3 Thermal conductivity κ of SiNWs as a function of the oxide layer thickness.

Fig. 5 Partial vibrational density of states of bare SiNW, SiNW with 2ML, and SiNW with 3 ML of oxide layer. (a) Si core region (from 11th to 13th atomic layer from the SiO₂/Si interface) and (b) Si surface region (from 2nd to 4th atomic layer).