Molecular Dynamics Simulation of Heat Transport in Silicon Fin Structures

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Abstract—**A series of molecular dynamics (MD) simulations has been conducted to investigate the transport process of heat from a heat source consisting only longitudinal optical (LO) phonon in Bulk and SOI Fin structures. The calculation results show that the heat transport from the Fin to the Si substrate is delayed when the buried oxide (BOX) layer exists even if the thickness is only one atomic layer. The kinetic energy distributions of LO and longitudinal acoustic (LA) phonons in SOI Fin structures are extracted from the MD simulations, and the result suggests that the heat transport process is impeded since acoustic phonon stays near the SiO_2/Si interface. That is, the retarded heat is an unavoidable in a SOI Fin, a nanowire, or any channel structure confined in an insulating material. Having a heat duct in a device can be effective to avoid the self-heating problem for advanced transistor structures.**

Keywords-component; self-heating effect, phonons, Fin stuructures, nanowires, SOI, molecular dynamics simulations

I. INTRODUCTION

Multi-gate transistors have attracted much attention as an alternative device to overcome disadvantages of conventional planner structures. In such devices, heat is emerging constraint on achieving processor performance improvement, because 1) the heat transport process of multi-gate devices differs from the one in planner bulk devices due to the large surface to volume ratio, and 2) multi-gate transistors, i.e., in silicon-on-insulator (SOI) Fins and nanowires, have isolated channels in an insulating layer with a relatively lower thermal conductivity than bulk Si. Takahashi *et al.* reported on the self-heating effects in SOI FinFETs and Bulk FinFETs using the device simulator, and they revealed that all the elements of the SOI FinFET, including channel, gate, source, drain, and buried oxide (BOX), are heated up due to the poor heat dissipation to the substrate [1]. Since heat gives unwanted influences on transistors' performance [2, 3], the self-heating effect must be prevented if multi-gate devices are considered as an alternative device structure.

Most of heat is usually generated at "hotspots", located near the drain and the channel interface in a nano-scale transistor. According to a theoretical study, 60 % of the phonons emitted from hot electrons near the drain region are longitudinal optical (LO) phonons [4], and interactions of these phonons with hot electrons create hotspots (Fig. 1) [5]. This is because 1) LO phonons have lower group velocity and higher energy than acoustic phonons, which carry most of heat in bulk Si, and 2) energy transfer from LO phonons to acoustic phonons rarely occurs since the mean free path of phonon is usually longer than 100 nm. Moreover, the phonon behavior is modulated near the SiO_2/Si interface due to the increased influence of phonon-interface scattering and oxide-induced strain in the Si nano-structures confined in oxide films [6, 7]. Thus, the analysis of the phonon spectra is essential for full understanding of the heat dissipation process in the nano-scale devices.

In this work, we conduct the Molecular dynamics (MD) simulations to investigate the transport process of heat in a hotspot region in Bulk and SOI Fin structures in terms of the phonon spectra. We also provide realistic pictures of phonon and heat behaviors in nano-scale devices by considering the anharmonic effects of phonons, i.e., phonon-phonon and phonon-interface scatterings, in MD simulations. Dependence

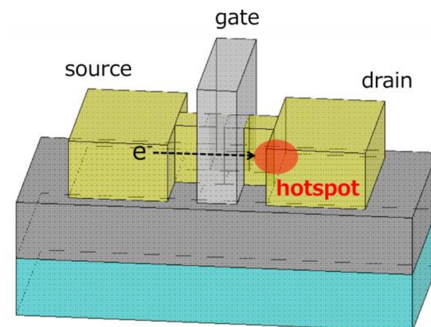

Fig. 1. A Hotspot in the multi-gate device. Due to the downsizing in channel length, the hotspot is generated near the drain region and is considered to affect the device performance.

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of the heat transport on the thickness of BOX layer and the kinetic energy distribution of LO and longitudinal acoustic (LA) phonons in SOI Fin structures in the process of the heat transport are also investigated in this report.

II. SIMULATION METHODS

Fig. 2(a) shows the Bulk Fin model viewed from an x-z plane. A two-dimensional periodic boundary condition is imposed on the system along the x and y direction. The simulation system consists of 6582 Si atoms and the oxide film. A fin model is designed by the following manner; 1) a Si lattice containing Fin structure is prepared without O atom, 2) oxide layers are formed by inserting O atoms into the midpoints of Si-Si bond from the top surface. Figure 2(b) shows the SOI Fin model. In the SOI Fin model, the BOX layer is formed by oxidizing a part of the Si substrate underneath the Fin structure. In this study, three models with different BOX thicknesses (two, three, and four atomic layers) are employed to investigate how heat transport in the SOI Fin model differs when BOX thickness varies.

A heat source only including LO phonon mode is placed in the center of the Fin region to represent a hotspot. The initial temperature of atoms in the hotspot region is set at 730 K in this study, since hot electrons with energy above 60 meV is known to couple strongly with 730 K LO phonon through inter-valley scattering in Si [5]. The direction of the wave vector of LO phonon mode is <100>. Atoms at the bottom layer of the system are fixed. In the regions besides the hotspot, the initial temperature of atoms is set at 0 K. Temperature is not controlled once the simulation begins.

The MD simulations on the SiO_2/Si system are carried out using an interatomic potential function for Si, O mixed systems [8]. The potential is an extended version of the Stillinger-Weber (SW) potential for pure Si systems [9], which comprises two- and three-body potential energy terms that depend on local environments. All parameters in the potential function were determined by ab initio molecular orbital calculations of small clusters. Details of the potential function are described in [8]. The extended SW potential has been employed to investigate SiO_2/Si interface structures, stress properties [10, 11] and the heat transport process [6, 7] in Si nano-structures.

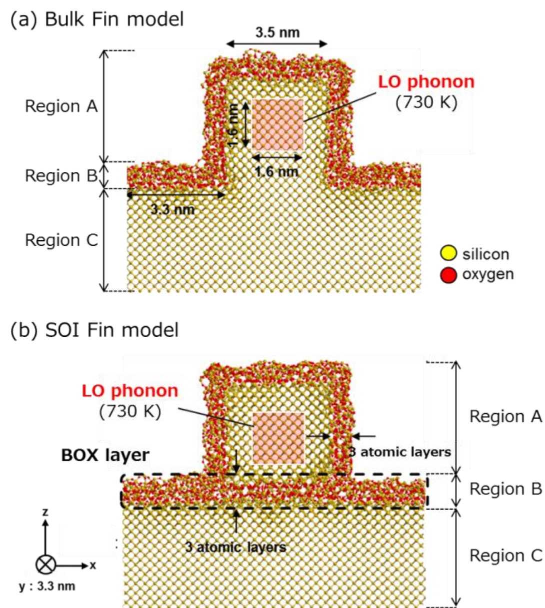


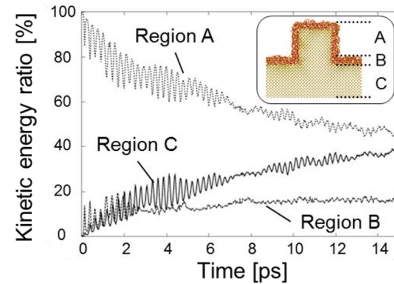
Fig. 2. Fin models with oxide films for MD simulations; (a) Bulk Fin and (b) SOI Fin models.

We perform a series of MD simulations on the systems for 15 ps to monitor how heat in the hotspot region flows to the bottom of Fin models. In order to investigate the effect of the presence of BOX layer, we split the model into three regions: Region A is corresponding to a Fin region, C is the Si substrate region, and B is the connecting region between Region A and C, as displayed in Fig. 2. For SOI Fin model, Region B is a BOX layer. We calculate the kinetic energy in each region at each time step and investigate spatial heat distributions in Fin structures.

III. RESULTS AND DISCUSSION

Fig. 3 shows the time evolution of the ratio of the kinetic energy in each region to the total kinetic energy of the system for (a) Bulk Fin and (b) SOI Fin models. The thickness of BOX layer in the SOI Fin is 3 atomic layers. The kinetic energy ratio, hence heat, in Region A decreases while heat in Region B and C increases as simulation time evolved. This implies that heat in the hotspot region diffuses from Region B to the bottom of the system. As seen in Fig. 3(a), heat in the

(a) Bulk Fin model



(b) SOI Fin model (with 3 atomic layers of BOX)

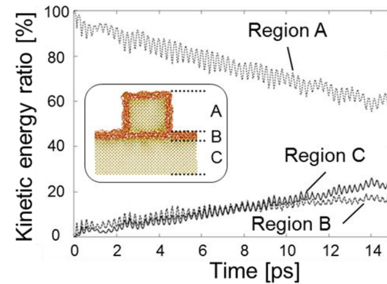


Fig. 3. Time evolution of the kinetic energy ration in Region A, B, and C in the (a) Bulk Fin and (b) SOI Fin models.

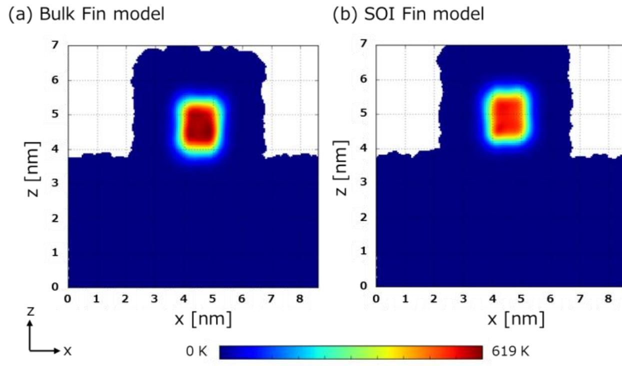


Fig. 4. Heat distributions viewed from an x-z plane for (a) Bulk Fin and (b) SOI Fin models at **0.05 ps**. In both models, heat is localized in the center of the Region A, that is Fin region.

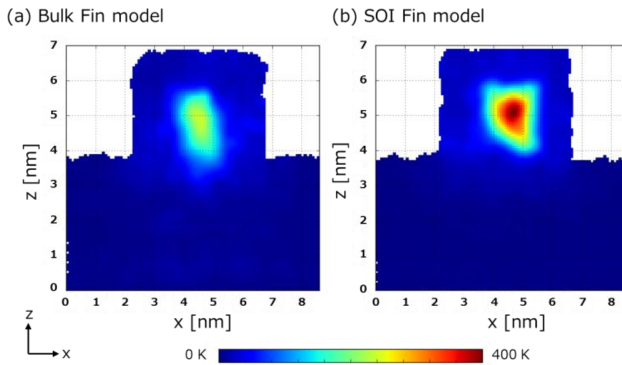


Fig. 5. Heat distribution for (a) Bulk Fin and (b) SOI Fin models at **4.5 ps**. In SOI Fin model, the heat diffusion from Region A to Region C is impeded by the BOX layer.

Region A diffuses more quickly to Region B and C in Bulk Fin than in SOI Fin. Fig. 4(a) and (b) show the heat distributions for Bulk fin and SOI fin models at 0.05 ps. Heat is localized at the center of Region A at such early time of the MD simulations. Fig. 5(a) and (b) show the heat distributions at 4.5 ps. Heat in the Bulk Fin diffuses to Region B and C, however, heat in the SOI Fin stays in Region A. This is because thermal resistance at the SiO_2/Si interface prevents heat to escape from Region A in a SOI Fin model.

We investigate dependence of the BOX thickness on the heat transport in the SOI Fin models. Fig. 6 (a) shows the time evolution of the kinetic energy ratio in Region A for SOI fin models with 2, 3, and 4 atomic layers of BOX. In Fig. 6 (a), the kinetic energy ratio in Region A decreases comparably for all atomic layer thicknesses and the diffusion rate of the heat is quite lower than that in the Bulk Fin model. This indicates that, during the transient heat transport process, heat flow is impeded despite only one atomic layer of BOX layer exists in the Fin structure. Fig. 6(b) shows the kinetic energy ratio in Region C as a function of time. As seen in the figure, the heat dissipation process to Region C, that is Si substrate region, is further delayed as the thickness of the BOX layer increases. This result corresponds that transient time of heat through Region B is proportional to the BOX thickness, suggesting that thicker the SiO_2 BOX film is, harder the heat dissipation takes place.

In order to investigate the decay and diffusion process of original LO phonon, we extract the kinetic energy distribution of LO and LA phonon modes in the SOI Fin models. Fig. 7(a) and (b) show the heat distribution of LO and LA phonon modes for Si atoms in SOI Fin with 3 atomic layers of BOX at 9.0 ps. In the figure, the temperature of O atoms is shown as 0 K. In this study, we determine the kinetic energy of phonon modes as following manner. First, we diagonalize the dynamical matrix estimated using the extended SW potential and obtain the polarization vectors of each phonon modes corresponding to eigen-vector of the dynamical matrix [7]. Second, we multiply the polarization vector by the velocity vector generated by MD simulations, and define the dot product as the velocity vector of each phonon mode. Thus the total kinetic energy is decomposed into LO and LA phonon components. In this study, the phonon kinetic energy is extracted for all Si atoms in the system, including those in the oxide film. Therefore, in the Fig. 7, the phonon distribution in the SiO_2 region is meaningless. As displayed in Fig. 7, heat generated by LO phonon stays at the center of the Fin region. By contrast, heat generated by LA phonon mainly localizes near the SiO_2/Si interface, suggesting that the scattering rate of LO phonon into acoustic phonon is enhanced at the SiO_2/Si interface due to increase in interface-phonon scattering. This

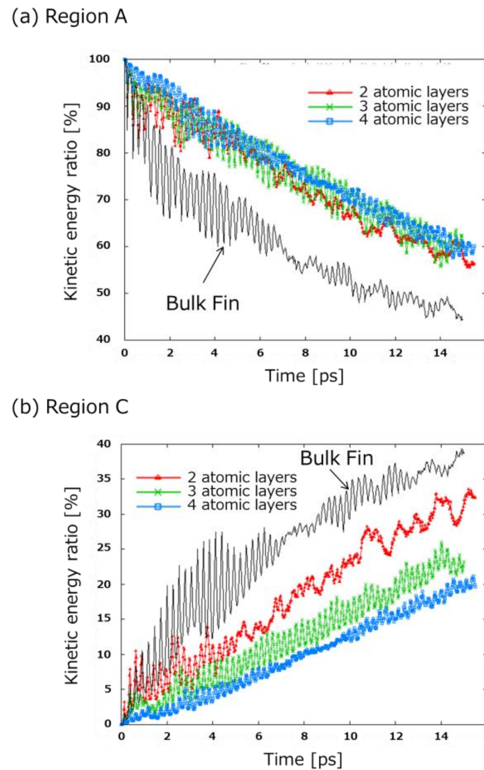


Fig. 6. Time evolution of the kinetic energy ratio in (a) Region A and (b) Region C for SOI Fins with 2, 3, and 4 atomic layers of BOX.

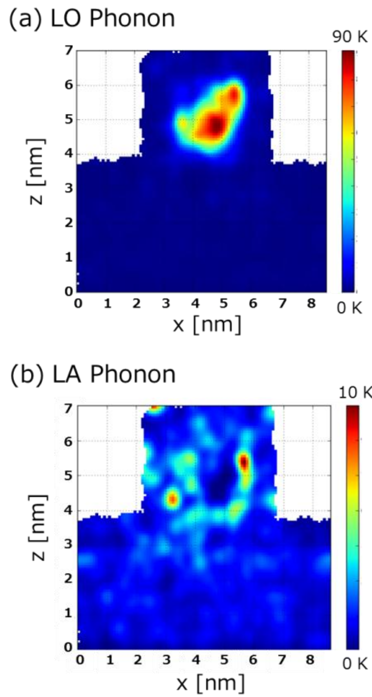


Fig. 7. Heat distributions of (a) LO and (b) LA phonon modes. We estimated the kinetic energy of each phonon mode using the dot product of the polarization vector of the phonon and velocity vector of atoms generated by MD simulations.

agrees well with our previous MD study [7]. The results in Fig. 7 also indicate that the heat transport in SOI Fin structures is retarded since acoustic phonons stays near the interface between Si from the Fin region and SiO_2 from the BOX layer.

Our results suggest that the heat dissipation process from the Fin to the Si substrate region is hindered by the presence of SiO_2/Si interface. Yet, acoustic phonon mode stays near the interface and heat is accumulated in the Fin region. It is concluded that the retarded heat is unavoidable problem in a SOI Fin, a nanowire, or even in an ultra-thin BOX layer transistor.

IV. CONCLUSION

We conducted the MD simulations on the heat transport process for hotspot regions in Bulk and SOI Fin structures in terms of the phonon spectra, and we analyzed the dependence of BOX thickness on the heat transport process. The results reveal that heat dissipation process to the Si substrate is impeded despite only one atomic layer of BOX exists in between the fin and the substrate. This indicates that thermal resistance at the SiO_2/Si interface prevents heat to escape from hotspot regions in a SOI Fin model. We extracted the heat distributions of LO and LA phonon modes using the polarization vector, and the results suggest that heat transport is impeded due to acoustic phonons to localize near the SiO_2/Si interface.

In conclusion, the retarded heat is unavoidable in a SOI Fin, a nanowire, or even in an ultra-thin body SOI structure. To overcome this issue, building a heat duct in a system to transfer heat outside the device region could be effective for an advanced device structure.

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