Extended Abstracts of the 2009 International Conference on Solid State Devices and Materials, Sendai, 2009, pp725-726

P-13-10

Simulation on the heat transport in a silicon nano-structure covered with oxide films

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1. Introduction

In a nanoscopic silicon metal-oxide-semiconductor field-effect transistor, electron-phonon scattering occurs predominantly at the drain region of transistor rather than at the channel region, because electrons transfer ballistically through the channel. 90% of the phonons emitted from hot electrons near the drain region are optical phonons. Since the optical phonons have low group velocity and high energy, hotspots are created near the drain region and affect device properties significantly [1]. Despite this concern, however, phonon behavior and heat transport in the nanoscopic devices, whose size is smaller than phonon mean free paths, have not been clarified. Importance of these heat problems is increasing due to the emergence of new device structures, such as thin film silicon-on-insulator or silicon nanowire. In these device structures, silicon core including drain regions are covered with oxide films, which have significantly lower thermal conductivity than bulk silicon, and the heat problems are expected to become even more prominent.

In this work, we investigate the heat transport in a silicon nano-structure, in particular in the system confined with SiO_2/Si interface, by mean of molecular dynamics (MD) simulation.

2. Simulation methods

Figure 1 shows the system we used for the simulations. We model the hotspot with a heat source localized at the central region of the silicon lattice, and temperature of silicon atoms in the region was held constant at 1000K. Temperature of silicon atoms at both ends of the silicon lattice was held constant at 300K, and other regions include SiO_2 were allowed to equilibrate with the three heat sources. To investigate how the heat of the central region diffuses to surroundings, we performed a series of MD simulations on these systems.

We imposed a two-dimensional periodic boundary condition on the system along the x and y directions. Thus the system is constrained only along the z direction and resembles a sheet.

Our original interatomic potential function for Si, O mixed systems [3, 4] was employed as an interatomic potential function for the MD simulations.

Simulation models consist of a silicon lattice covered with oxide films at top and bottom. The silicon lattice contained 6400 atoms, and its dimension was 10.9x2.72x4.38 nm^3. Three models with different thickness of the oxide films (two, five, and eight layers) were employed in order to compare how heat transport in the silicon core depends on the oxide thickness.

Heat distribution in the silicon core was analyzed for the three models with different oxide thickness. The result of the analysis was presented in a graph whose horizontal axis represent a distance from the left edge of the silicon lattice and longitudinal axis represents mean kinetic energy of atoms existing in the region. The heat distribution was analyzed at 0.001, 3.0, 6.0, and 9.9 ps.

In order to quantitatively compare the differences in heat distribution, we fitted the plots with a Gaussian curve and evaluated its full width at half maximum (FWHM).

3. Results and discussion

Figure 2(a), (b), and (c) show oxide silicon model viewed from x-z plane (left) and heat distribution in the silicon core (right). In the heat distribution graphs, heat is highest at center regions and converges to 300K at both ends. Evaluation at subsequent time steps revealed that heat diffuses outward from the center.

Figure 3(a), (b), and (c) show Gaussian fit curves to the heat distribution in models with two, five, and eight atomic layers of oxide film, respectively. The FWHMs at each time step are summarized in Table I. It was clearly observed that FWHM increases with time evolution, indicating that heat diffuses to the surroundings from the central region.

Comparing the FWHMs of the three models at each time step, FWHM was nearly equal initially but began to vary as simulation proceeded. The broadening of the curve was slower in models with thicker oxides. This means that when oxide thickness is increased, the heat diffusion is impeded, and thus the heat tends to pool around the heat source. Our calculation results are in agreement with the fact that thermal conductivity of an oxide film is lower than bulk silicon.

4. Conclusions

We investigated heat transport in silicon covered with oxide films and its dependency on the oxide thickness by

means of MD simulation. We found that heat diffusion was retarded as oxide films became thicker. The calculation results suggest that heat problem in nanoscopic devices is key problem to improve the device properties.

Acknowledgements

We acknowledge Grants-in-Aid for Science Research on Particular Areas “Post Scale” (Grants No.20035007) from Minister of Education, Culture, Sports, Science and Technology.

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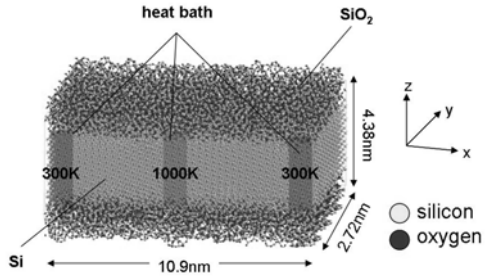

Fig. 1 $SiO_2/Si/SiO_2$ structure employed in MD simulations

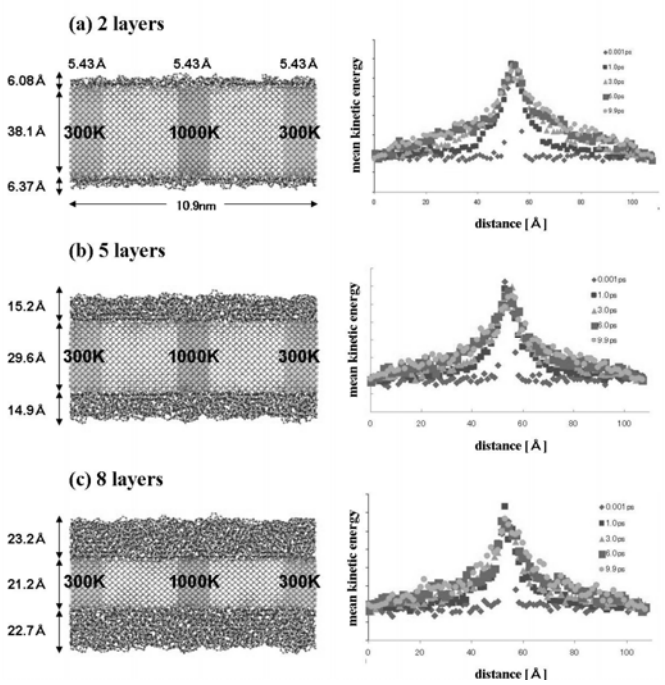

Fig. 2 Structure models and heat distribution graphs of oxide silicon models with (a) two, (b) five, and (c) eight atomic layers of oxides.

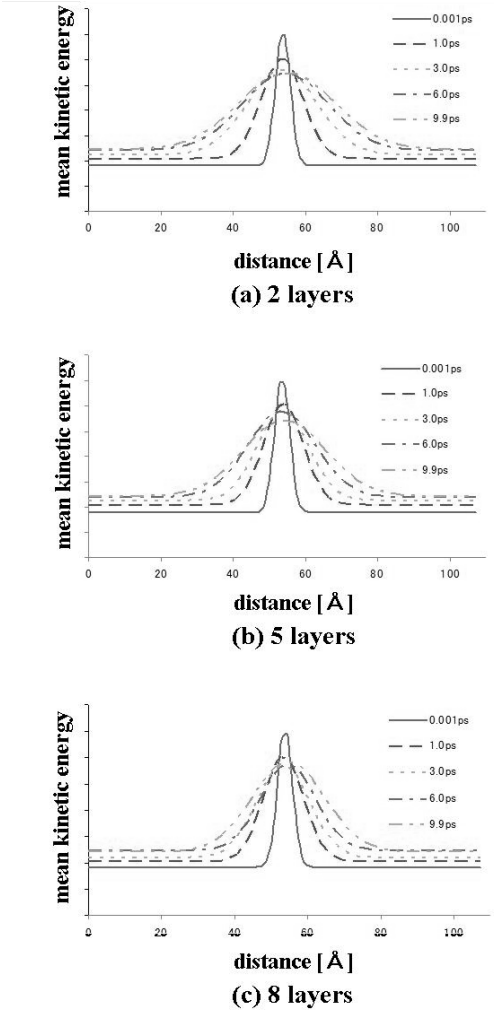

Fig. 3 Gaussian curve fits to the calculated heat distribution. Number of oxidation layers is (a) two, (b) five, and (c) eight layers.

Table I FWHM of the three models at each time steps.

	2layers	5layers	8layers
time[ps]	FWHM[Å]		
0.001	4.83	4.87	4.80
1.0	13.5	12.8	13.0
3.0	22.4	16.5	17.0
6.0	27.3	21.8	17.5
9.9	30.7	26.5	23.2