# Molecular Dynamics Simulation on LO Phonon Mode Decay in Si Nano-structure Covered with Oxide Films

T. Zushi, I. Ohdomari, T. Watanabe/Waseda University
Faculty of Science and Engineering
Institute for Nanoscience and Nanotechnology
Tokyo, Japan
zushi@watanabe.nano.waseda.ac.jp

Y. Kamakura, K. Taniguchi/Osaka University
Faculty of Engineering
Osaka, Japan

***Abstract*—A series of molecular dynamics (MD) simulations is conducted to investigate the dynamics of longitudinal optical (LO) phonon in Si nano-structure confined with oxide films. This work is motivated by heat issues in nanoscopic devices; it is considered that the LO phonons with low group velocity are accumulated in the nanoscopic device and the electric property deteriorates. We estimate the relaxation time of the LO phonon and investigate its dependency on the oxide thickness. The calculation results show that the LO phonon decays faster as the oxide thickness increases and turns into acoustic phonon. The result indicates that the presence of $SiO_2$ films promotes the scattering of the phonon and this is effective to diminish the optical phonon.**

## I. INTRODUCTION

With the rapid development in integrated circuit fabrication technology, the size of individual devices is reduced to nanometer scale, and the channel length of devices has fallen below the phonon mean free paths. In such nanoscopic devices, electrons and phonons in the channel region are considered to travel quasi-ballistically, and phonon behavior is changed from those observed in conventional planar bulk devices [1]. Despite this concern, phonon properties, such as dispersion relation, group velocity, and relaxation time in nanoscopic devices have not yet been clarified in detail.

In a nanoscopic silicon metal-oxide-semiconductor field-effect transistor (MOSFET) whose channel length is below 100 nm, electron-phonon scattering occurs predominantly at the drain region of the transistor rather than at the channel region, because electrons transfer ballistically through the channel. According to a theoretical study, 60% of the phonons emitted from hot electrons near the drain region are optical phonons [2], and interactions of these phonons with hot electrons create so-called "hotspots" (Fig. 1). This is because, first, optical phonons have a lower group velocity and a higher energy than acoustic phonons that carry most of the heat in a crystal, and, second, energy transfer from optical phonons to acoustic phonons rarely occurs in such a small region [3], since phonon mean free paths are usually longer than 100 nm. Since the creation of the hotspot is considered to degrade the performance of transistors [3], it is important to clarify the phonon behavior and heat transport in the nanoscopic devices.

Molecular dynamics (MD) simulation is a powerful tool to obtain the realistic picture of the phonon behavior in condensed materials, since it includes anharmonic effects of phonons, i.e., phonon-boundary scattering and phonon-phonon scattering. Recently, MD simulation studies have been performed actively to investigate the phonon properties in silicon [4-6, 8]. These MD studies focused on the longitudinal optical (LO) phonon decay, because the decay process of the LO phonon into acoustic phonon is considered to be the potential bottleneck to heat transfer [7] and to limit the thermal diffusion rate. Shinha et al. [8] investigated the scattering mechanisms of LO phonons at hotspot in pure Si and showed that the LO phonon turns into transverse acoustic (TA) phonon and longitudinal acoustic (LA) phonon.

However, the presence of insulating oxide films which cover the Si lattice has never been considered in these previous studies. In the state-of-the-art nanoscopic devices

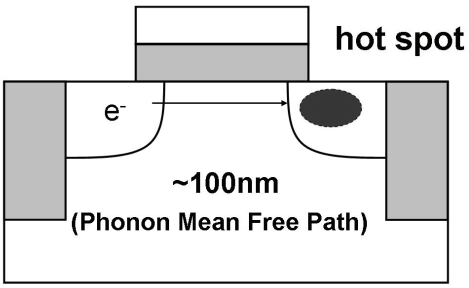


Fig. 1 The hotspot in nanoscopic devices. Due to the decreased channel length, the hotspot is created in the drain region and is considered to affect the device properties.

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utilizing thin film silicon-on-insulator and silicon nanowire, a large part of Si lattice touches the oxide films whose thermal conductivity is significantly lower than bulk silicon, so that the diffusion of the heat from the hotspot hard becomes difficult. To obtain more practical situation in the nanoscopic devices, interface between Si and the insulating oxide films should be included in the simulation systems.

In our research group, we have been investigating the heat transport [9] in the silicon nano-structure including explicitly the oxide layers in the simulation system. In the present work, we investigate the dynamical behavior of the LO phonon in the Si nano-structure sandwiched by oxide films and how the rate of mode decay depends on thickness of the $SiO_2$ film

## II. Simulation Methods

Fig. 2 shows the simulation system of the Si lattice covered with oxide films. A two-dimensional periodic boundary condition is imposed on the system along the x- and y- directions. Thus, the system is replicated throughout the x-y plane to an infinite sheet.

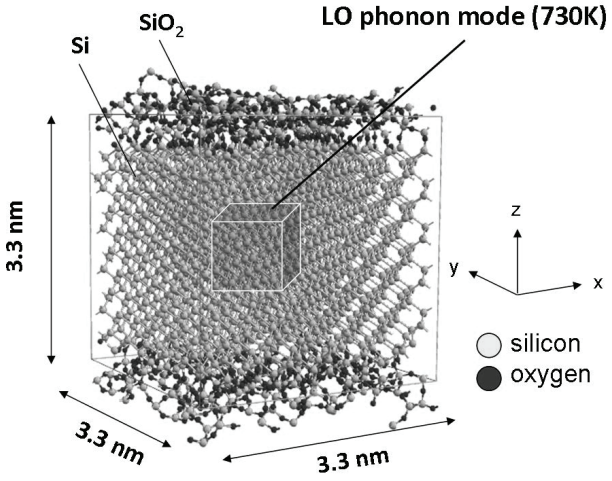


Fig. 2 $SiO_2$/Si/$SiO_2$ structure employed in MD simulations.

The simulation model was built as follows. First, we prepared a Si lattice consisting of 1728 atoms with the dimension of 3.3 x 3.3 x 3.3 $nm^3$. Next, oxide films are formed by inserting O atoms into the midpoints of Si-Si bond from the top and bottom surfaces. The total thickness of the system in the z- direction varies depending on $SiO_2$ film thickness.

To model the hotspot a heat source consisting of only LO phonon mode is placed in the central region of the model, as shown in Fig. 2. The initial temperature of atoms at the hotspot is set to 730 K. This temperature is chosen because hot electrons with energy above 60 meV is considered to be involved in intervalley scattering with the 730 K LO phonon most effectively in Si [3]. The direction of the wave vector of the LO phonon mode is set to <100>. The dimension of the heat source is 1.1 x 1.1 x 1.1 $nm^3$. In the other region, the initial temperature of Si and O atoms is set to 0K, thus these atoms are frozen at the beginning of the MD simulation.

In the present work, two models with different thickness of the oxide films (three and eight layers) are employed, and the decay rate of the LO phonon mode is measured in both models. The decay rate of the LO phonon is calculated from the time evolution of the phonon mode amplitude A(**k**,*p*,*t* ) [6]:

$$A(\mathbf{k},p,t)=\sum_j\left(\mathbf{r}_j(t)-\mathbf{r}_{j0}\right)\cdot\mathbf{p}_j(\mathbf{k},p)\cdot\exp\left(i\cdot\mathbf{k}\cdot\mathbf{r}_{j0}\right), \quad (1)$$

where the summation runs over the atom indices *j* within the heat source region, **k** is the specific wave vector, $\mathbf{r}_j(t)$ the atom's position, $\mathbf{r}_{j0}$ lattice position and $\mathbf{p}_j(\mathbf{k},p)$ the corresponding polarization vector.

After the manner of Henry and Chen [6], we calculate the relaxation time using the mode amplitude. The relaxation time is given by

$$\tau(\mathbf{k},p)=\frac{\int\langle\delta A(\mathbf{k},p,t+t')\cdot\delta A(\mathbf{k},p,t)\rangle dt'}{\left\langle\delta A(\mathbf{k},p,t)^2\right\rangle}, \quad (2)$$

where $\delta$ A(**k**,*p*,*t*) is the deviation from the average amplitude.

MD simulation is conducted by employing an interatomic potential function for Si, O mixed systems [10]. The potential

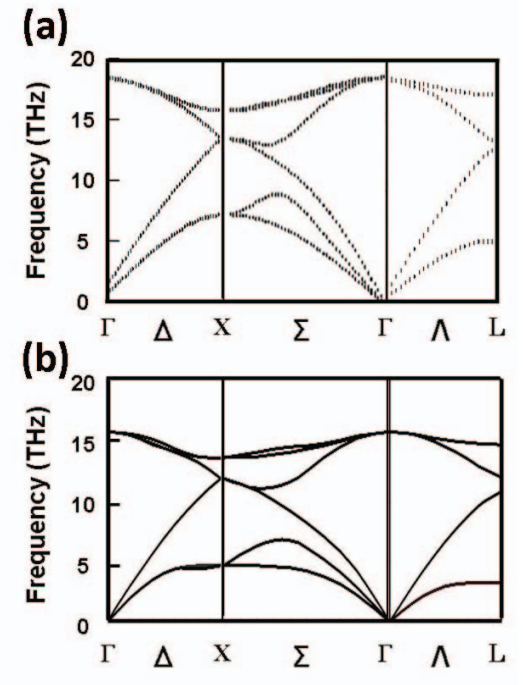


Fig. 3 (a) Phonon dispersion relation calculated from the dynamical matrix which is estimated using the Si subset of the extended SW potential. (b) Phonon dispersion relation calculated based on the bond-charge model [17].

is an extended version of the Stillinger-Weber (SW) potential [11], which comprises two- and three-body potential energy terms that depend on local environment of each atom. All parameters in the potential function were determined by *ab initio* molecular orbital calculations of small clusters. The extended SW potential has been employed in large scale modeling of $SiO_2$/Si interface structures to investigate the stress properties of the $SiO_2$ film [12-16].

Fig. 3 shows the phonon dispersion relation obtained by diagonalizing the dynamical matrix estimated by using the Si subset of the extended SW potential. Although the frequency, which is given by the square root of the corresponding eigenvalue of the dynamical matrix, is slightly overestimated by the extended SW potential, the over all relation agrees qualitatively with the relation calculated based on the bond-charge model [17].

## III. RESULTS AND DISUCCUSION

Fig. 4 shows the time evolutions of the autocorrelation function of LO phonon amplitude calculated by (1), together with the $SiO_2$/Si/$SiO_2$ model used in the simulation. The amplitude of the LO phonon mode decays in both models as the MD simulation proceeds.

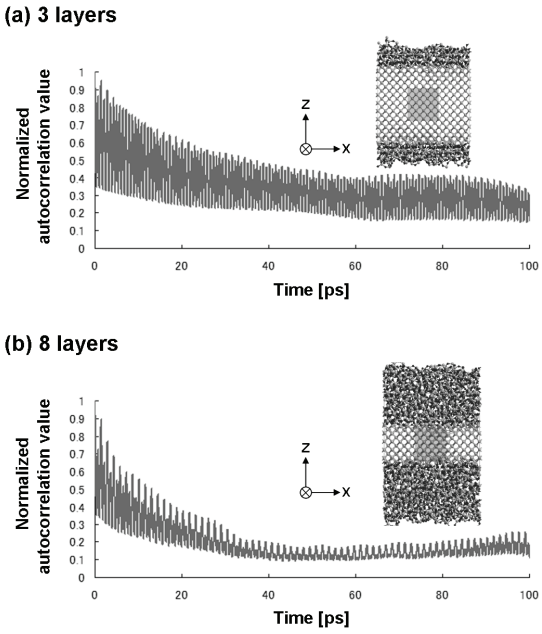


Fig. 4 Structure models and autocorrelation function of the LO phonon mode amplitude. (a) Three and (b) eight atomic layers of oxides.

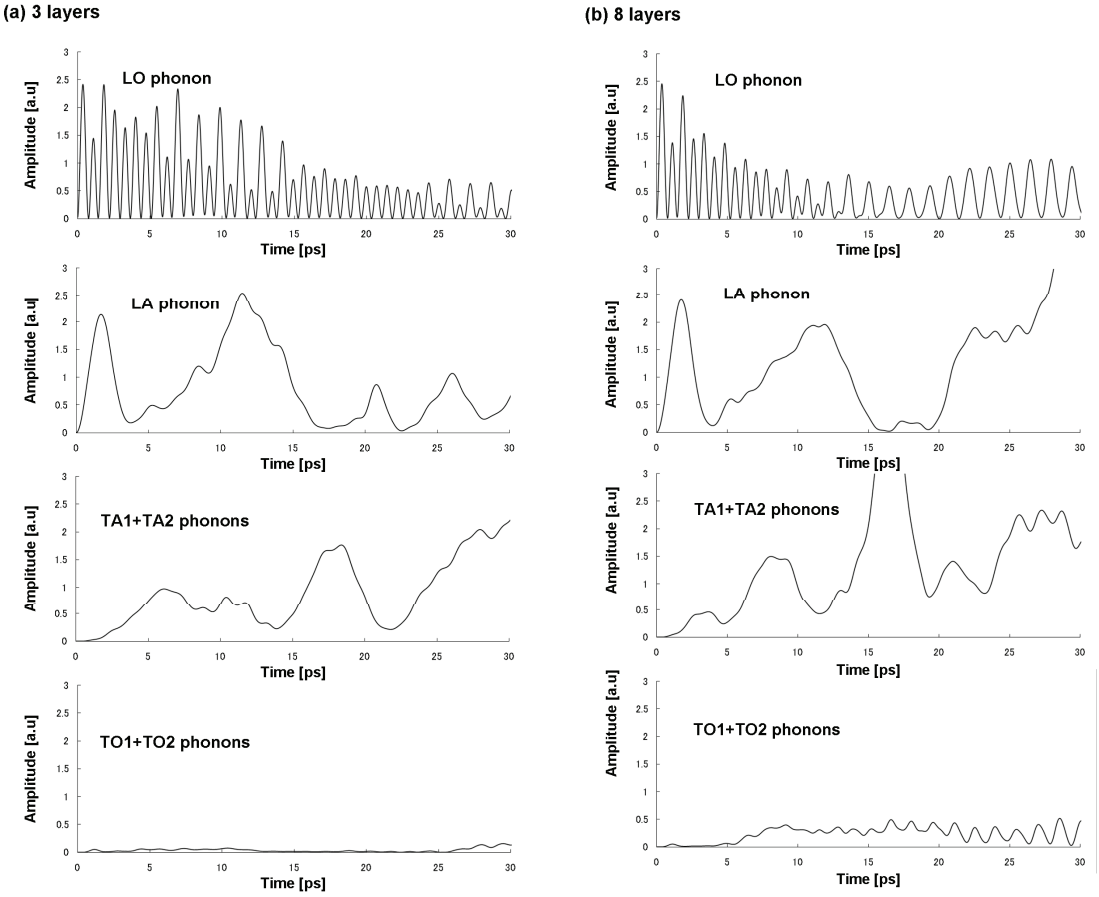


Fig. 5 Time evolution of the amplitudes for the LO, LA, TA and TO phonons. (a)Three and (b) eight atomic layers of oxides.

Comparing the time evolutions in the two models, initial amplitude is nearly equal to each other but the rate of the decay is found to increase with the oxide thickness. The relaxation times estimated using (2) are 22.3 and 8.84 ps for 3 and 8 oxide layer respectively. The results mean that the scattering rate of the LO phonon mode in $SiO_2$/Si/$SiO_2$ structures is affected by the thinness of remaining Si layer.

This decay corresponds to population transfer from the original LO mode into other modes. To investigate the phonon mode that LO phonon decays into, we calculate amplitudes of other phonon modes, i.e. LA, TA, and transverse optical (TO) phonon modes. Time evolutions of the amplitude of the representative modes are shown in Fig. 5 (a) and (b) for 3 and 8 oxide layers systems, respectively. Here we focus on phonon modes whose wave vectors are equal to that of original LO phonon, i.e., $0.3x(2\pi/a)<100>$, where $a$ is the lattice constant.

In the Fig. 5, doubly degenerated TA phonons (TA1 and TA2) and TO phonons (TO1 and TO2) are shown individually. It is clear that the large part of LO phonons decays into acoustic phonons, i.e., LA and TA phonons. In addition, the population transfer from LO to TO phonons rarely occurs. These trends agree with results of other Monte Carlo and MD studies [8, 18] assuming in Si bulk.

The rate of population transfer from the LO phonons to acoustic phonon increases with oxide thickness. The mean amplitude of LA phonon over 30 ps is 0.80 in arbitrary unit for 3 oxide layers model. In the 8 oxide layers model, it increases to 1.30. The mean amplitude of TA phonons (the sum of TA1 and TA2) are 0.86 and 1.33 for 3 and 8 oxide layers models, respectively. Thus the decay of the LO mode into acoustic phonon modes is more enhanced in the thicker oxide model.

The present results reveal that the presence of $SiO_2$ films is effective to diminish the hotspots consisting of LO phonons. In this sense, existence of $SiO_2$/Si interface is favorable to solve the heat issue in nanoscopic devices. It should be noted, however, that our previous study shows that the heat diffusion is retarded with decreasing the Si lattice thickness [9]. In nanoscopic devices, population transfer from the LO mode to acoustic modes can easily occur, so that the retardation of the following heat transport process via the acoustic phonons would be rather problematic.

## IV. CONCLUSION

We performed MD simulation on the phonon dynamics in Si lattice considering the presence of oxide films. A heat source consisting of only LO phonon mode is placed in the center of the Si lattice part, and the time evolution of the LO phonon mode amplitude were observed. It was found that the rate of the amplitude decay increases with the oxide thickness. In addition, it has been revealed that the LO phonon predominantly decays into acoustic phonons. These results indicate that the existence of $SiO_2$/Si interface is rather favorable to solve the heat issue in nanoscopic devices.


## ACKNOWLEDGMENT

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