Trial application of tight-binding method to Si-cluster surrounded by SiO_2 in optimized atomistic network

Si-cluster surrounded SiO_2 is quite unique.

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***Abstract*—A tight-binding method is applied to optimized Si-cluster surrounded by SiO_2. As a result, it is found that the energy band structure is quite different from that of Si-substrate. It is regarded that the band-gap is invaded from the conduction band by intrinsic interfacial states.**

Keywords-component; tight-binding; molecular-dynamics;Si-dot; floating-gate; interfacial-states

I. INTRODUCTION

Semiconductor industry may be grown-up until the device-scaling is terminated. To prolong the scaling, new materials and structures are proposed this decade. A high-K and low-K materials are replacing the gate oxide and the isolation insulator, respectively. An ultra-thin body SOI [1] or a FIN [2] is replacing silicon-substrate, and Schottky source-drain [3], [4]will be adopted for reducing the junction leakage. From 30nm-to-10nm generations, the mechanism of electron-transportation is regarded as ballistic. Beyond 10nm generation (nano-devices era), the oxide or another insulator will replace the Schottky source-drain for reducing the leakage current further. Since the gate width and the gate length are less than 10nm and the channel is disconnected from the source and the drain, the channel is turned out to be a floating Si-dot between the source and the drain, as shown in Figure 1. (Left).

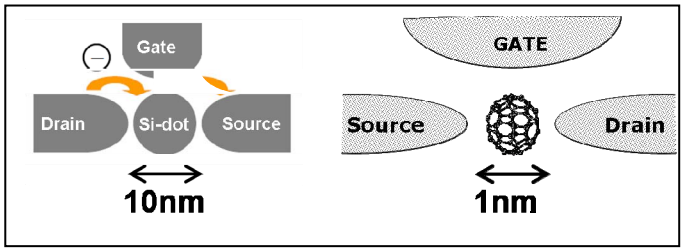

Figure 1. Hopping transport via Si-dot

The transport mechanism is accordingly a hopping transport of electrons via a floating Si-dot which causes the coulomb oscillation [5]. Beyond 1nm generation (molecular-devices era), the channel will be turned out to be a molecular-cluster, for example, C_{60}, as shown in Figure 1. (Right), in which the transportation will be the electron hopping influenced by the atomistic perturbation. An actual Si-cluster in such aggressively scaled transistors is accordingly surrounded by the oxide or another insulating film.

On the other hand, a floating gate of memory cell may also be aggressively shrunk to be a small Si-cluster surrounded by an insulating layer in generations of 20nm-to-10nm. In such small Si-clusters, the boundary is going to dominate the physical and the electrical properties with the device-scaling. It is illustrated in Figure 2. , the ratio of boundary is changed from 33.1% (=40/ (40+81)), 39.5%, and 49.0% as the cell is made smaller. Although we have several material-scientific methods for studying such clusters, *i.e.*, the first principles method, the tight-binding method, the molecular-dynamics method, and so on, we have less knowledge on the impact of cluster-boundary that is significant beyond 20nm generations. In this paper, we demonstrate a ***mixed method of molecular dynamics and tight-binding*** to study the properties of Si-dot surrounded by SiO_2 in such aggressively scaled transistors.

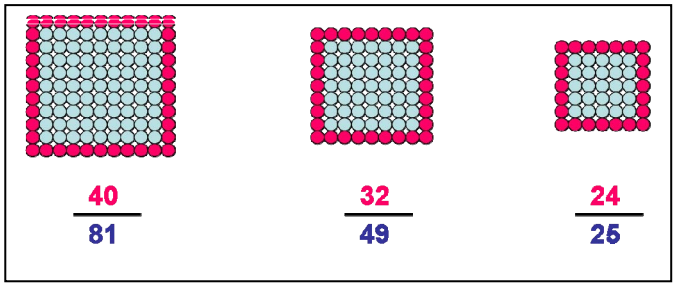

Figure 2. The ratio of boundary is changed with the scaling

II. CALCULATION METHOD

First of all, we need to prepare a cluster of many atoms with the pre-determined crystal geometry, the pre-determined crystal orientation, and the pre-determined boundary condition. To insert a Si-cluster into SiO_2-cluster, we adopt the following algorithm:

1) A considered volume, V_1, involves an inner volume, V_2, i.e., $V_2 \subset V_1$.

2) If a component of cluster, p, belongs to both V_1 and V_2, i.e., $p \in V_1$ and $p \in V_2$, we replace p with another component, q.

3) If $p \in V_1$ and $p \notin V_2$, we leave p there. If $p \in \partial(V_1 \cap V_2)$, we remove p from the interface.

Shown in Figure 3. are simple examples prepared using the present algorithm.

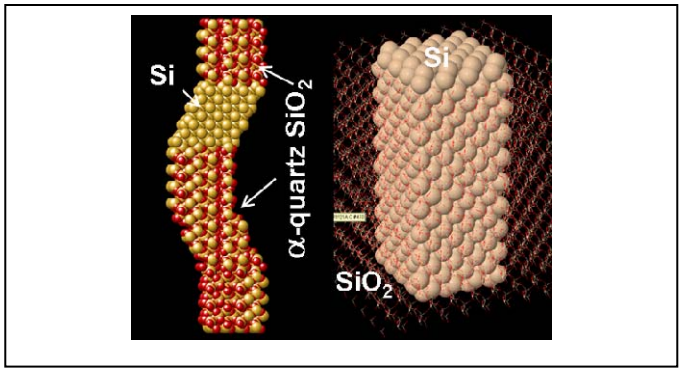

Figure 3. Simple examples prepared

Next, we optimize the bonding network of the considered atoms using the molecular-dynamics method with the reactive force-field [6], so that the system energy is reduced and the Si/SiO_2 interface is relaxed to remove the artificial lone pairs after the optimization, as shown in Figure 4. . Finally, we calculate the density-of-states (DOS) and the partial density-of-states (PDOS) using the tight-binding method in which we regulated the matrix elements of Hamiltonian according to Vogl *et al* [7].

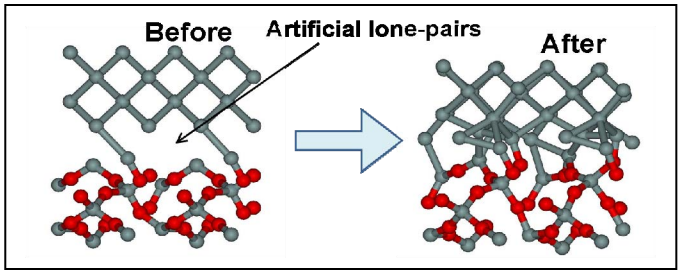

Figure 4. Optimization at the Si/SiO_2 interface

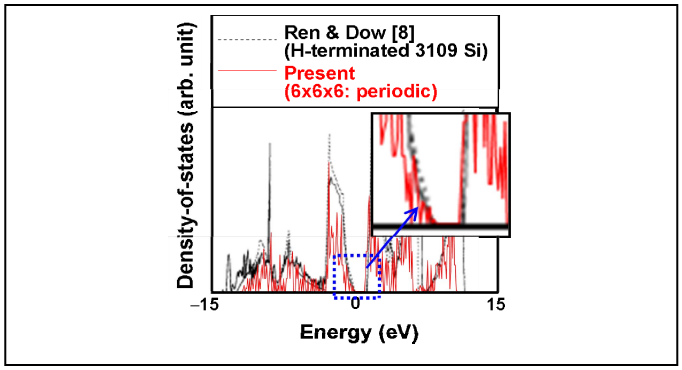

Figure 5. Comparison with the literature

III. RESULTS

To confirm the validity of the present tight-binding program, Figure 5. exhibits a good agreement between the calculated DOS of Si-crystal and that of extensively cited literature [8]. It is shown in Figure 6. that the size-dependency of Si-cluster DOS, in which the band-structure is getting similar to the bulk-Si around 0eV in the H-terminated 4x4x4 cluster. The H-termination is accordingly adopted to reproduce the bulk band structure while studying the small clusters. It is shown in Figure 7. that the boundary states invade the bulk band-gap from the valence band, as the Si-H bonding energy at the boundary is decreased. This invasion from the valence band may be associated to the lone pairs shown in Figure 4. , and sounds artificial. In Figure 8. , we compare the calculated DOS of α-quartz SiO_2 with that of first principles method, and then have a good agreement in SiO_2 band-gap.

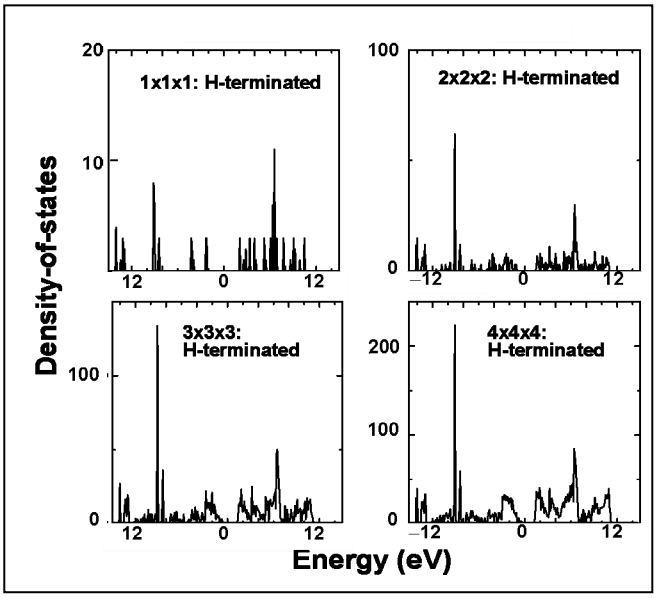

Figure 6. Size dependency of DOS of H-terminated Si-cluster

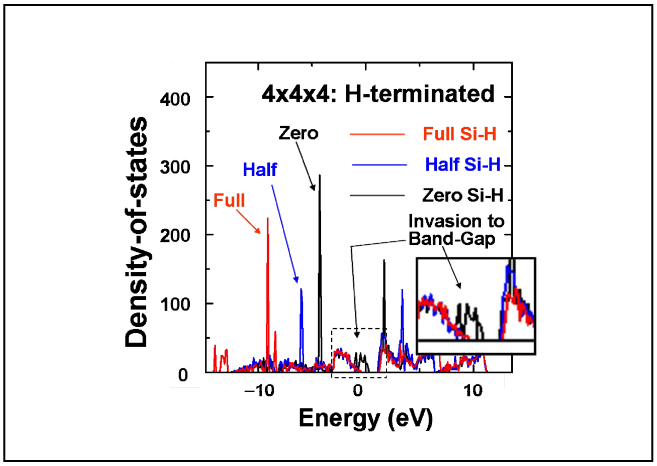

Figure 7. Si-H boundary effect

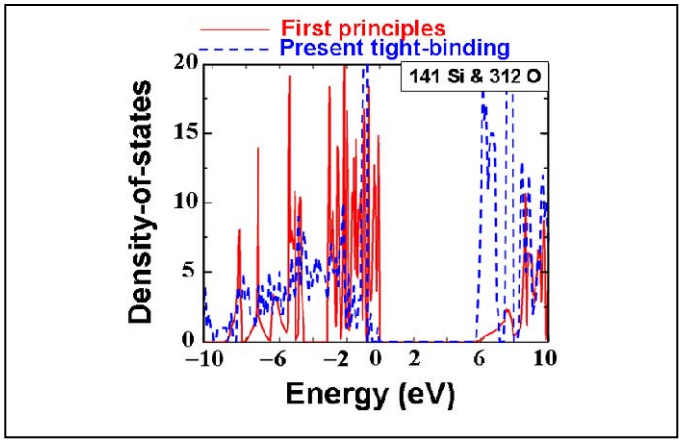

Figure 8. DOS of α-quartxz SiO_2

In Figure 9. , we insert a *Si*-cluster into *α*-quartz crystal of SiO_2 and optimize the whole network composed of atomistic bonding using the molecular-dynamics with the reactive force-field [6]. In Figure 10. , we compare the DOS shown in Figure 8. with the PDOS of SiO_2-side interface in this Si-SiO_2 cluster after the optimization. It is noted that the interfacial states invade SiO_2 band-gap from the conduction band, which may degrade the insulation quality of the oxide. Since the number of atoms in Figure 8. is much smaller than the present Si-SiO_2 cluster, the PDOS is also much smaller than that of the interface. In Figure 11. , we compare the PDOS of the inner Si-cluster with that of Si-side interface after the optimization. It is found that the interfacial states invade the band-gap around 0eV (corresponding to the bulk Si band-gap) from the conduction band. This is decisively different from the apparent invasion from the valence band that is shown in Figure 7. . The number of the interfacial states is decreased after the optimization, since the artificial lone pairs are removed from the interface. However, after the optimization, we have the intrinsic interfacial states that may have a significant influence on the electrical properties of Si-dot surrounded by SiO_2, *i.e.,* the transportation mechanism of nano-devices.

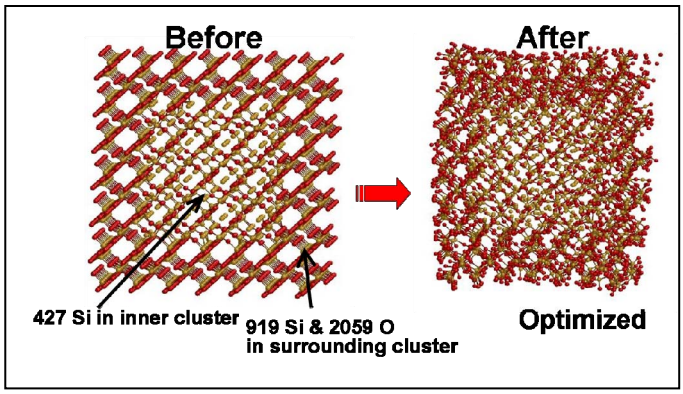

Figure 9. Optimization of Si-SiO2 cluster

Finally, we compare the Si-SiO_2 cluster with the Si/SiO_2 interface. The simulation samples are shown in Figure 12. , in which the left is the sample of Si/SiO_2 interface before the optimization and the right is that after the optimization. There are 774 Si-atoms, 212 O-atoms, and 513 H-atoms for the termination of the boundary. The thickness of SiO_2 is 1nm, and that of Si-pillar is 4nm.

The calculated PDOS of these optimized samples is shown in Figure 13. . The energy band gap is clearly left in the PDOS of Si/SiO_2 interface even after the optimization, while the conduction band edge and the valence band edge are slightly unclear. On the other hand, the band gap of Si-SiO_2 cluster is invaded from the conduction band, as expected. In the last sample, we have 685 Si-atoms, 1412 O-atoms, and 442 H-atoms for the termination of the boundary. The size of inner Si is 2nm and the thickness of the surrounding SiO_2 is 1nm. Therefore, the band-gap shrink from the conduction band edge is the property of the Si-cluster surrounded by SiO_2. This suggests that the band structure of small floating gate or Si-dot is quite different from that of Si substrate.

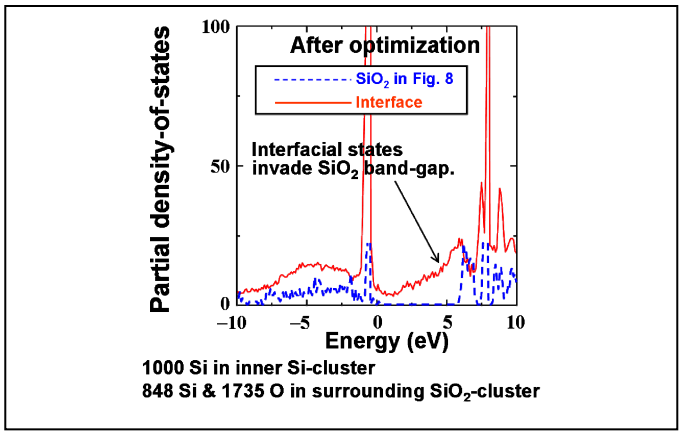

Figure 10. PDOS of SiO_2-side interface after optimization

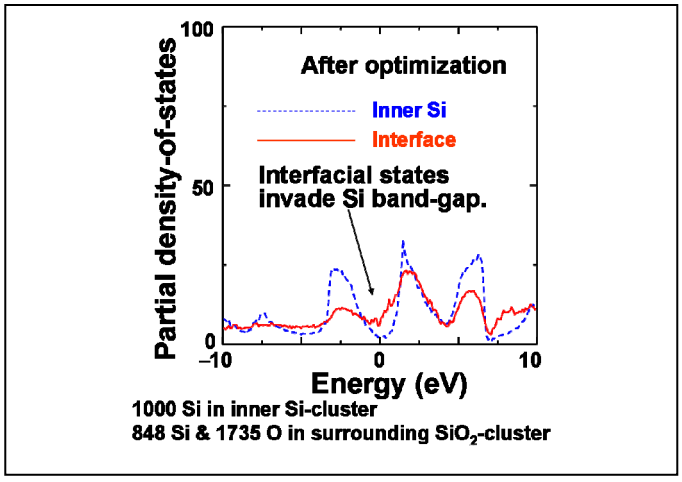

Figure 11. PDOSs of inner Si-cluster & Si-side interface

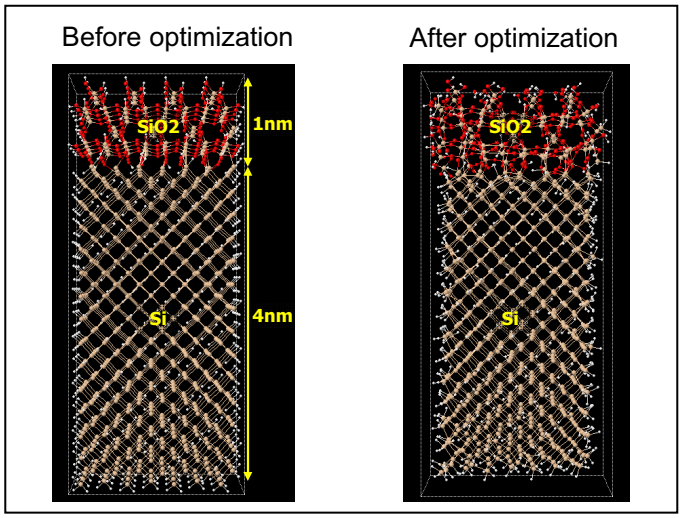

Figure 12. Simulation sample of cluster and interface

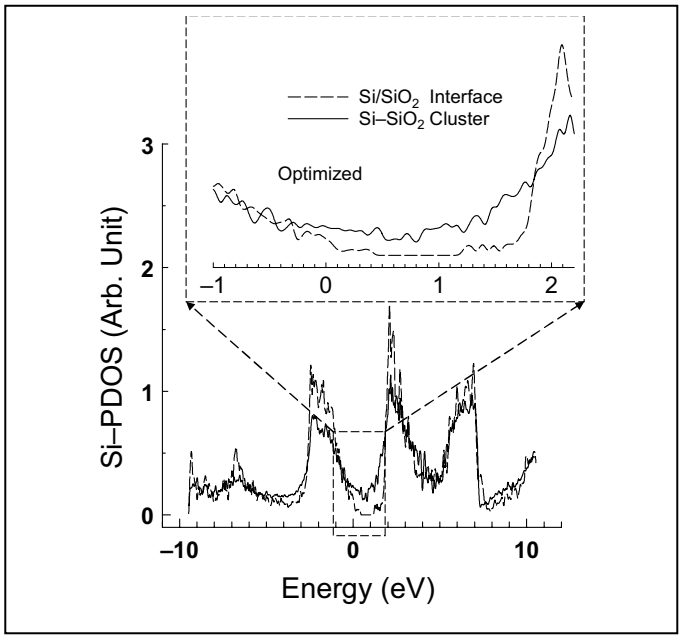

Figure 13. Si-PDOS of optimized Si-SiO_2 cluster and Si/SiO_2 interface

IV. Concluding Remarks

We demonstrated a trial application of the tight-binding method to Si-SiO_2 clusters in which whole atomistic bonding network is optimized by the molecular-dynamics to suppress the influence of extrinsic interfacial states due to the lone pairs that are involved when the cluster is artificially prepared. The trial result suggests that the intrinsic interfacial states invade Si and SiO_2 band-gaps from the conduction bands, which is quite different from the artificial invasion from the valence band due to the extrinsic interfacial states that are removed from the interface after the optimization. This also suggests that the band structure of small floating gate or Si-dot is quite different from that of Si substrate. Significant in future study are therefore the cluster size dependency of this effect and the computational limitation for larger cluster. On the other hand, since the present tight-binding method assumes that the parameters confirmed in crystal are valid in optimized system a-priori, we need to improve the computational technique in order to study this issue more carefully.

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