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A First Principles Study on Electronic Band Structures of Nano-Scaled SOI Films

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1. Introduction

Ultra-thin body structure such as FinFETs has attracted much attention because of the superior immunity to short channel effect and the mobility enhancement due to the volume inversion. Recently, sub-1nm body MOSFETs have been successfully fabricated to experimentally examine the thinning limit of SOI film [1]. However, the carrier transport mechanisms in such an extremely scaled SOI-MOSFETs have not been sufficiently understood yet, because the device behavior is increasingly sensitive to atomic-scale phenomena such as SOI-thickness-fluctuation, Coulomb scattering, local bond distortions, microscopic structure of interfaces and quantum effects. In this paper, we studied the electronic band structures and transport parameters of nano-scale SOI films based on the first principles calculation.

2. Theoretical Details

All calculations in this study were performed by using a first principles simulation package called VASP (Vienna Ab initio Simulation Package) [2]. The electron-electron exchange and correlation interactions were treated within the generalized gradient approximation (GGA). The Kohn-Sham equation was solved based on the density-functional theory and a plane-wave basis set using ultra-soft pseudopotentials and projector-augmented-wave (PAW) method [2]. In the present calculations, the pseudo wave functions are expanded in terms of the plane-wave basis set corresponding to a kinetic-energy cutoff of 300 ~ 360 eV.

3. Simulation Models

Fig. 1 (a) shows the atomic structure of a Si nano-film model sandwiched in between two SiO_2 layers. The crystalline model of the SiO_2 layers is assumed to be a β-cristobalite-like structure [3]. The dangling bonds at the Si/SiO_2 interfaces are passivated by hydrogen. We employed a supercell method to simulate the Si nano-film geometry. We may add that the atomic structures of β-cristobalite SiO_2 and hydrogen were determined by using a first principles MD simulation based on the Car-Parrinello method. In this paper, a simpler model shown in Fig. 1 (b) is also simulated for comparison, where all of surface Si atoms are assumed to be terminated by hydrogen atoms, which form a dihydride Si-H structure at the surfaces. To apply the supercell technique to this model, vacuum layers with a sufficient thickness are included above and below the structure.

4. Simulation Results

Fig. 2 shows the calculated electronic band structures of Si nano-film with a thickness of 0.64 nm (Si 5 atomic layers), where (a) and (b) correspond to the results for the SiO_2 / Si [001] / SiO_2 model (SOI model) and the hydrogen-terminated model (H-terminated model), respectively. The apparent difference in the dispersion curves between the two models is due to the different shape and breadth of the Brillouin zone. Here, it should be noted that the band-gap is direct at the Brillouin zone center in both models. This characteristic can be explained in terms of the anisotropic effective mass of bulk Si [4]. For the conduction band valleys of bulk Si, the longitudinal effective mass is about 5 times as large as the transverse effective mass. In the Si nano-film, the six valleys in bulk Si are folded onto equi-wavenumber planes due to the quantum confinement effects as shown in Fig. 3. The folded transverse valleys have a larger effective mass in the confinement direction than the folded longitudinal valleys. The difference in the effective mass gives the order of the conduction band minima, and then gives the direct band gap of the Si nano-film.

Next, Figs. 4 and 5 show the calculated dependences of the band-gap energy and transverse effective mass on the Si layer thickness T_{Si}. Due to the quantum confinement effects, the band-gap energy monotonically increases as the T_{Si} becomes less than a few nanometers. On the other hand, as shown in Fig. 5 the transverse effective mass of the conduction band minima is found to be almost identical to the bulk effective mass of $m_t = 0.19 m_0$ until T_{Si} = 1 nm, and then abruptly increases by an amount of ~ 30 % for T_{Si} < 1 nm. Since the increase of the effective mass is not predicted in the simple H-terminated model, the atomic structure at Si/SiO_2 interfaces could affect the electron transport in sub-1nm thick SOI films. The increase in transport effective mass could be a performance-degrading factor in ultimately scaled SOI-MOSFETs.

5. Conclusions

By performing the first principles calculation on the electronic band structures of nano-scaled SOI films, we found that the Si nano-film has a direct band gap. We also found that the transverse effective mass increases abruptly when the SOI film becomes less than 1 nm. The present results indicate that an atomic-scale modeling of the Si/SiO_2 interfaces is important to understand the electron transport mechanisms in ultra-thin body MOSFETs.

References

[1] K. Uchida, J. Koga and S. Takagi, *Teck. Dig. of IEDM*, (2003) 805.

[2] G. Kresse and J. Furthmüller, Phys. Rev. **B54** (1996) 11169.

[3] F. Sacconi, A. Di Carlo, P. Lugli, M. Stadele, and J. M. Jancu, IEEE Trans. Electron Devices, **51** (2004) 741.

[4] T. Ohno, K. Shiraishi, and T. Ogawa, Phys. Rev. Lett., **69** (1992) 2400.

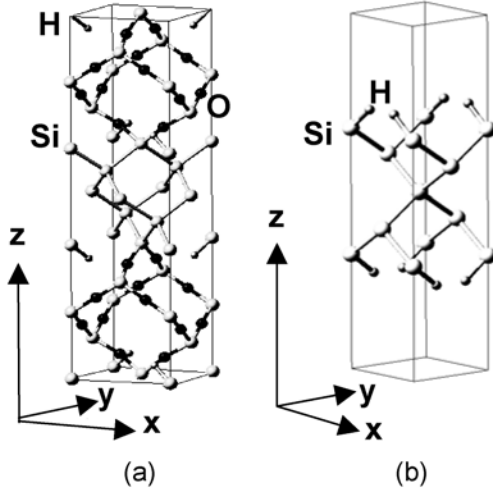Fig. 1 Atomic structures of (a) Si nano-film model sandwiched in between two SiO_2 layers and (b) hydrogen-terminated Si nano-film model. The Si, O and H atoms are depicted as large gray, small black and smaller gray spheres, respectively.
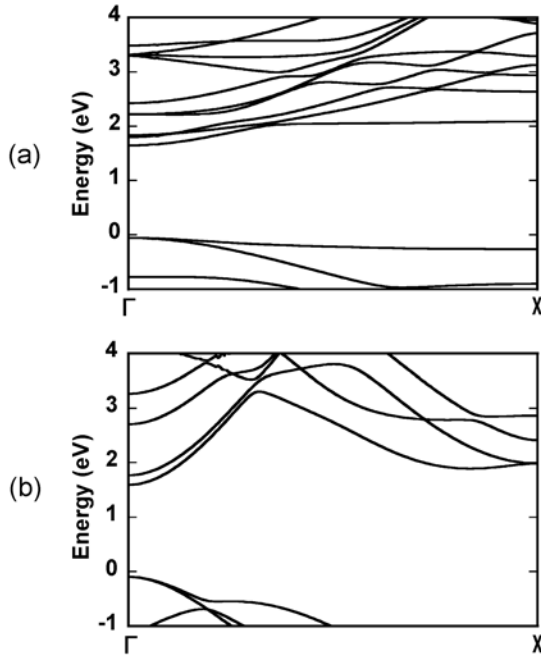

Fig. 2 Calculated band structures of Si nano-film with a thickness of 0.64 nm (Si 5 atomic layers). (a) and (b) correspond to the β-cristobalite $SiO_2 / Si\,[001] / \beta$-cristobalite SiO_2 model (SOI model) and the hydrogen-terminated model (H-terminated model), respectively.
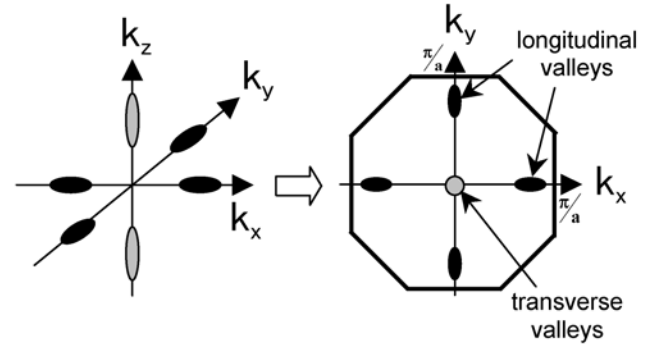

Fig. 3 Schematic of six equivalent valleys in bulk Si conduction band folded onto equi-wavenumber planes. The octagon in the right side figure represents the first Brillouin zone of bulk Si.
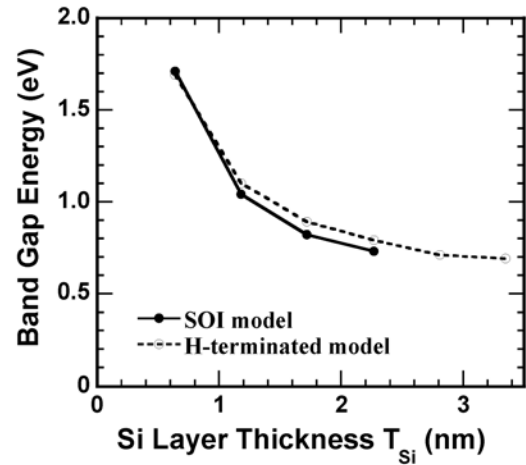

Fig. 4 Calculated T_{Si} dependences of band-gap energy. The solid and open circles denote the SOI and H-terminated models, respectively.
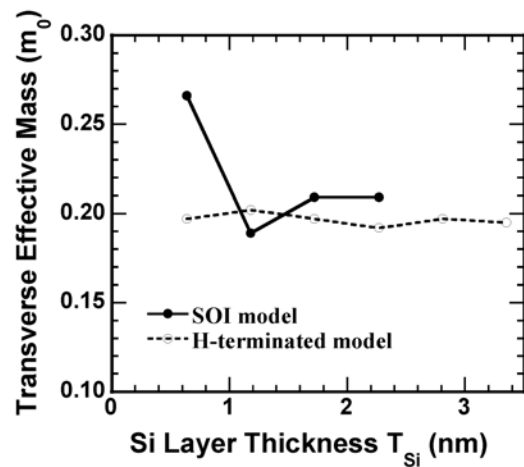

Fig. 5 Calculated T_{Si} dependences of transverse effective mass at conduction band minima. The solid and open circles denote the SOI and H-terminated models, respectively.