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Ab-initio simulation of phonon properties of ultra-thin silicon films

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1. introduction

The International Technology Roadmap of Semiconductors (ITRS2005) [1] predicts that downscaling of CMOS will be pursued further, and the gate length of the high-performance MOSFETs will reach 9 nm in 2016. Along with such an aggressive device miniaturization in the lateral dimensions, thickness of silicon channels has also been reduced continuously, and the SOI (Silicon-On-Insulator) MOSFET with the channel thickness of as thin as five silicon atom layers has recently been reported [2].

Apparently the conventional continuum model does not work for such nanometer-scale silicon structures, and atomistic modeling is certainly needed for taking account of their discrete natures as well as quantization effects. Another important consequence of the atomistic discreteness of silicon nanostructures may be observed for their phonon properties. Phonon dispersion relationship has recently been studied for ultrathin silicon films by using the continuum model [3], but there have been very limited number of reports on phonon calculations based on the first principle calculations.

In this paper we report for the first time on the ab-initio simulation of the phonon properties of ultra-thin silicon films and clarify the difference between those for bulk silicon and for ultra thin films.

2. Method

In the present work we adopted the DFT program SIESTA [4,5] optimized for the grid computer TSUBAME at Tokyo Institute of Technology [6]. Phonon dispersion relationships and the density of states (DOS) of phonons were calculated in the following way.

We first made an atomistic model of the unit cell for an ultra thin film of Si such as Fig.1 [7]. We then optimized the atomic structures and obtained the most stable one by using SIESTA. After that a two-dimensional 3 x 3 super cell was formed to take the effect of first and second nearest neighbor cells into consideration.

The force constant matrix was then created by repeating the electronic structures calculation with shifting the individual atoms slightly in the x-, y-, and z-directions slightly. Finally, the phonon dispersion relationships were calculated in the particular directions in the first Brillouin zone. The associated phonon DOS was calculated by integrating the eigenvalues in the first Brillouin zone

3. Results

Figure 2 shows the phonon dispersion curves calculated for a ultra thin film of silicon in the direction from the Γ point to [100] and [110] directions. It should be noted that a phonon band gap is clearly seen at near 100 cm^{-1} in [110] direction, which does not exist in that for bulk silicon. The physical origin of the phonon band gap is still under discussion, but it may result from the formation of periodic Si dimmers formed on the reconstructed surface of the film. Figure 3 shows a blow-up of the dispersion curves near the Γ point in comparison with the results obtained by using the continuum model. It can be seen that these results agree well in such a small k region.

Figure 4 shows the phonon dispersion curves calculated near the Γ point for bulk silicon (dotted curves) and the ultra thin film (solid lines). It should be noted that the lowest acoustic branch exhibits a quasi-quadratic dependence that is attributable to the bending mode of the thin film [8] and contrasts with the linear dependence for bulk silicon. This results in the shift of the edge of phonon DOS towards the lower energy (Fig. 5).

4. Conclusions

We succeeded in the calculation of phonon dispersion and density of state of ultra thin film of silicon by using ab-initio calculation. The simulated results clearly showed the unique phonon properties such as phonon banc gap formation and quadratic acoustic branch.

5. References

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6. Acknowledgements

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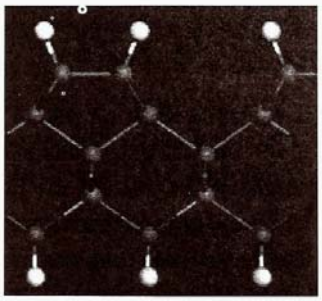

Fig.1 An atomistic model of ultra thin film of silicon. Gray balls are silicon, white balls are hydrogen.

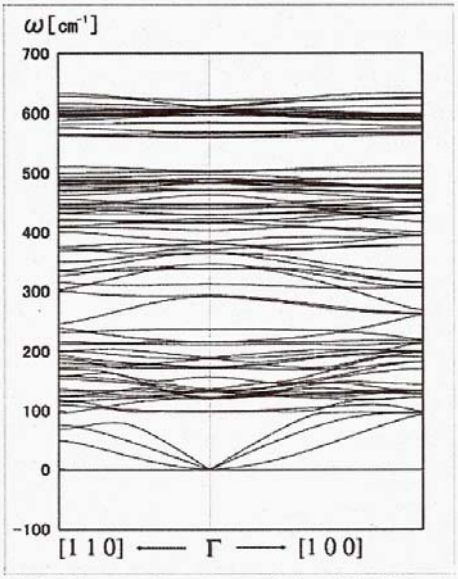

Fig.2 Phonon dispersion of ultra thin film of silicon

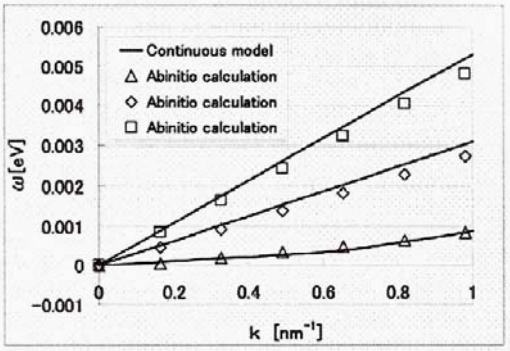

Fig.3 Comparison of calculation results near gamma point between in the case of continuous approximation and our case

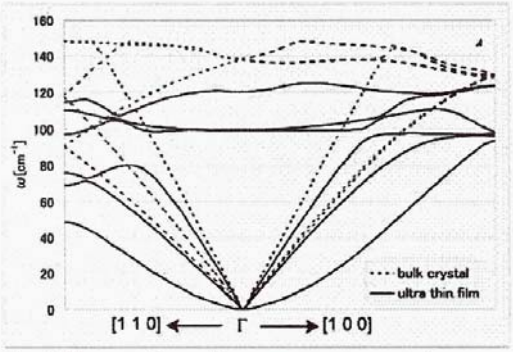

Fig.4 Phonon dispersion near gamma point comparing between the case of bulk silicon and ultra thin film of silicon

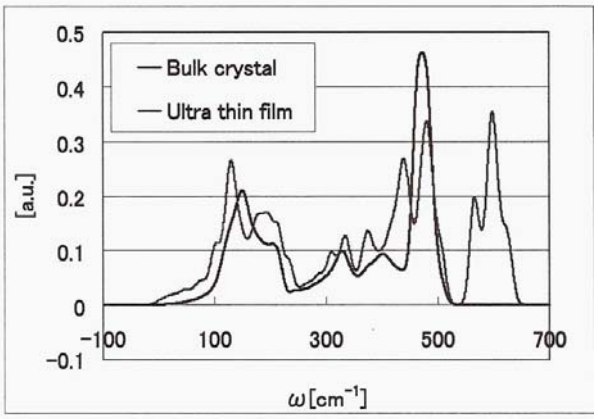

Fig.5 Density of state of phonon comparing with that of bulk silicon