Atomistic study of phonon states in hydrogen-terminated Si ultra-thin films

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1. Introduction

Along with aggressive downscaling of the physical gate length of MOSFETs, thickness of Si channels has also been reduced continuously, and the SOI MOSFETs with the channel of as thin as five Si atomic layers has recently been reported [1]. Phonons in such thin Si layers are expected to behave in a different manner to those for bulk Si. However, virtually no study has been reported to date on their properties based on the *ab initio* simulation. As a new first step towards clarifying them, we here report on the *ab-initio* analysis of phonon properties for ultra thin Si films with hydrogen-terminated surfaces for the first time.

2. *Ab initio* simulation of phonons

Figure 1 shows Si thin film structures of 3 to 10 atomic layers in thickness used for the present analysis. To construct the initial atomistic model, a few atom layers were first extracted from bulk crystal, and each two valence bonds of surface Si were terminated by hydrogen atoms. The Si(0 0 1) 2x1 dimer structures [2] were then formed on the film surface, and the entire atomic structures were optimized by using the DFT (density-functional theory) simulator SIESTA [3,4]. Note that there are two stable structures for the 6- and 10-layer-thick films with different relative dimer configurations on the two opposite surfaces. We adopted the DZP (double zeta polarized) basis sets of Si and H optimized for bulk Si and the water molecule [5]. In order to obtain eigenvalues and eigenvectors for phonons, we used VIBRATOR, which is associated with SIESTA and based on the *ab initio* force-constant method [6]. Using this method, we first calculated the phonon dispersions of bulk Si in an excellent agreement with the experimental data [7] (Fig. 2). Particular efforts were made to speed-up the calculations for thin films as the surface dimers inevitably increase the number of atoms in the unit cell. We have, for example, 48 atoms in the unit cell for the 5-atomic-layer film. The phonon calculations need construction of a super cell, and so we had to carry out the self-consistent calculations for quite large-scale structures. The multiple k-point calculations also require a few super cells to achieve a reasonable accuracy. We adopted the SIESTA parallelized on the TSUBAME grid cluster [8].

3. Phononic properties of Si ultrathin films

We obtained a set of numerical results of the phonon dispersions, phonon DOSs, and the eigenvectors for all the film structures. The most remarkable feature is phonon bandgaps observed for the films thinner than 7 atomic layers. Figure 3 shows the dispersion relationship calculated for the 4-atomic-layer-thick film in comparison with those for bulk Si. The phonon bandgap is observed only in the (1 -1 0) direction for the energy from 66.5 to 86.8 cm^{-1}, which is defined between the energy maximum of the acoustic branches and the energy minimum of the right above optical-like branch. We found that the formation of the phonon bandgaps are closely related to the Si dimers which line up in the (1 -1 0) direction. In contrast to the bulk Si atoms, the surface Si atoms are covalently-bound alternately in the direction and therefore hold the structural and mechanical periodicity of twice as long as that for bulk Si. This hypothesis is confirmed by the fact that the phonon bandgaps are observed also for the (1 1 0) direction for the films with odd number of Si atomic layers (i.e., 3, 5 and 7 layers) because the Si dimers are formed in the (1 1 0) direction on the opposite surface. The magnitude of the bandgaps decreases with increasing the film thickness and finally vanishes for the thickness above 8 atomic layers. This is because the impact of the surface dimers on the entire dispersion relationships is reduced relative to that of the bulk Si atoms. We also found that the 6-layer-thick films exhibit the singularities in the phonon properties due to their special symmetry in atomic structures, resulting in the phonon bandgap disappearance. Another notable feature is the softening of the acoustic phonons with reducing the film thickness. Figure 4 compares the lowest acoustic branches calculated for all the film structures. This acoustic mode represents atomic vibrations perpendicular to the film surface, which corresponds to the Flexural mode in the continuum approximation, and therefore the effects of the surface Si atoms are enhanced with decreasing the film thickness. This results in the increase in the phonon DOS in the low energy regime as shown in Fig. 5.

4. Conclusion

We have conducted the *ab initio* simulation of 'nanophonons' for the first time for the H-terminated ultrathin Si films of 3 to 10 atomic layers in thickness and have revealed that the phonon bandgaps are formed as a result of the Si dimers on the surface.

References

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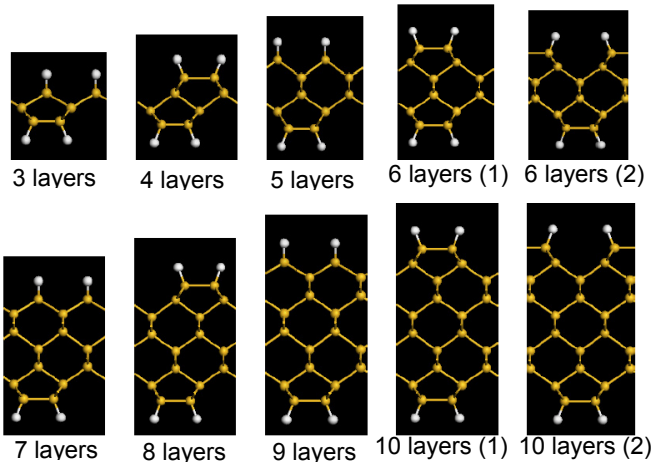


Fig.1 Atomistic structures of H-terminated ultrathin silicon films ranging from three to ten silicon layers.

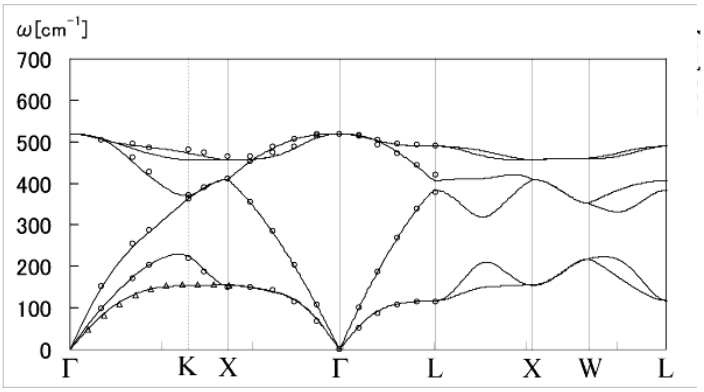
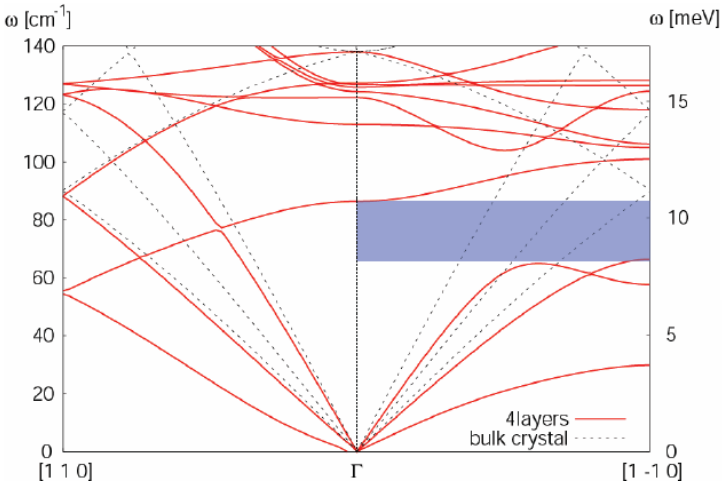


Fig.2 Phonon dispersion curves simulated for bulk silicon (solid lines) compared with experimental data (open circles and triangles) [7].



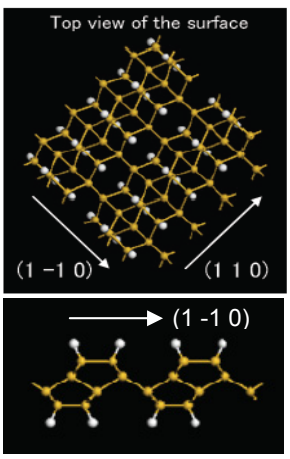


Fig.3 (Left) Phonon dispersion curves simulated for a 4-layer-thick silicon film (solid lines). The dotted lines are the dispersion curves for bulk silicon, which are redrawn by folding the original curves in Fig. 2 into the Brillouin zones defined for the Si thin films. A hatched grey area shows a phonon band-gap. (Right) Atomistic images of the silicon thin film.

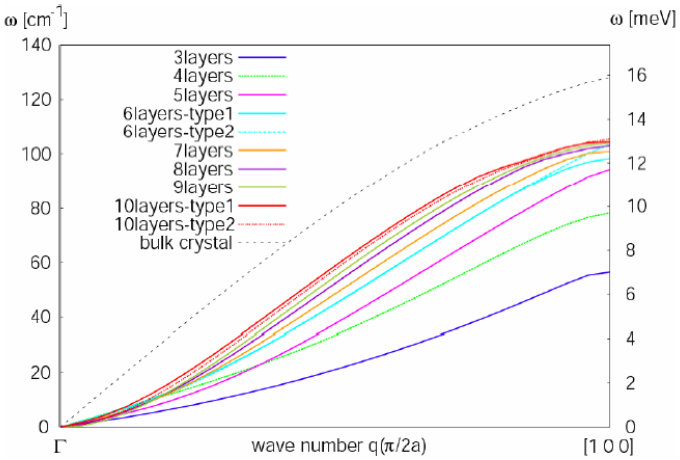


Fig.4 The lowest acoustic branches calculated with various values of film thickness in comparison with that for bulk silicon.

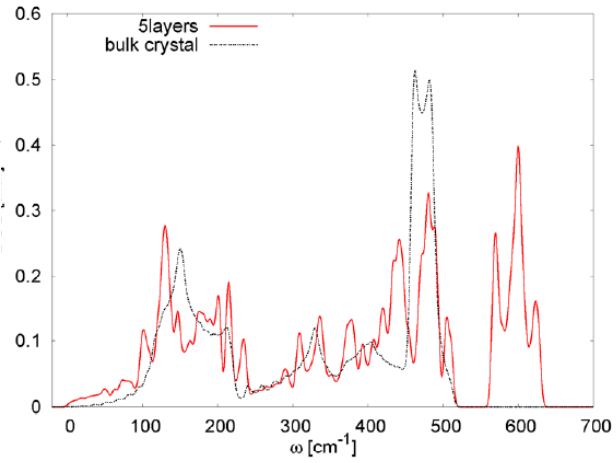


Fig.5 Phonon density-of-states (DOS) calculated for a five-layer-thick silicon film.