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# Impacts of Surface Orientation on Band Gap and Band Structure of Ultra-Thin Silicon Films

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**INTRODUCTION** Silicon thin films and silicon-based superlattice structures have attracted much attention in recent years because of their many potential applications including the area of nano-photonics. Such silicon-based superlattices are of fundamental interest, also may have practical use because of their ideal interface compatibility with standard semiconductor technology. Light emission from Silicon-based superlattice, such as Si/$SiO_2$ and Si/$Si_3N_4$ superlattices is an attractive new field. [1-5] In light emission from nanostructured silicon, both crystalline and amorphous silicon superlattice structures are used, and crystalline superlattice structures are with high light emission efficiency. In Si/$SiO_2$ and Si/$Si_3N_4$ superlattices, the peak emission wavelength is controlled by the silicon layer thickness. The size effects on band gap of silicon thin films and light-emission peak wavelength are invested by simulations [1] and experiments [2-5]. The band gap of a silicon layer decreases with an increase of layer thickness and induces red-shift in the light-emission peak wavelength. Although some studies have been done, many important and fundamental questions remain unsolved. For example, how does quantum confinement effect and band structure depend on silicon thin-film orientation? In this work, we investigate systematically the electron band structure and band gap of nanostructured silicon films with first-principles calculations, discuss the impacts of surface orientation on band structure and size effect.

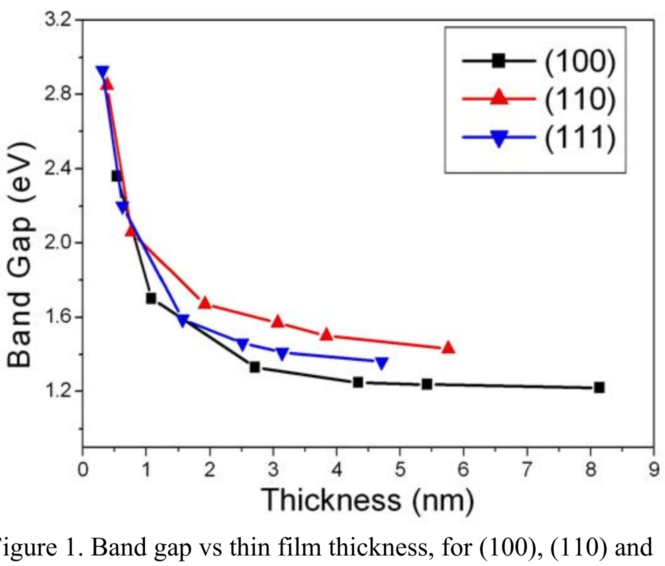


Figure 1. Band gap vs thin film thickness, for (100), (110) and (111) films.

**Computation Method and Model** Repeated free-standing Si slabs with (100), (110), and (111) surface orientations are used for the calculation. The supercell consists of $N$ ($N$=1-10) unit cells in the direction perpendicular to the Si(100)/(110)/(111) surfaces, with a vacuum region of 18 Å to avoid interaction between the silicon film and its images in neighboring cells. The (1×1) unit cell is adopted parallel to the surface. The lattice constant in the plane for the slab is assumed to be that for bulk silicon crystal. We focus on the films with thickness less than 7 nm because in most light-emission devices, the thickness of silicon film is from 2 to 7nm. [3-5] Therefore understanding the band structure of silicon film in this scale is indispensable. For presentation in the figures, the number $N$ of unit cells in the conventional cell is related to the slab thickness. The up and down sides of the slab are terminated with H atoms placed at a standard bond length of 1.48 Å to eliminate artificial dangling bonds. This Si-H bond length corresponds to that in the $SiH_4$ molecule. This hydrogen-saturated slab model has been successfully used to study the electronic and optical properties of nanostructured films. [6] Geometry optimization of silicon layers are studied by using density-functional theory (DFT) with the generalized gradient approximation (GGA) of Perdew-Burke-Enzerhof (PBE) form. All the possible structures are optimized by the BFGS algorithm, which provides a rapid means to find the lowest-energy structure and supports cell optimization in the CASTEP code. [7] The ion-electron interaction is modeled by norm-conserving pseudopotentials. The plane-wave cutoff energy is taken as 350 eV, and a 5×5×1 Monkhorst-Pack k-point sampling is used for integration of the first Brillouin zone. Good convergence was obtained with these parameters. The optimization is performed until the forces on the atoms are less than 0.01 eV/Å and all the stress components are less than 0.02 GPa; the tolerance in the self-consistent field calculation is $5.0\times10^{-6}$ eV/atom.

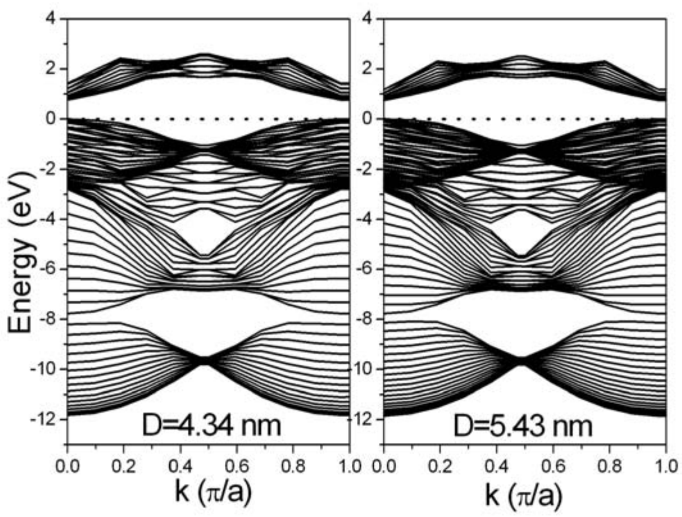


Figure 2. Band structure of Si (100) thin film. Here the highest occupied states (valence band maximum) are aligned at 0 eV.

**Results and Discussion** Figure 1 shows the calculated band gap of silicon films as a function of the film thickness. It should

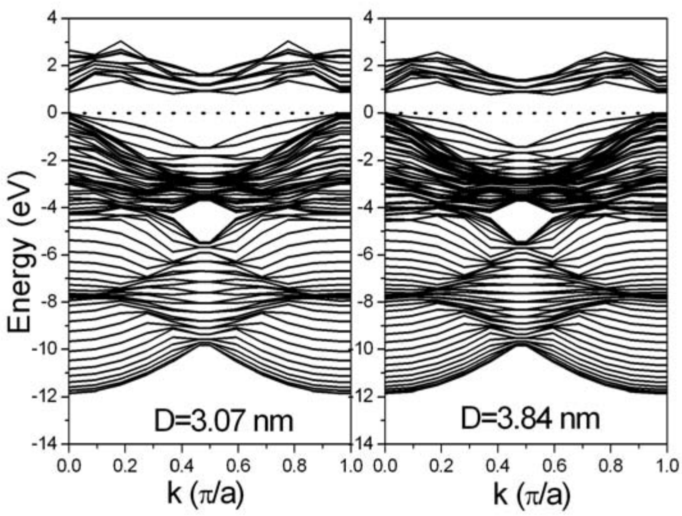


Figure 3. Band structure of Si (110) thin film.

be noted that the calculated band gap is substantially lower than the true band gap. This magnitude of underestimation is typical of the Kohn-Sham equations. In the present investigation, a 0.6 eV correction is used to shift the theoretical bulk limit of the band gap to 1.12 eV, which is in agreement with experimental value, as Ref. 1 adopted. The quantum-confinement effect is pronounced in the band gap. A large increase of band gap (from 1.2 to 2.8 eV) is observed in the nanostructured Si films. At small thickness, the small increase of thickness can induce large decrease on band gap. Contrast to the high sensitivity at that region, the band gap versus film thickness curves are almost flat at the large thickness region (>3 nm) as show in Figure 1. Over 3 nm thickness, the band gap of Si (100) film converges to 1.2 eV. And the band gap (BG) of (110) film is larger than that of (111) film, and larger than that of (100) film ($BG_{110}$>$BG_{111}$>$BG_{100}$). The dependence of band gap on growth orientation is remarkable.

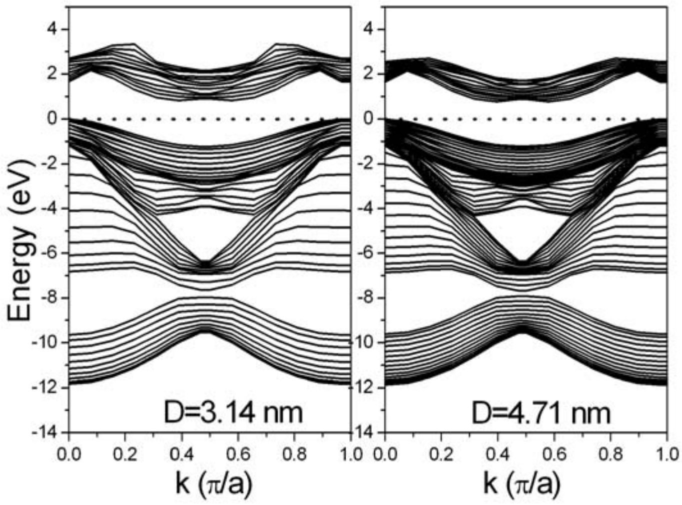


Figure 4. Band structure of Si (111) thin film.

Besides band gap, band structure is also an important factor affects the light emission. Silicon is generally considered to be unsuitable for optoelectronic applications because of the indirect nature of band gap. However, when silicon is in the form of nanostructures, the optical and electrical properties are quite different from that of bulk silicon, and light emission from nanostructured silicon has attract wide interests. System with direct band gap is with high efficiency in light emission. Here we show the impacts of surface orientation on the band structure. Figure 2-4 show the band structure of Si (100), (110) and (111) films. It is clear that the (100) thin film is with typical direct band gap, which will benefit the light emission process. However, (111) thin film is typical indirect band gap. The (110) thin film is with direct band gap, while the second lowest conduction band edge is very close to the conduction band minimum. As direct band gap system is with great benefit of light emission, and indirect band gap prevents efficient electron-photon energy conversion due to low emission rate, we propose that in silicon photonics light emission application, (100) orientated silicon thin film is with remarkable advantages over (110) and (111) orientated thin films.

**Summary** In summary, we have studied the impacts of surface orientation on band gap and band structure of silicon thin films. When the film thickness is larger than 3 nm, the band gap versus film thickness curves are almost flat. And the band gap (BG) of (110) film is larger than that of (111) film, and larger than that of (100) film ($BG_{110}$>$BG_{111}$>$BG_{100}$). The dependence of band gap on grow orientation is remarkable. Moreover, the (100) film is with typical direct band gap, and (111) orientated thin film is with indirect band gap. As direct band gap system is with large light emission efficiency, our results show that in silicon photonics light emission application, (100) orientated silicon thin film is with remarkable advantages over (110) and (111) orientated thin films.

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