AB INITIO ANALYSIS ON IDEAL STRENGTH OF NANOSCALE THIN FILM

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ABSTRACT

The ideal strength, which is the possible maximum strength of the material, gives a fundamental information about the mechanical properties. Since the material strength is sensitive to its structure, it is necessary to evaluate the critical stress. We define this as "structural ideal strength" and aim to conduct systematic studies to clarify it. To achieve this goal, we are to carry out rigorous evaluation on the structural ideal strength of typical structures. In this paper, we present the effect of surface structure to the mechanical properties. *Ab initio* tensile simulations are carried out for silicon thin films with the thickness of 1.77nm, 1.23nm and 0.68nm, having (001)-p(2x1) asymmetry surfaces. At the initial state without external load, the thin films are slightly deformed compared to bulk due to the existence of the surfaces. The stress-strain relationship during tension indicates that a thinner Si thin film has a lower Young's modulus. The ideal strength decreases as the film becomes thinner. Atomic and electronic structures do not show significant change before unstable deformation takes place.

1. Introduction

Manufacturing and application of materials with fine and complex structure in the nanometer scale have been intensively developed. It is, then, of great importance to elucidate the mechanical properties of nanomaterials.

In general, the ideal strength of materials is defined as the critical stress of unstable deformation in perfect crystals under uniform deformation[1-2]. The ideal strength, which is the possible maximum strength of the material, gives us a fundamental information about the mechanical properties. Rigorous evaluations of the ideal strength of materials have been performed so far by means of *ab initio* analysis[3-7], which is highly precise theoretical calculation based on quantum mechanics[8].

Since the material strength is sensitive to their structure, it is necessary to evaluate the critical

stress. We define this as "structural ideal strength" and aim to conduct systematic studies to clarify it. To achieve this goal, we are to carry out rigorous evaluation on the structural ideal strength of typical structures.

In this paper, we investigated the effect of surface structure to the mechanical properties. *Ab initio* deformation simulations are performed on nanoscale silicon thin films which show significant surface reconstructions.

2. Simulation procedure

Ab initio tensile simulations are carried out for silicon thin films with (001)-p(2x1) asymmetry surfaces. Figure 1 shows three simulation models consisting of 14, 10 and 6 atomic layers parallel to the surfaces (Models A, B and C). The vacuum layer with the thickness of 1.0nm is included in each model, which is thick enough for eliminating the effect of the periodic boundary condition in the *y* direction. The initial lattice constant is 0.5456nm. While the surface configuration is relaxed by an *ab initio* calculation, the cell size is adjusted so that the normal stresses are zero to create the initial state. Then, the cell is stretched gradually in the *x* direction, which corresponds to [110], while the atom configuration is relaxed and the normal stress in the *y* direction is kept zero.

The *ab initio* calculations are performed using VASP[9]. The exchange-correlation energy is evaluated using GGA by Perdew and Wang[10], an ultra-soft pseudopotential[11] is employed with the cutoff energy for plane waves of 300eV, 15 k-points arranged with Monkhost-Pack method[12] are selected, and the atom configuration is relaxed with the conjugate-gradient method.

3. Result and discussion

The relaxed atom configuration and bond structure under no external load is depicted in Fig. 2. The spheres are the atoms and the bond structure is shown by the curved surface on which charge density is 0.45 x 10^{-3}nm^{-3}. The asymmetric dimers of the p(2x1) structure are formed on the surfaces. The film is contracted in the *x* direction and stretched in the *y* direction. Figure 3 shows relationship between the stress, $?_x$, and the strain, $?_x$, during tension in the [110] orientation. The stress-strain relationship of Si single crystal is also shown for comparison. The Young's modulus of the Si thin film is evaluated from the inclination of the curve at $?_x$=0. The modulus becomes smaller as the thickness decreases, indicating that the existence of surface softens the films. In the

cases of Models A and B, the stress increases with the increase of the strain to reach its maximum magnitude. Then, the stress decrease rapidly, which indicates unstable deformation. On the other hand, in the case of Model C, the stress shows slight decrease around $?_x$=0.1, then shows fluctuation with the increase of the strain before the stress decrease rapidly when $?_x$>0.2. The maximum stresses of Models A, B and C are 13.5GPa, 12GPa and 10GPa, respectively, meaning that the ideal strength decreases as the film becomes thinner.

Figure 4 shows change in atomic and electronic structures in the Si thin films during the tensile deformation. The curved surface on which charge density is $0.425 \times 10^{-3} nm^{-3}$ is depicted. In all the cases, atom and electronic structures do not change significantly before bond breaking (indicated with dashed lines in the figure) takes place at the unstable deformation. This means that the deformation of the Si nanoscale thin films is brittle, where structural change does not occur during tension.

4. Summary

To investigate the effect of surface structure to the mechanical properties, we conducted *ab initio* tensile simulations for silicon thin films. Results are summarized as follows:

(1) A thinner Si thin film has a lower Young's modulus.

(2) The ideal strength decreases as the thickness becomes smaller.

(3) Atomic and electronic structures do not show significant change before unstable deformation takes place.

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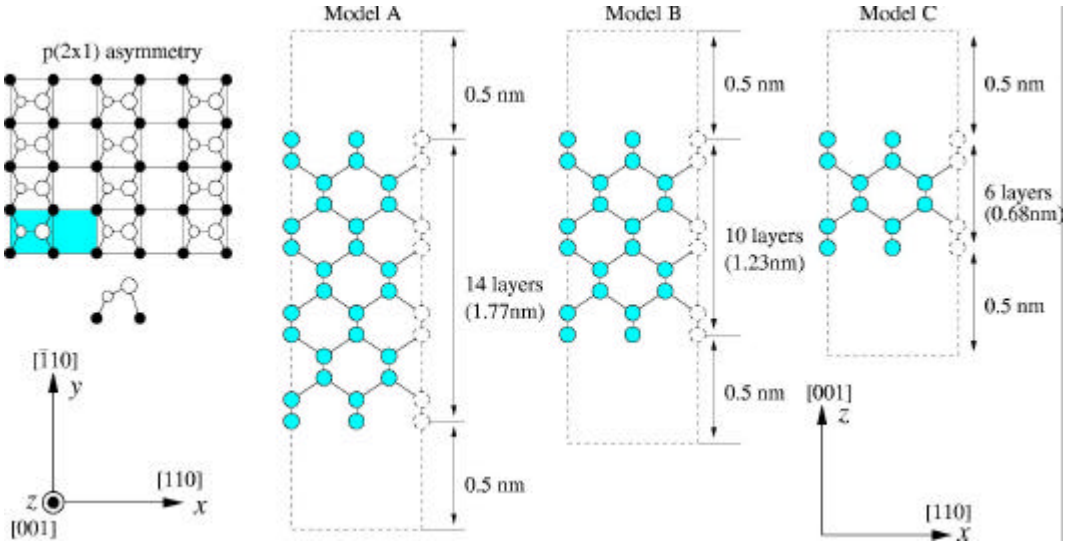

Figure 1 Simulation models.

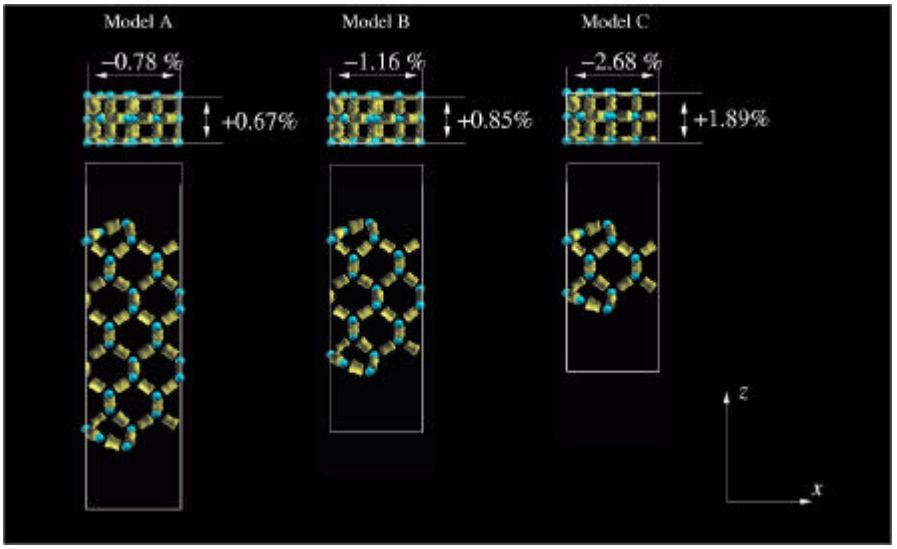

Figure 2 Atomic and electronic configuration after relaxation..

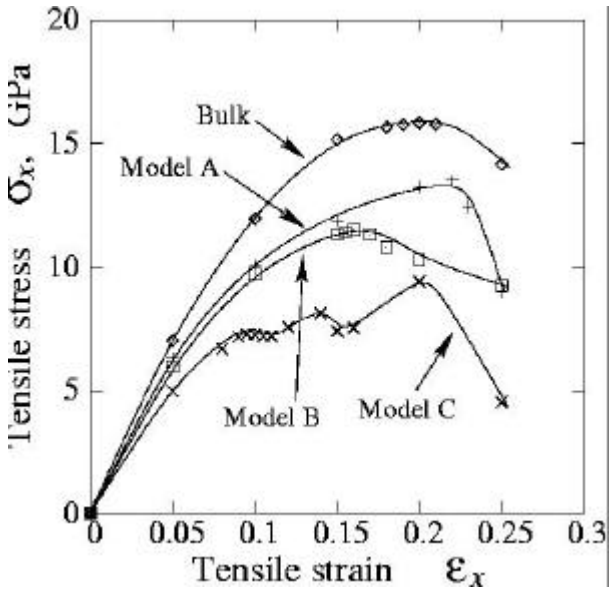

Figure 3 Stress-strain curve.

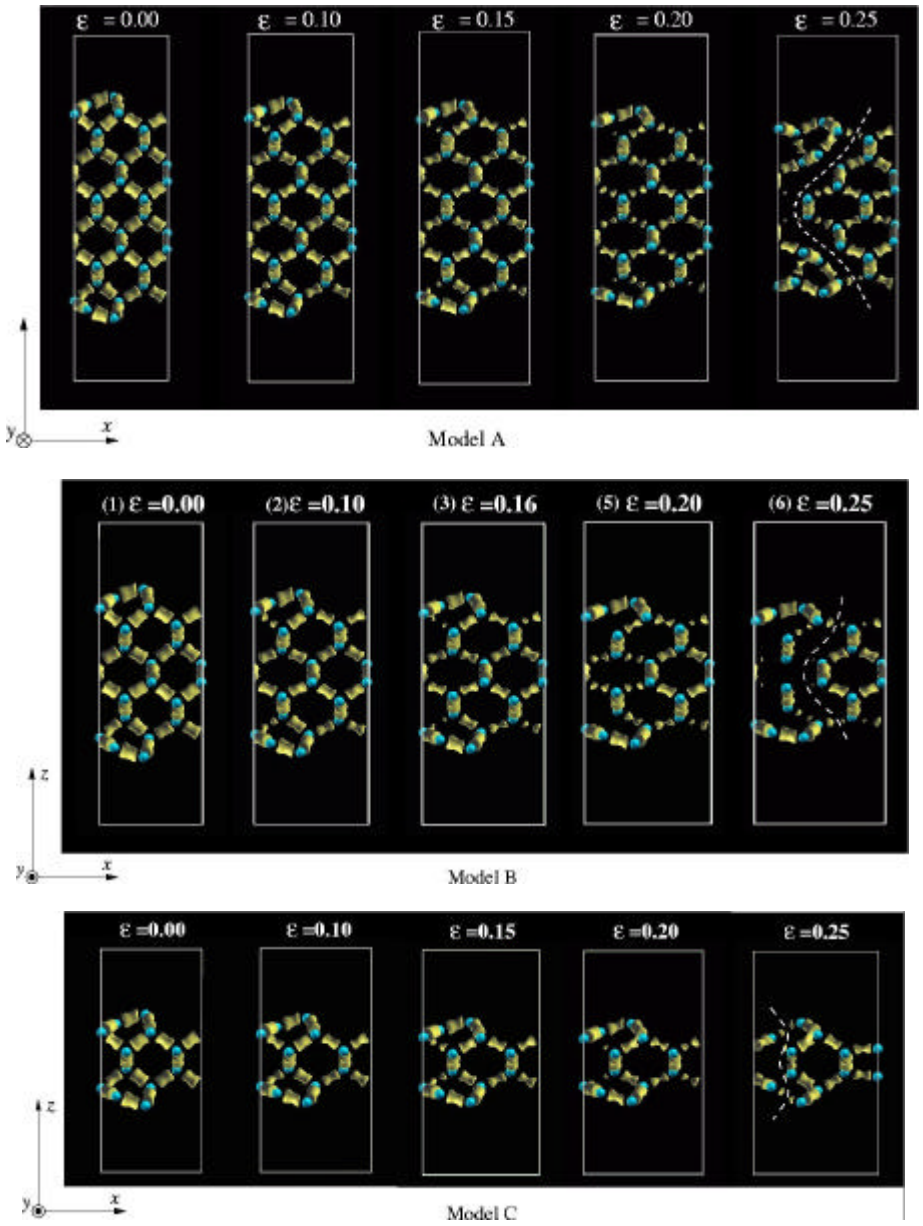

Figure 4 Change in configuration during tension.