Ab Initio Simulation on Ideal Shear Strength of Silicon

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ABSTRACT

Single crystal of silicon is commonly used for the substrate of electronic devices. Large stress is induced in the substrate due to thermal mismatch of device component. It is well known that a defect such as dislocation brought about by the stress aggravates the electronic property of silicon. It has been reported that the ideal shear strength can be correlated to the resolved shear stress to introduce the dislocation in the substrate. In this study, in order to evaluate the ideal shear strength, homogeneous shear deformation of silicon single crystal (slip plane: (111), slip direction: $[\bar{1}01]$) is simulated by the *ab initio* calculation based on plane waves. Especially, the focus is put on the effects of normal stress and the inner displacement of atoms in the cell under the shear strain. The normal stress strongly affects on the instability strain, and the inner displacement remarkably decreases the strength. The peak stress of silicon crystal is about 10GPa at the shear strain of 0.3. The band gap becomes narrow as the strain increases. Since it disappears at the shear strain of 0.2, the deterioration of electronic property is more sensitive to the shear deformation than the mechanical one.

Keywords: *Ab initio*, Silicon, Ideal strength, Shear deformation, Inner displacement, Band gap

1 Introduction

Silicon single crystal is commonly used for substrate of electronic devices. Because an integrated circuit consists of various micro-materials, their deformation mismatch brings about stress concentration in the substrate during processing and/or service. An atomic scale defect, e.g. dislocation, which sometimes nucleates due to the high stress, causes fatal malfunction of the devices[1]. Therefore, it is of great importance to elucidate the mechanical property of silicon under high shear stress.

In this study, homogeneous shear deformation of silicon single crystal is simulated by the *ab initio* calculation and the shear ideal strength is examined taking into account effects of the normal stresses and the inner displacement of atom position in the unit cell of crystal.

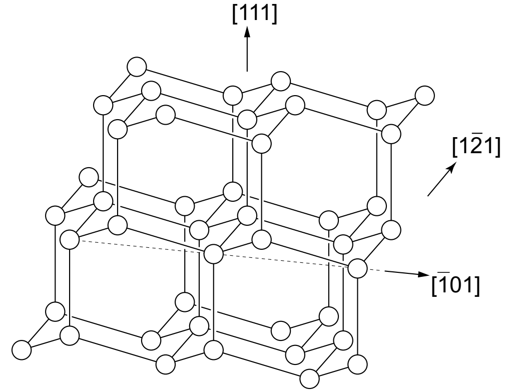


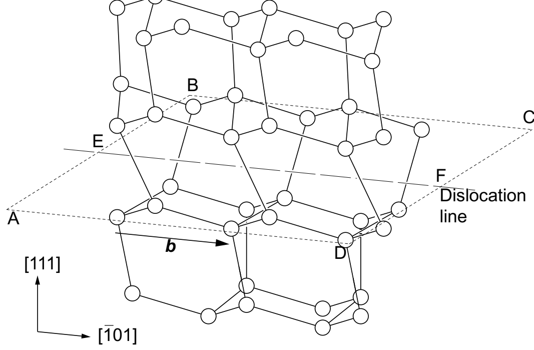
Figure 1: Schematic illustration of silicon lattice.

2 Simulation procedure

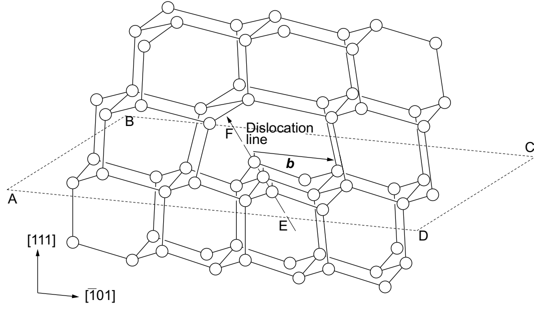
Figure 1 shows a rotated view of the silicon crystal where the base is set on a {111} plane. The dislocations usually observed are the screw type and the 60° one with the slip plane of {111} and the slip direction of $\langle 110 \rangle$ as shown in Fig.2[2], respectively. The dislocation line is parallel to the Burgers vector in the former, while the angle between them is 60° in the latter. The edge dislocation, of which the slip plane is {100}, is hardly found.

The shear deformation is applied on the slip direction of the simulation cell shown in Fig.3. The cell includes 12 atoms, and the cell size is $L_x \times L_y \times L_z = \frac{\sqrt{2}}{2}a \times \frac{\sqrt{6}}{2}a \times \sqrt{3}a$ where a indicates the lattice constant. The periodic boundary condition is applied in order to simulate the bulk behavior. The *ab initio* calculation is conducted using the norm conserving pseudopotential proposed by Hamann[3] and the plane wave basis set[4,5]. In order to accelerate the iteration of the self-consistent calculation, the conjugated gradient method proposed by Bylander *et al*[6] is adopted. The cut-off energy of plane waves is 20.0Ry, and 30 $\boldsymbol{k}$-points $(5 \times 3 \times 2)$ are selected in the brillouin zone[7]. The exchange-correlation energy is estimated by the function proposed by Perdew and Zunger[8] based on the Local Density Approximation (LDA)[4,9].

For searching the equilibrium state under no external load, total energy is calculated by varying the lattice constant. Then, the shear strain, γ_{zx}, which corre-



(a): Screw dislocation.



(b): 60 ° dislocation.

Figure 2: Schematic illustration of dislocation in silicon.

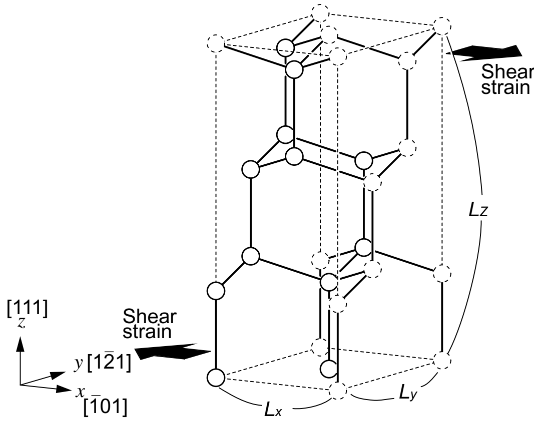


Figure 3: Simulation cell.

sponds to the slip direction of the dislocations, is applied to the cell. As discussed in the next section, two factors such as (1)the normal stresses, and (2)the inner displacement of atoms in the cell, strongly affect the mechanical property of silicon. Therefore, three types of simulation are conducted:

[**Simulation 1**] Shear deformation keeping the cell volume. Inner displacement is not taken into account.

[**Simulation 2**] Shear deformation under the normal stresses of zero. The inner displacement is not taken into account.

[**Simulation 3**] Shear deformation under the normal stresses of zero. The inner displacement is taken into account by relaxing atom position.

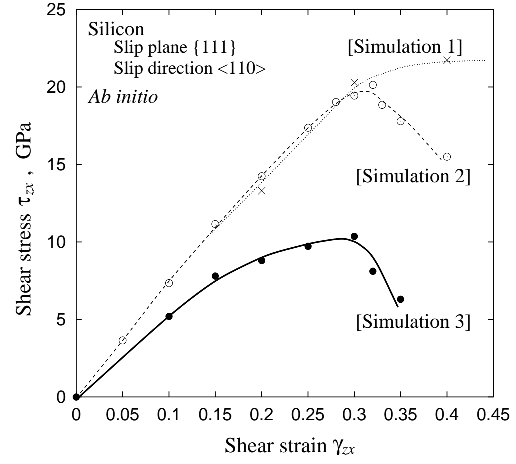


Figure 4: Stress-strain curve in the shear of silicon single crystal.

Simulation precedures are as follows:

[**Simulation 1**] Shear strain, γ_{zx}, is applied to the cell while its width (L_x), depth (L_y) and height are kept constant. The atoms are fixed at the perfect lattice points in the sheared cell.

[**Simulation 2**] At each shear strain, the normal strains (the width, depth and height) are adjusted for reducing the normal stresses by the trial and error. The atoms are fixed at the perfect lattice points in the sheared cell.

[**Simulation 3**] At each shear strain, the normal strains are adjusted for the normal stresses to be zero and relaxed configuration of the atoms due to internal displacement is found by molecular dynamics calculation, where the atomic temperature, T, is controlled to be 50K by velocity scaling method every step and kinetic energy is removed every 10 steps.

In the [Simulation 2] and [Simulation 3], the normal strains are adjusted until all the normal stresses in the x, y and z directions after the relaxation process of the atomic configuration become under 0.5GPa.

3 Result and discussion

Figure 4 shows the stress-strain relation under the shear deformation. Here, the stress is evaluated by the Nielsen's method[10]. The symbols "X" (dotted line) indicate the result in [Simulation 1] without the normal-stress control and the internal relaxation. The stress continues to increase even at the shear strain of 0.4 and the magnitude of stress reaches 22GPa. In [Simulation 2] under the normal-stress control shown by the open circles (dashed line), the $\tau_{zx} - \gamma_{zx}$ relation is in good accord with that in [Simulation 1] up to $\gamma_{zx} = 0.3$. However, the stress turns to decrease after the shear strain exceeds 0.3. Figure 5 shows the normal stresses observed in [Simulation 1]. The normal stress in [Simulation 1] keeps 0 up to shear strain of 0.3. However,

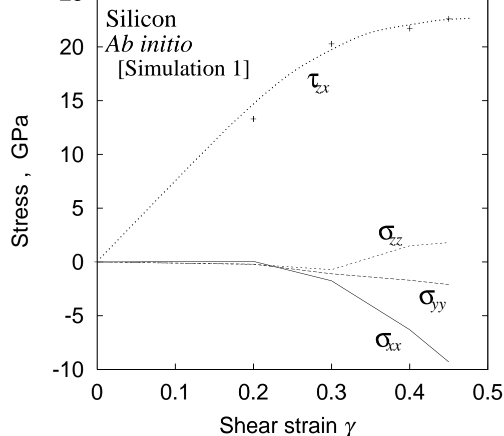


Figure 5: Change in the normal stresses during the shear deformation in [Simulation 1].

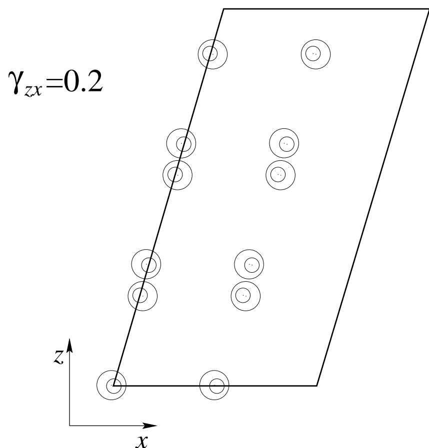


Figure 6: Atom configuration before (smaller circles) and after (larger ones) the internal relaxation at γ_{zx} = 0.2.

beyond the shear strain of 0.3, the normal stresses in [Simulation 1] deviate from 0 and concurrently its shear stress is different from that in [Simulation 2] as shown in Fig.4. This points out that the normal stresses strongly affect on the shear behavior at high strain.

The $\tau_{zx} - \gamma_{zx}$ relation after the relaxation of atom configuration in the cell ([Simulation 3]) is shown by the solid circles (solid line) in Fig. 4. Compared with the result in [Simulation 2], the shear stress is much lower at the same mugnitude of strain, and the relation deviates from the linearity at smaller strain. Figure 6 shows the comparison of the atom configurations projected on the $x - z$ plane in the cell before and after the internal relaxation at $\gamma_{zx} = 0.2$. Though there is little difference in the location of atoms, the subtle configuration remarkably changes the mechanical behavior of silicon.

From the inclination in the linear region of $0 < \gamma_{zx} < 0.1$ in [Simulation 3], the shear elastic coefficient in the $[\bar{1}01]$ direction is roughly estimated as 52GPa. Although the shear modulus evaluated in another report is 64.5 GPa[11], the direction was not described. Because the anisotropy and the internal displacement have to be taken into account for the exact behavior of Si in the specific direction, it is not appropriate to discuss the comparison, here.

Figure 4 also shows that the peak stress (the ideal shear strength of silicon single crystal) is at $\gamma_{zx} = 0.3$ about 10GPa at 0K. An experiment was conducted by Ohta *et al*[12] to elucidate the critical shear stress of the dislocation nucleation at a notch root in silicon substrate at $T = 1173$ K. The criterion measured was about 2GPa. Considering the temperature dependence, the ideal shear strength might be a reasonable candidate of the criterion.

Figure 7 shows a three-dimensional image of the bonds (high charge density regions) between atoms (white spheres) in the simulation cell. The brown cylinders indicate the surface with the charge density of $\rho = 0.073$a.u.$^{-3}$. Each atom possesses four bonds, and three of them, A, B and C, are depicted in the figure. The break of bond A is evidently observed at $\gamma_{zx} = 0.3$ though the other bonds, B and C, won't be disrupted. Moreover, the bond B becomes thicker as the strain grows while the bond C stays in the similar size. This means that the charge transfers from the bonds A to B during the shear deformation. Especially, the remarkable growth of bond B takes place during $\gamma = 0.2 \sim 0.3$, when the stress-strain relation deviates from the linearity. In other words, the charge transference brings about the decrease of elastic coefficient and weakens the resistance against the shear deformation. This also corresponds the moment when the inner displacement of atom position in the cell begins to increase.

Change in density of states (DOS) during the shear deformation in [Simulation 3] is shown in Fig. 8. There is the band gap of about 0.6eV at initial, which is about half of the magnitude experimentally observed (1.17eV). It has been reported that the calculation on the basis of the LDA used in this simulation usually underestimates the magnitude of band gaps[9,13]. However, this is good enough for our purpose that is to comprehend qualitatively the effect of shear deformation on the electronic property. The gap gets narrow as the strain increases, and it disappears when the shear strain reaches 0.2. This points out that the deformation deteriorates the electronic property of the silicon crystal. Attention should be paid that the break down takes place at much smaller shear strain than that at the maximum stress ($\gamma_{zx} = 0.3$). This suggests that the electrical deterioration may appear before the disorder of atomic configuration introduced by the dislocation nucleation.

4 Conclusion

In order to evaluate the ideal shear strength, homogeneous shear deformation of silicon single crystal (slip

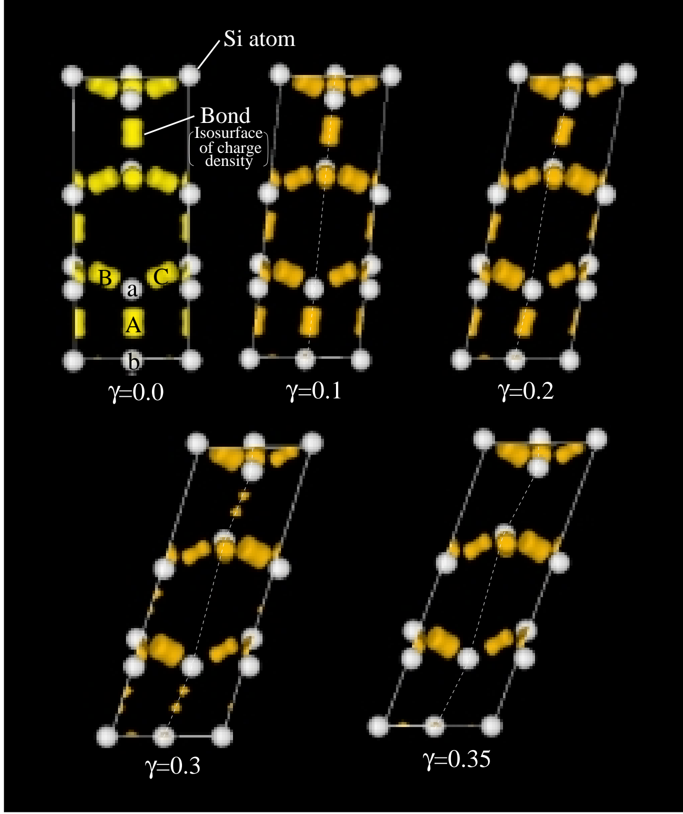


Figure 7: Change in bonds during the shear deformation.

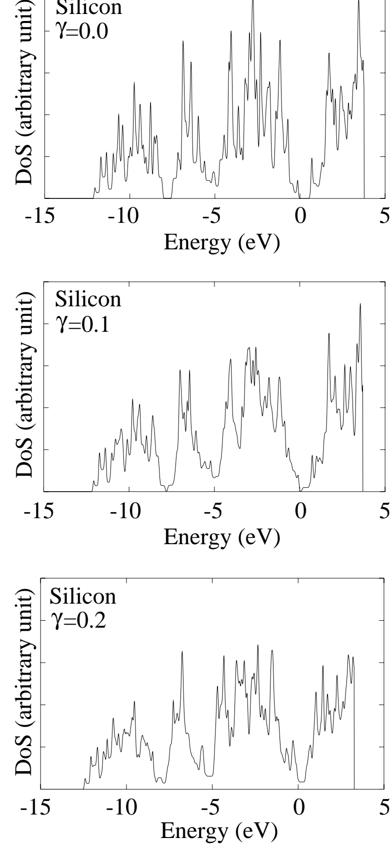


Figure 8: Change in density of states during the shear deformation.

plane: (111), slip direction: [$\bar{1}$01]) is simulated by the *ab initio* method. The results are summarized as follows:

1) The lattice constant at the equiribrium state evaluated by the *ab initio* calculation coincides well with the experimental one.

2) The shear elastic constant evaluated by the *ab initio* calculation shows fairly good agreement with the experimental data. 1) and 2) prove the validity of the simulation.

3) The normal stresses strongly affect the critical shear strain which gives the maximum shear stress.

4) The inner displacement in the crystal is subtle but it remarkably affects on the shear stress.

5) The ideal shear strength is evaluated as 10GPa taking into account the normal stresses and the inner displacement.

6) The band gap of silicon crystal disappears at $\gamma \sim 0.2$. This means that the electronic property is more sensitive to the shear strain than the mechanical one.

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