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Tensile response of bi-crystalline Si nanofilms with twist and tilt grain boundaries

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ABSTRACT

This present work studies the effects of grain boundaries (GBs), notches and temperature on the mechanical properties of silicon (Si) nanofilms via molecular dynamics simulations. Both $\sum 25\,(710)\langle 010\rangle$ tilt and $\sum 25(001)\langle 001\rangle$ twist GBs are considered. It is found that the single-crystalline Si nanofilm has relatively low fracture strength of ~11.6 GPa at room temperature, and fracture occurs through the dislocation sliding mechanism regardless of the existence of notches. At the same temperature, the bi-crystalline Si generally has lower fracture strength than that of the single-crystalline due to the presence of GBs, which changes the crystallographic orientation of the Si nanofilms. Moreover, strength of the bi-crystalline Si depends on the type of the GBs, and it fractures through either the dislocation sliding or cleavage mechanism, depending on the presence of notches. The temperature reduces the fracture strength of the nanofilms but does not change the failure mechanism.

1. Introduction

In the recent years, integrated circuit (IC) packaging has been moving towards three-dimensional (3D), which involves the stacking of chips to achieve a smaller system size. The advantages of 3D ICs over the conventional ICs include increased function density, reduced package profile and interconnect length and enhanced electrical performance [1].

Silicon (Si) is the most fundamental material used in 3D ICs and its properties are essential to their functionality and performance. As the system size approaches the nanoscale level, properties of Si are strongly influenced and can no longer be predicted from those obtained from its bulk phase [2–6].

In addition, like many crystalline materials, Si may have many intrinsic defects, such as grain boundaries (GBs), point defects and dislocations. It can also contain extrinsic defect, such as cracks, caused by mishandling, manufacturing and operating processes [7]. These structural defects can significantly influence the deformation process and the subsequent failure mechanism [8–10]. The effects of these structural defects on the material properties can be even more impactful at nanoscale.

Furthermore, the increase in vertical integration and reduction in size of these 3D ICs have resulted in high density interconnection, giving rise to an increase in heat density during operation. Generally, 3D ICs consist of multi-layers of different materials. When subjected to high heat density, Si experiences thermomechanical stresses as a result of the difference in coefficients of thermal expansion between these layers. Under such stresses, the mechanical properties of Si can be weakened and eventually lead to failure of the ICs. Hence, the performance of the 3D ICs will be adversely affected. Therefore, it is important to study the mechanical properties and fracture behaviour of Si under stresses at the nanoscale level to improve the reliability of these 3D ICs.

So far, many studies have been conducted to understand the mechanical properties of Si. Kim et al. [2] studied the influence of polycrystalline size and anisotropy of Si on its effective elastic constants. The results showed that when polycrystalline size decreases and anisotropy increases, there is a large scatter of elastic constants. Kozhushko et al. [11] measured the critical fracture strength of single-crystalline Si along different crystallographic directions and the determined critical strength varied between 5 and 7 GPa. Liu and Shen [12] investigated the effect of axial orientation and surface condition on the yield strength of Si nanowires (NWs). The results demonstrated that different crystallographic directions lead to different failure mechanisms. Moreover, they showed that the yield strength is dependent on the size and crystallographic direction. This disparity among fracture behaviours signifies that the crystallographic orientation plays an important role in competition with surface effect. Ivashchenko et al. [13] also found that the

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enhancement of mechanical properties of the homopolar nanocrystalline Si structures is attributed to their deformation anisotropy.

Kuo et al. [14] showed that the presence of vacancy defects has marginal effect on the mechanical and fracture behaviours of Si NWs. When the cross sectional of the NWs decreases, vacancy defects can considerably weaken the ultimate strength of these NWs. Kim et al. [15] studied the effects of temperature and tilt angle on the structural order of tilt GB structure in silicon oxide.

In spite of these previous works, little is known about the effects of structural defects, particularly the GBs, on the mechanical properties of Si. The coexistence of multiple types of defects is seldom considered and the coupling effect between temperature and these defects are still not fully understood. Therefore, this work is devoted to studying the effect of GBs, notch and temperature on the mechanical properties and fracture behaviour of crystalline Si nanofilms at the nanoscale via molecular dynamics (MD) simulation. Both $\sum 25(710)\langle 010\rangle$ tilt GB and $\sum 25(001)\langle 001\rangle$ twist GB are considered. The stress–strain curves are plotted and the deformation processes are examined to analyse and explore failure mechanisms.

2. Modelling

Fig. 1 shows the computational cells for the notched single- and bi-crystalline Si nanofilms with $\sum 25(001)\langle 001\rangle$ twist GB or $\sum 25(710)\langle 010\rangle$ tilt GB. The dimension of the computational cells is set as $15.3 \times 3.8 \times 54.3$ nm. The GBs are arranged to be parallel to the x-y plane (Fig. 1b). The grains of the bi-crystals are of the same size. The $\sum 25$ twist GB is constructed by using the coincident site lattice (CSL) model through rotating the upper grain by +8.13° and the lower grain by −8.13° about the [001] axis, as shown in Fig. 2a. Similarly, for the $\sum 25$ tilt GB, the upper and lower grains of the cell are rotated at the angles of +8.13° and −8.13° about the [010] axis, respectively (Fig. 2b).

A penetrating notch along the y-direction is introduced on the left surface (parallel to the y–z plane) of the nanofilm and located on the same x–y plane as that of the GB introduced. The notch has a depth of $2a$ with a being the lattice constant of bulk Si. Periodic boundary conditions are applied in both y- and z-directions, while free boundary condition is used along the x-direction to model an infinite large thin film. The simulations are conducted by using the large-scale atomic/molecular massively parallel simulator (LAMMPS). The atomic interactions between the Si atoms are described by *the Stillinger–Weber* (*SW*) potential [16].

During the simulations, the initial structures are first relaxed to obtain the state with minimum local potential energy. Afterwards, the system is equilibrated at constant 300 K and zero normal stress tensor components by using isothermal–isobaric (NPT) ensemble for 40 ps. Upon achieving equilibration, the system is switched to constant volume and temperature (NVT) ensemble and the uniaxial tensile strain is applied along the z-direction at a constant strain rate of 10^8 s^{-1}. The tensile strain on the nanofilm is realized by deforming the simulation cell with the same strain rate along the z-direction.

As the free boundary condition is applied in the x-direction, the volume of the specimen may vary during the deformation process, despite NVT ensemble being employed.

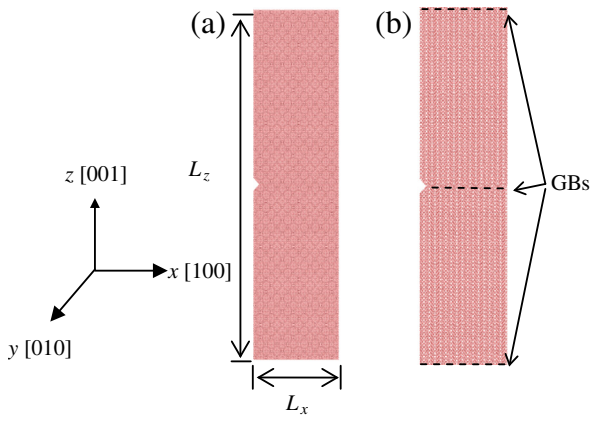

Fig. 1. Computational cells for notched (a) single-crystalline and (b) bi-crystalline Si nanofilms before deformation.

3. Results and discussion

Fig. 3 shows the stress–strain relations obtained at 300 K for both the Si nanofilms with and without notch. For single-crystalline nanofilms, the stress–strain curves are depicted by lines while for bi-crystalline Si nanofilms by lines and symbols. It is found that for smooth (without notch) single-crystalline nanofilm, the fracture strength is approximately 11.8 GPa which is close to that for the monocrystalline Si thin film subjected to [011] loading (~13 GPa) [17]. The strength of smooth bi-crystalline nanofilm with the tilt GBs is slightly lower (~10GPa), while for the smooth nanofilm with twist GBs, its fracture strength is comparable to that of the smooth single-crystalline nanofilm. This is due to the fact that for both the bi-crystalline nanofilm with twist GBs and single-crystalline nanofilm, the (001) plane is perpendicular to the loading direction, in spite of the change in the crystallographic orientation of the grains due to the twist GB.

With the addition of a notch, the fracture strength of the single-crystalline nanofilm decreases significantly by 40%, resulting in a much lower strength as compared to the bi-crystalline cases. For the bi-crystalline nanofilms with twist GBs, their fracture strength is reduced by ~20%, while those for the nanofilms with tilt GBs stay almost unaffected. In other words, the presence of a notch in the Si nanofilm with twist GBs is more detrimental to its strength than that for the Si nanofilm with tilt GBs.

Interestingly, the slope of the stress–strain curve, i.e., the Young's modulus E, of the single-crystalline nanofilm decreases dramatically with the presence of notch and becomes lower than those of the bi-crystalline nanofilms. Similar phenomenon has previously observed in the MD simulations of fracture behaviours of Si nanofilms with micronotches [18]. This significant reduction in E is probably due to the effect of surface inhomogeneity induced by defects, such as a notch. It is previously found that the elastic constants of Si thin films are lowered by the effect of inhomogeneity near the surface and by the resulted changes of the internal atomic displacement [19].

For the validation of the above simulation results, the Young's modulus E for the single crystalline and bi-crystalline samples are calculated using a theoretical model and compared with the E obtained from the MD simulation. Theoretically, the E of bulk single crystalline Si can be calculated by using the following formula [20]:

$$\frac{1}{E_{hkl}} = s_{11} - 2\left[(s_{11} - s_{12}) - \frac{1}{2}s_{44}\right](m^2n^2 + n^2p^2 + m^2p^2) \quad (1)$$

The terms m, n and p are the "direction cosines": the cosine of the angle between the direction of interest [hkl] and the X-, Y- and Z-axes while the term s_{ij} represents the compliance constant. The values of s_{ij} are obtained from Ref. [20]. The 'effective' moduli of the bulk bi-crystalline structure can be estimated by using the elastic Hooke's law [21]:

$$\mathbf{E}_{eff} = f\mathbf{E}^{\mathbf{I}}(\mathbf{E}^{*})^{-1}\mathbf{E}^{\mathbf{II}} + (1-f)\mathbf{E}^{\mathbf{II}}(\mathbf{E}^{*})^{-1}\mathbf{E}^{\mathbf{I}} \quad (2)$$