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Grain size effects on indentation-induced plastic deformation and amorphization process of polycrystalline silicon

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ABSTRACT

The deformation behavior and amorphization process of polycrystalline and single-crystalline silicon are investigated using molecular dynamics (MD) simulations and compared with the previous nanoindentation experiments. In order to unravel the grain size effect on the deformation mechanism, the indentation simulations of polycrystalline silicon with the different grain sizes are performed, and all grains follow the inverse Hall-Petch relation. The results reveal that Young's modulus of polycrystalline silicon is much greater than Young's modulus obtained in the ⟨1 0 0⟩ direction single-crystalline silicon due to the random crystallographic orientation and strong anisotropy of polycrystalline silicon at nanoscale. The nucleation of amorphization in both single-crystalline and polycrystalline silicon appears always beneath the indenter due to the maximum shear stress, controlling the plastic deformation during the indentation process. The horizontal expansion of amorphization region is faster and larger than the vertical expansion of amorphization region due to two reasons: the limit of indentation stress along the depth direction is compared with along the width direction; the grain boundary is the most possible path of weak connection, and produces the complex stress distribution for the propagation of amorphization region. The smaller grain size leads to the stronger gradient strain, especially in the region of upper surface.

1. Introduction

Silicon has dominated the many microelectronic devices, such as computer systems and solar cells [1]. Before obtaining such devices, the bulk crystal silicon undergoes usually sliced, ground, and polished, to achieve an atomic level surface integrity [2]. However, the complex machining process can introduce the stress concentration, which affects strongly the response of the microelectromechanical systems (MEMS) and nanoelectromechanical systems (NEMS) devices [3]. Hence, a deeply understanding of the nanomechanical response of silicon plays a significant role in increasing the reliability of MEMS/NEMS and improving the technology of microelectronic device manufacturing [2–9].

So far, the nanoscale mechanical response in silicon is investigated by various experimental techniques, such as using in-situ quasistatic nanoindentation [4], scanning spreading resistance microscopy [5], high temperature creep [6], and transmission electron microscopy [7–9]. In addition to the above experiments, the deformation and phase transformation mechanisms of silicon are revealed by some simulations, e.g., finite element method (FEM) [10–13], MD simulation [14–17], and multiscale simulation using quasi-continuum (QC) method [18–20]. Some important theoretical modelings [21–23] also discuss the deformation mechanism of silicon during nanoindentation and nanoscratching. In addition, in brittle materials an ultra-precision material removal process can achieve micro-accuracy and nanometer finish but produces the machining damages [24–27], which contain the visible surface damage formed on the ground surface and the invisible subsurface damage formed below the affected machined zone. However, to date, the effects of grain size on the nanoindentation induced-deformation are still not well understood for brittle materials. The grain size influences significantly the plastic deformation mode, the fatigue resistance, thermal conductivity, and yielding strength revealed by the experiment and theoretical method [28–32].

In the present study, we clarify the grain size effect on the plastic deformation and amorphization process using the MD simulation, which is wide popularity to capture the evolution

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processes of simultaneously microstructures at nanoscale. We also compare the elastic modulus of silicon obtained from MD simulations and experiments, and find that the two results correlate well. In addition, the gradient strain and stress fields generated in the subsurface of substrate control the nucleation and propagation of the amorphization.

2. Computational details and models

Fig. 1 shows the MD simulation models of the nano-grained silicon under the indentation process. The samples containing approximately 717, 810 atoms have dimensions of 81.4 × 65.2 × 2.7 nm^3, where the thickness of the grains is larger than the cutoff distance along the z direction. The diamond indenter containing approximately 344, 427 atoms has a configuration of a cylindrical shape with the radius of 15.0 nm, which could be considered as a rigid body because of silicon substrate much softer than diamond indenter [15,16]. The nano-grained structures are constructed by the Voronoi method [33], where a set of grain centres are randomly built, and the space area closer to a given grain centre compared to other grain centre is filled with silicon atoms in a diamond cubic structure with a randomly selected crystallographic orientation [34]. The nano-grained structures have 10, 30, and 90 grains, and the corresponding average grain sizes are 21 nm, 7 nm, and 2.3 nm. Hence, the samples can be divided into four cases: (1) Case 1, single-crystalline silicon; (2) Case 2, polycrystalline silicon with average grain size of 21 nm; (3) Case 3, polycrystalline silicon with average grain size of 7 nm; (4) Case 4, polycrystalline silicon with average grain size of 2.3 nm. According to the previous work [35], the yield strength of polycrystalline silicon (Case 2-Case 4) complies with the inverse Hall-Petch relation. Periodic boundary conditions are applying along x and z directions, and free boundary conditions are applying along y directions. All the samples are categorized into three parts, namely, Newtonian region governed by Newton's second law, thermostat region for heat dissipation, and boundary region for supporting the substrate (see Fig. 1).

For the nanoindentation process, the three different atomic interactions are used: (1) the Si—Si interaction in the silicon substrate is described by the Tersoff potential [7,14–17,36–38], which is widely used in studying the indentation induced deformation [7,37]. (2) the C—C interaction in the tool is ignored because of a rigid indenter [7,14–16,36]. (3) the Si—C interaction is set by the Morse potential [7,15,36–39], where Morse potential parameters are D = 0.435 eV, α = 4.6487 $Å^{-1}$ and r_0 = 1.9475 Å.

The all MD simulations during the nanoscale indentation are computed by the open-source Large-scale Atomic/Molecular Massively Parallel Simulator code [40]. According to the Maxwell-Boltzmann distribution, the velocities of all atoms are randomly set. The initially temperature of MD simulation is 293 K. Prior to the indentation, sample is first subjected to energy minimization using the conjugate gradient method, and then NVT dynamics are performed for 100 picoseconds in order to the relaxation. A time step is 1 fs, and the indentation at a constant speed of 50 m/s is applied along y-direction. The microstructural evolution is presented via the Ovito software, and the local atomic structure is analyzed by the indentify diamond structure in Ovito [41].

3. Result and discussion

To study the indentation-induced deformation of polycrystalline silicon, the elastic module of single-crystalline and polycrystalline silicon should be investigated in advance, which has been reported to play a key role in the amorphization and phase transformation in fact. The elastic properties of polycrystalline silicon is the macroscopic property dominated by the Si—Si chemical bonding at nanoscale, for example, the increasing number of Si—Si bonds per volume can increase Young's modulus. Here, the expressions of bulk module, shear module, and Young's module can be obtained as follows [42–45]:

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \tag{1}$$

$$G = \frac{1}{2}(G_V + G_R) \tag{2}$$

$$E = \frac{9BG}{3B + G} \tag{3}$$

where C_{11}, C_{12}, and C_{44} are the elastic constants. Voigt shear modulus and Reuss shear modulus are $G_V = (C_{11} - C_{12} + 3C_{44})/5$ and $G_R = 5(C_{11} - C_{12})C_{44}/[4C_{44} + 3(C_{11} - C_{12})]$, respectively.

As shown in Fig. 2, the Young's module and shear module of polycrystalline silicon are larger than that of single-crystalline silicon, while the bulk module and B/G of polycrystalline silicon are smaller than that of single-crystalline silicon. For different grain sizes, there is no obvious difference in Young's module, shear module and bulk module. The results of theory and simulation reveal the maximum value of Young's module of silicon in the ⟨1 1 1⟩ direction, and the minimum value in the ⟨1 0 0⟩ direction [46,47]. Hence, the polycrystalline silicon can possess a considerable amplitude of Young's module due to the random crystallographic orientation and strong anisotropy at nanoscale, in general, much greater than the value of Young's module obtained in single-crystalline silicon along the ⟨1 0 0⟩ direction.

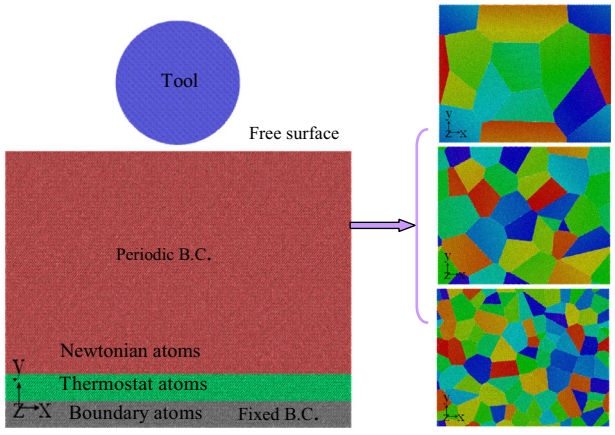

Fig. 1. The MD model of indentation in single-crystalline and polycrystalline silicon.

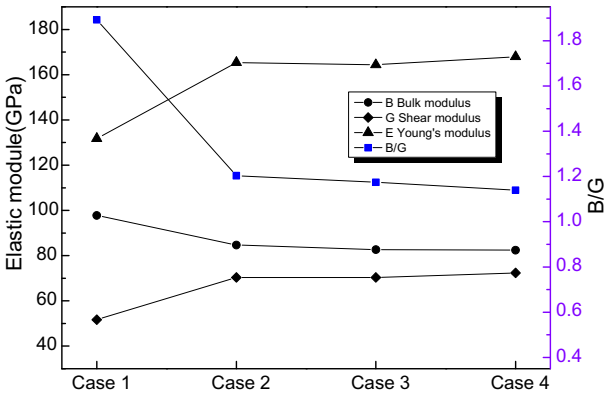

Fig. 2. The elastic module of single-crystalline and polycrystalline silicon.