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Computational Materials Science 30 (2004) 16–20

COMPUTATIONAL MATERIALS SCIENCE

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Computer study of microtwins forming from surface steps of silicon

J. Godet *, L. Pizzagalli, S. Brochard, P. Beauchamp

Laboratoire de Métallurgie Physique de Poitiers, UMR 6630, BP 30179, SP2MI Bld., P. & M. Curie 86962, Futuroscope Chasseneuil Cedex, France

Abstract

A model silicon sample with a free {1 0 0} surface containing atomic steps along the ⟨1 1 0⟩ dense directions has been submitted to a uniaxial compression stress, by numerical simulation. Silicon is modelled using the Stillinger–Weber empirical interatomic potential. An elementary microtwin has been nucleated from this surface step, although the resolved shear stress is in the anti-twinning direction. The microtwin is formed by two perfect 1/6 ⟨1 1 0⟩ 60° dislocations, gliding in two neighboring planes of the shuffle set, and rearrangement of the atoms belonging to the plane of the glide set in-between. An explanation of this plastic event has been found in examining the structures obtained in calculations of bulk silicon submitted to large ⟨1 1 2⟩ {1 1 1} homogeneous shear.

The formation of dislocation at surface defects is a process of particular importance in nanostructured materials submitted to large stresses, such as whiskers or heteroepitaxial thin films (as those used for microelectronic devices). In these nanostructures, the dimensions are too small for the Franck–Read mechanism of dislocation multiplication to operate. The dislocation can then form at surface or interface defects, such as surface steps or cleavage ledges. For instance the formation of dislocation from cleavage ledges has recently been observed during plastic deformation of silicon at low temperature [1].

The very first stages of dislocation nucleation are still out of the scope of experimental investigations, so that the atomic scale simulations are expected to provide useful informations. In a previous study performed on metals [2], it has been shown that dislocations can be nucleated at surface steps under the simple application of a uniaxial stress. As the applied stress increases, the elastic strain concentrates in one of the two {1 1 1} planes passing through the step edge. This localization is characteristic of the pre-nucleation of the dislocation.

In a similar work realized on silicon [3], where a uniaxial tensile stress was applied on a stepped surface, it has been shown, as one could expect, that the behavior of silicon is different from that of metals. The elastic deformations observed in the (1 1 1) planes near the step in silicon, although not

* Corresponding author. Tel.: +33-05-4949-6757; fax: +33-05-4949-6691.

E-mail address: julien.godet@etu.univ-poitiers.fr (J. Godet).

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doi:10.1016/j.commatsci.2004.01.004

quite uniform due to the proximity of the step, are not localized as in metals. However the surface step does have some effect: it weakens the structure, resulting in the fracture of the system in the vicinity of the step for a strain around 22.9%. Nevertheless no dislocation has been formed.

Using the same methodology as in traction, we have investigated the plastic effect of a surface step in a silicon sample submitted to a uniaxial compression stress. The aim of this paper is to discuss the plastic events obtained in the simulation of a compression test, in the light of the computed behavior of bulk silicon sample submitted to large homogeneous shear; both calculations are done with the same interatomic potential.

In this work, a 2×1 reconstructed (1 0 0) silicon surface has been considered. The step is along the $\langle 1\,1\,0\rangle$ dense direction. Periodic boundary conditions have been used along both directions in the surface plane. Two facing steps have been introduced on the free surface to ensure periodic conditions, and the opposite surface has been frozen to represent the bulk crystal. Two different steps have been tested, the rebonded D_B step and the non rebonded D_B step [4]. As the results are similar for these two steps, only the latter is commented. The uniaxial compression stress σ_{22}, contained in the surface plane and normal to the step line direction, is applied through the deformations calculated using linear anisotropic elasticity [5]. To model silicon, the empirical potential of Stillinger–Weber [6] is used. All the calculation presented here are performed at 0 K. More information on the computational methodology can be found in the previous study in traction [3].

Up to a compression strain ϵ_{22} of -7.0% along the stress direction, no modification in the crystal structure is observed. Beyond this limit, plastic deformations occur, initiated at the surface steps (Fig. 1). First, the step edge sinks down into the bulk (Fig. 1B) with the glide events localized in the (1 1 1) planes in the vicinity of the step (Fig. 1C). Finally we can observe the formation of a microtwin (Fig. 1D) which reduces the step height. Note that in the $\{1\,1\,1\}$ planes, the applied compression σ_{22} produces a shear stress oriented along a $\langle 1\,1\,2\rangle$ direction normal to the step, in the anti-twinning orientation. The analysis of the atomic displacements shows that this microtwin has been formed by two edge dislocations with the same Burgers vector, $1/6\,\langle 1\,1\,2\rangle$. Each dislocation has moved, not in the central glide plane, but in the shuffle planes on both sides of the glide plane, thereby forming the microtwin. The central glide plane is transformed into its twinned variant. The denominations shuffle plane and glide plane refer

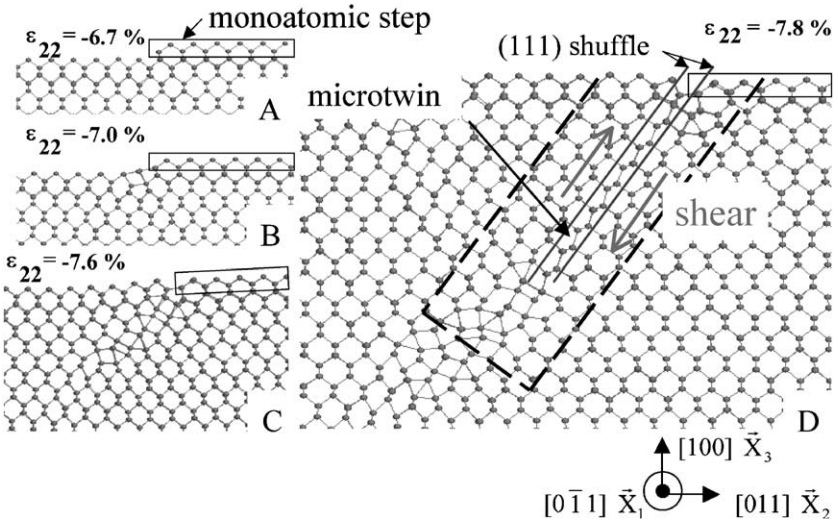

Fig. 1. Evolution of plastic deformations from the non rebonded D_B step, for a uniaxial compression stress. The dashed line delimits the zone shown in Fig. 6.

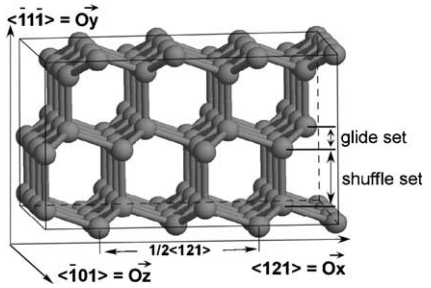

Fig. 2. Cell geometry used for the calculation of sheared bulk silicon.

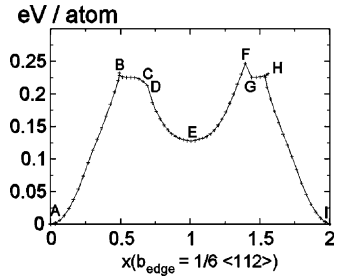

Fig. 3. Energy per atom versus shear amplitude measured by the displacement along the $\langle 1\,1\,2\rangle$ anti-twinning direction, from perfect crystal (A) to twinned crystal (I) (see corresponding geometries in Fig. 4, $\mathbf{b}_{\mathbf{edge}} = 1/6\langle 1\,1\,2\rangle$ see Fig. 5).

respectively to the widely and narrowly spaced $\{1\,1\,1\}$ atomic planes (Fig. 2) after Hirth and Lothe [5].

In order to understand the microtwin formation, we have performed calculations of the bulk silicon sheared in the $(1\,1\,1)$ planes along $\langle 1\,1\,2\rangle$ direction in the anti-twinning orientation. We have considered a periodic bulk system whose axes are $[1\,2\,1]$, $[\bar{1}\,1\,\bar{1}]$ and $[\bar{1}\,0\,1]$ (Fig. 2). Silicon is still modeled using the empirical potential of Stillinger–Weber. The system is increasingly sheared along the $\langle 1\,2\,1\rangle$ anti-twinning direction in the $(1\,1\,1)$ planes by applying a ϵ_{xy} shear in increment of 2.4% strain steps. Only the σ_{xy} stress component must be different from zero so as to get a pure shear; the five other components of the stress tensor must be zero. σ_{xz} and σ_{yz} necessarily vanish due to the crystal symmetry; thus it still remains three independent components of the stress tensor σ_{xx}, σ_{yy} and σ_{zz} to cancel. After each shear increment, the atomic positions are optimized using a simple gradient method and the convergence is reached when the resulting force on each atom is less than 10^{-3} eV/Å. The stress components σ_{ii}, with $i = 1$–3, are cancelled by rescaling the simulation box dimensions along each corresponding direction. This operation set forms a minimization cycle. To relax the system, this cycle is repeated until the energy difference between two cycles is less than 10^{-4} eV/atom.

The energy per atom versus the shear amplitude measured by the displacement along the $\langle 1\,1\,2\rangle$ anti-twinning direction is plotted in Fig. 3. Fig. 4 shows the evolution of the structure during the shearing of the crystal. At the beginning of the

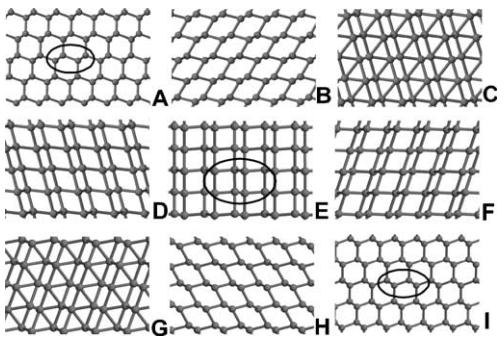

Fig. 4. Snapshot of the bulk structure during the shear process from perfect crystal (A) to twinned crystal (I).

deformation, the crystal is deformed mainly in the $(1\,1\,1)$ planes of the shuffle set with a very slight height reduction of glide and shuffle sets (Fig. 4B). The glide set projection in the plane of the sheet shows two kinds of bonds, a long bond and a short bond, the latter is called a 'trimer' because it binds a silicon atom to two of its nearest neighbors. Fig. 4C and D shows that the shear constrains the 'trimers' of each glide set to pile up. Then, an pseudo-hexagonal phase is obtained by a non shifted stacking of hexagonal planes corresponding to a local minimum of energy (Fig. 3E). In this crystal phase the two atomic planes of the glide set merge in a unique atomic plane. When shearing continues, as seen in Fig. 4F and G, the crystal structure follows a symmetrical path with respect to the (Oy) axis of the structures shown in Fig. 4D and C. In Fig. 5, the formation of new bonds in different stages is detailed. It can be seen that the

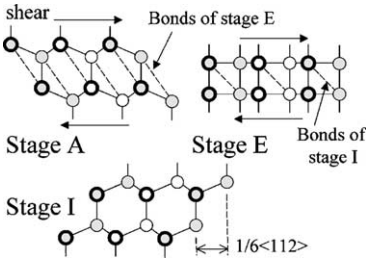

Fig. 5. Ball and stick sketches of the twinning mechanism. The open circles represent atoms contained in the sheet plane. The atoms belonging to the upper plane of the glide set in stage A are shown with bold edges so as to illustrate the inversion of the glide set.

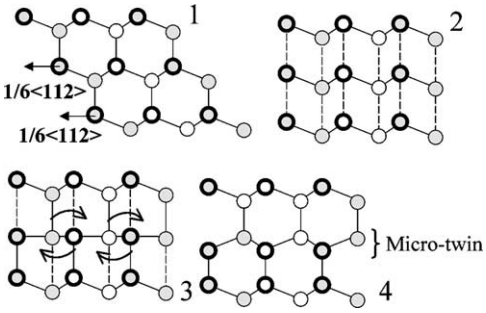

Fig. 7. The stages of the microtwin formation (see caption of Fig. 5).

new bonds in the shuffle set connect two rows initially shifted about 2/6 $\langle 1\,1\,2\rangle$. Finally, the energy curve is quasi-symmetric from the perfect crystal to the twinned crystal. The phase change is obtained by a glide in the shuffle set plane and the rotation of the 'trimers' in the glide set plane, with an intermediate phase where the glide set planes merge in a unique plane.

The different phases of sheared bulk silicon can be compared with the microtwin formation obtained from the surface step on silicon submitted to a uniaxial compression stress (Fig. 6). Before plastic deformation, in the initial stage of the bulk deformation, the crystal structure is the cubic diamond phase (Figs. 4A and 6A). Then the head of the microtwin shows a crystal configuration where the glide set is merged in a unique plane as in the pseudo-hexagonal phase of bulk (Figs. 4E and 6E). Finally, the microtwin shows the same configuration as the twinned crystal after the shear (Figs. 4I and 6I). The trimers of the glide set are the symmetrical to those in the perfect crystal (Fig. 6I and A). This analysis shows that the microtwin has been formed by two dislocations in the lower and upper planes of the shuffle set, with Burgers vectors of 1/6 $\langle 1\,1\,2\rangle$ each, and by the symmetrical inversion of the trimers of the glide set. To form this microtwin a set of two shuffle planes and one glide plane are necessary, as illustrated in Fig. 7. Thus the Burgers vectors in the shuffle sets calculated for the microtwin are twice smaller than those observed for the twinned bulk silicon. This study emphasizes the glide ability of the shuffle set at 0 K.

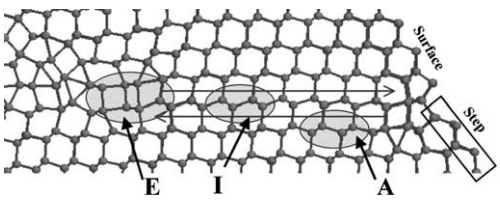

Fig. 6. Zoom on the microtwin obtained during plastic deformation from surface step (Fig. 1).

This findings are in good agreement with the ab initio calculation of the free energies of generalized stacking faults in Si [7]. It shows that the dominant mode of nucleation and motion of dislocations is in the shuffle set at low temperature. Moreover the transmission electron microscopy observations of Rabier et al. [8] seem to show the same behavior when silicon is plastically deformed at low temperature under high confining pressure.

To conclude, when the silicon crystal is submitted to a uniaxial compression stress, a plastic deformation appears for an absolute strain lower than in traction. A microtwin is obtained from the surface step. The study of the sheared bulk silicon explains the formation of this microtwin: it stems from glides in the lower and upper planes of the shuffle set and the rotation of the 'trimers' in the plane of the glide set, with an intermediate phase where the glide set merges in a unique plane. This calculation confirms that at 0 K, the surface step is a favored site for dislocation nucleation in a stressed crystal. Furthermore, in silicon these glide events are localized in the (1 1 1) planes of the shuffle set.

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