Fall 10-6-2015

Toward the understanding of the brittle to ductile transition at low size in silicon: Experiments and simulations

Firas El Nabi
CNRS – University of Poitiers, firas.abed.el.nabi@univ-poitiers.fr

Laurent Pizzagalli
CNRS – University of Poitiers

Sandrine Brochard
CNRS – University of Poitiers

Cristophe Tromas
CNRS – University of Poitiers

Ludovic Thilly
CNRS – University of Poitiers

See next page for additional authors

Recommended Citation

[1] F. Oestlund et al., Adv. Funct. Mat. 19 (2009) 1. [2] J. Rabier et al., Physica Status solidi c 10(2013) 1. [3] F. Abed El Nabi et al., Modelling Simul. Mater. Sci. Eng. 23 (2015) 025010

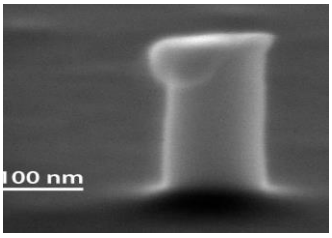
Authors
Firas El Nabi, Laurent Pizzagalli, Sandrine Brochard, Cristophe Tromas, Ludovic Thilly, Julien Godet, Michael Texier, and Olivier Thomas

TOWARD THE UNDERSTANDING OF THE BRITTLE TO DUCTILE TRANSTION AT LOW SIZE IN SILICON: EXPERIMENTS AND SIMULATIONS

Firas Abed El Nabi, Pprime Institute – CNRS – University of Poitiers, FRANCE
firas.abed.el.nabi@univ-poitiers.fr
Laurent Pizzagalli, Pprime Institute – CNRS – University of Poitiers, FRANCE
Sandrine Brochard, Pprime Institute – CNRS – University of Poitiers, FRANCE
Christophe Tromas, Pprime Institute – CNRS – University of Poitiers, FRANCE
Ludovic Thilly, Pprime Institute – CNRS – University of Poitiers, FRANCE
Michael Texier, Département de Physique - Aix-Marseille Université - FRANCE
Olivier Thomas, Département de Physique - Aix-Marseille Université - FRANCE
Julien Godet, Pprime Institute – CNRS – University of Poitiers, FRANCE

While bulk silicon is brittle at temperatures below 600-700K, the compression of nanopillars has shown that a decrease of the diameter below few hundreds of nanometers could change the silicon behavior from brittle to ductile [1,2]. This size effect cannot be explained by the initial defect density like in metals, because pristine silicon nano-objects do not contain residual defects. In these conditions the cracks and/or the dislocations nucleation should take origin at the surface. The identification of the parameters governing the brittle to ductile transition in size and the understanding of the mechanisms are the key points to further develop the MEMS and NEMS technology or to prevent the failure of microelectronic components based on the silicon strained technology. Nowadays the respective improvements in simulations and experiments allow to investigate the mechanical properties of objects of similar sizes, close to hundreds of nanometers. We have then used both approaches - experiments and simulations – to understand the mechanisms at the origin of cracks and dislocations nucleation in such nanopillars. Experimentally, <110> nanopillars with diameters of 100 nm and heights of 300 nm are obtained by lithography. They are deformed in compression by a flat punch nano-indentor under controlled-displacement mode at room temperature, and analyzed by scanning electron microscopy and high resolution transmission electron microscopy. In simulation, nanopillars up to 44 nm in diameter and height are investigated under compression and tension in controlled-displacement too, with a temperature ranging from 1 to 600K. The atomic interactions in silicon are modeled by two different semi-empirical potentials, Stillinger Weber and a Modified Embedded-Atom-Method (MEAM), both fitted to better reproduce the ductile and brittle properties of bulk silicon.

Under compressive load (Fig. 1), both approaches reveal a ductile behavior with similar stress-strain curves, and large shear bands of amorphous silicon along the slip plane. In addition the simulations enlighten the formation of stacking fault plane in the anti-twining shear stress direction at the onset of plasticity, not yet confirmed by experiments (work in progress). The simulations under tensile load (Fig. 2) show the nucleation of perfect dislocations from the surface that can lead to cavity opening when they interact [3]. We observe first that the height of the nanopillars must be higher than 20 nm to allow the cavity opening, and second that the brittle to ductile transition is controlled by the diameter of the nanopillars, as observed experimentally in compression. The deformation of pillars with large diameters operates by cavity expansion leading to the brittle fracture, while pillars with smaller diameters are deformed by dislocations gliding leading to ductile fracture. Finally, the simulations in temperature seem to corroborate the fact that the size of the brittle to ductile transition could increase with temperature, as presumed experimentally [2].



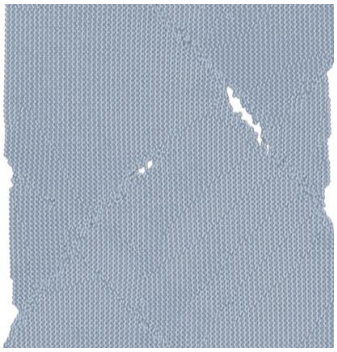


Figure 2: <110> silicon nanopillars under tensile strain at 10K (diameter 44 nm). The simulations reveal cavities formation initiated by dislocations interactions.

Figure 1: <110> silicon nanopillar under compressive strain at room temperature. Left: molecular dynamics (diameter 12 nm), right: experimental nano indentation.

[1] F. Oestlund et al., Adv. Funct. Mat. 19 (2009) 1.
[2] J. Rabier et al., Physica Status solidi c 10(2013) 1.
[3] F. Abed El Nabi et al., Modelling Simul. Mater. Sci. Eng. 23 (2015) 025010.