

NANOMECHANICS

Small-scale transformations

Under shear stress, silicon nanocrystals become amorphous through an intermediate hexagonal crystalline phase.

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There are two long-standing unsolved issues in our understanding of the mechanical properties of silicon at room temperature. One is whether or not pure, silicon single crystals are intrinsically brittle; the second is how important phase transformations are in their room-temperature ductility. It can be shown that as stresses approach the theoretical values for bond breaking, the nonlinear behaviour in the stress versus strain, usually observed prior to fracture, can be due to either phase transformations or dislocation nucleation. Theoretical physicists and material scientists have pondered about the nature of these permanent displacements for decades^{1,2}. But it is now ever more important to characterize them, because they could make the next generation of silicon semiconductors inoperable. Writing in *Nature Nanotechnology*, Scott Mao, Ting Zhu, Chongmin Wang and co-workers now provide important insights on this nonlinear regime with nanoscale precision³. Using a sophisticated experimental set-up that couples an *in situ* electron microscope with a nanomechanical testing device, they reveal that amorphization of a single nanocrystal of silicon at room temperature involves a transitional phase transformation into a hexagonal phase.

The researchers — who are based at the University of Pittsburgh, the Georgia Institute of Technology and the Pacific Northwest National Laboratory — use <100> silicon nanopillars 86 nm in diameter and apply shear stress to induce amorphization. It is notoriously difficult to induce amorphization of the hexagonal crystalline phase due to the ease of motion of partial dislocations in the {111} slip systems that results in a plastic deformation that relaxes the rise in stresses. The researchers observed the sequence of the mechanical deformations inside a high-resolution transmission electron microscope while using diffraction contrast methods to follow the evolution of secondary phases, dislocations and amorphous islands.

The main finding was that the normal diamond-cubic structure of silicon changes to metastable hexagonal silicon possessing the same unit-cell structure observed at high pressure (Fig. 1a). Within this structure,

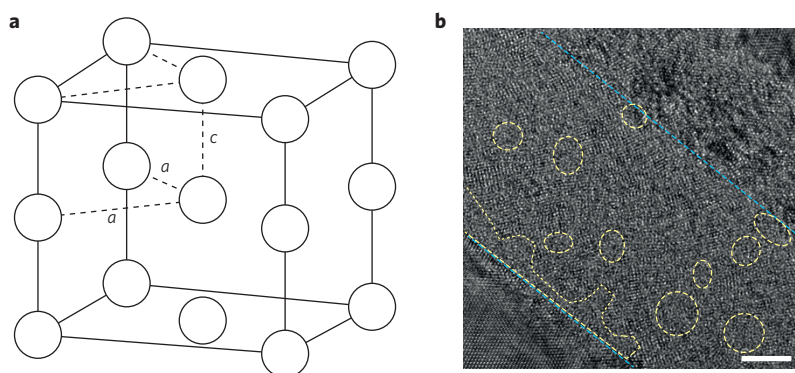


Figure 1 | Hexagonal silicon in nanostructures under shear stress at room temperature. **a**, The lattice structure of hexagonal silicon with $a = 0.255$ nm and $c = 0.239$ nm, with $2c$ the vertical dimension⁶. **b**, Formation of amorphous silicon domains (yellow) in a hexagonal silicon shear band (blue). Scale bar, 5 nm. Panel **b** reproduced from ref. 3, Nature Publishing Group.

dislocations are formed that do not glide. Therefore, when the shear stresses approach the theoretical limit, the crystal lattice becomes amorphous (Fig. 1b). A dislocation density of roughly $4 \times 10^{16} \text{ m}^{-2}$ is sufficient to cause the amorphous transition.

The implications of this finding could be profound for any device using silicon crystalline nanostructures, including future 10, 7 or 5 nm technology for three-dimensional silicon transistors — expected for commercialization in about 10 years. For these devices, important mechanical complications have already been identified, and discussed within the community. Since amorphous silicon might form in these systems, how would properties such as strength and ductility respond? For example, one could start with a diamond-cubic crystalline silicon and decide to include a certain percentage of a different allotrope (say, a hexagonal phase) or even amorphous silicon to achieve certain, unique properties. (An analogous line of thinking has already been used at the micrometre scale about 30 years ago when researchers found that controlled crystallization of amorphous phases improved fracture toughness in silicon nitride⁴.)

Another possible scenario could be playing with silicon purity. It is known for example that phosphorus or arsenic atoms, as n-dopants, or hydrogen atoms can have

a large effect on the activation energies and activation velocities of dislocations. Here, temperature-dependent experiments should be able to provide valuable information⁵, which, in conjunction with computational approaches, similar to the one used by Mao and colleagues, can in principle enable identifying the right atomic compositions to achieve a desired mechanical property.

Overall, the work of Mao and colleagues, and in particular their instrumental approach, might just be the proverbial tip of the iceberg for what is to come in our understanding and controlling of the mechanical properties of silicon and other materials at the nanoscopic level. □

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