Seeing silicon crystal transform to amorphous

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A team of researchers led by the University of Pittsburgh's Scott X. Mao has observed at atomic scale a previously unknown mechanism of shear-driven crystal to amorphously transform in silicon. The paper "In situ observation of shear-driven amorphization in silicon crystals," published in *Nature Nanotechnology*, represents a milestone in the in situ study of amorphization of silicon.

Shear-driven amorphization has been observed in large-scale covalently bonded materials during contact loading and/or severe plastic deformation such as surface scratching, indentation, and ball milling. However, the underlying mechanism of this transformation and its interplay with other deformation mechanisms such as dislocation slip was unknown.

"We chose silicon because it is widely applied in MEMS and electronics and its diamond-cubic structure is representative of other semiconductor materials," said Mao, the paper's corresponding author and William Kepler Whiteford Professor in the Department of Mechanical Engineering and Materials Science within Pitt's Swanson School of Engineering. "This knowledge is crucial to help control the crystal to amorphously transform in the synthesis of amorphous silicon and application of silicon crystals. It also holds broad implications for other covalently bonded materials, especially diamond-cubic structured materials."

By using state-of-the-art in situ atomic-scale transmission electron

microscopy, Mao's team at Pitt showed that shear-driven amorphization in diamond cubic silicon is led by a shear induced phase transformation to diamond hexagonal silicon, and dislocation nucleation dominated deformation in the latter phase that resulted in amorphous silicon.

To better understand the dependence of this amorphization mechanism to loading orientations, Ting Zhu conducted advanced computer simulations using molecular dynamics that showed the mechanical behavior of the silicon nanostructure at the atomic level. Zhu is a professor in Georgia Tech's George W. Woodruff School of Mechanical Engineering and School of Materials Science and Engineering. Zhu's simulation revealed distinct active dislocation modes prior to amorphization in silicon nanopillars under different loading orientations.

Such atomic-scale observation had not been possible in the past due to the brittle nature of bulk silicon and difficulties in maintaining the conditions for atomic-scale TEM imaging during continuous mechanical straining.

"By reducing the size of covalent crystals to nanoscale, we eliminated fracture-producing flaws and acquired relatively high deviatoric stress in the silicon crystal. This opens up new opportunities for studying amorphization without a need of pressure confinement," said Mao. "The silicon nanopillars used in our study were epitaxial fastened on silicon wafer. This sample geometry, combined with advanced nanomanipulation techniques, enables very stable sample orientation required for high resolution TEM imaging during continuous compression of the silicon crystals at high stress level."

The techniques demonstrated in this study provide a powerful method for future study of mechanical responses in covalently bonded materials. "Our atomic-scale observation provides unprecedentedly detailed information of how silicon deform and transform to amorphous; it

should motivate further experimental and modeling investigation of mechanical responses in covalently bonded materials," said Mao.

Other researchers in this study include Chongmin Wang, a senior scientist at the Environmental Molecular Sciences Laboratory at the Pacific Northwest National Laboratory; Yang He and Li Zhong, Pitt Ph.D. students in Mao's lab; and Feifei Fan, a former Georgia Tech Ph.D. student in Zhu's lab and current assistant professor at the University of Nevada, Reno.

More information: Yang He et al. In situ observation of shear-driven amorphization in silicon crystals, *Nature Nanotechnology* (2016). DOI: 10.1038/nnano.2016.166

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