Dislocation creates 'whirlpool' that pulls surface atoms into crystal

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6/7/04 CHAMPAIGN, Ill. — Developing novel ways to control the motion of atoms on surfaces is essential for the future of nanotechnology. Now, researchers at the University of Illinois at Urbana-Champaign have found a phenomenon of dislocation-driven nucleation and growth that creates holes that spiral into a surface and pull atoms into crystalline solids.

The newly discovered mechanism – identified as a series of spiral steps around dislocations terminating at the surface of titanium nitride, a technologically important material used in microelectronics and hard coatings – could potentially be put to use in controlling surface morphology and in preparing nanoscale structures on surfaces.

“The spiral step dynamics strongly suggests that the cores of surface-terminated dislocations behave like ‘whirlpools’ sucking surface atoms into the crystal structure,” said Suneel Kodambaka, a postdoctoral research associate and lead author of a paper that announced the team’s findings in the May 6 issue of the journal Nature.

Dislocations are imperfections in a crystal structure where there is a missing or an extra half plane of atoms in the lattice. Dislocations can strongly influence nanostructural and interfacial stability, mechanical properties and chemical reactions.

“We found that the presence of a dislocation could reverse the behavior and evolution of the nearby surface substructure,” said Ivan Petrov, a research professor and director of the Center for Microanalysis of Materials at the Frederick Seitz Materials Research Laboratory on the U. of I. campus.

To study the dynamics of dislocation motion and morphological evolution in single crystals at high temperature (1,300 to 1,400 degrees Celsius), the researchers used low-energy electron microscopy – a technique that can visualize the surface at the atomic level.

“We saw steps form at the dislocation site and expand into spiral structures,” Kodambaka said. “This type of spiral growth had been seen previously under applied stress, and when depositing or evaporating material; but never during annealing, when the crystal is neither gaining nor losing material.”

Resembling steps on a spiral staircase, each step was one layer of atoms thick and rotated around the dislocation core. The spiral slowly spun while growing inward, like a bathtub drain sucking water.

“The dislocation provides a path for atoms to move from the surface to inside the crystal,” Petrov said. “The spiral structure is a manifestation of the moving material. It is a vortex that consumes surface atoms and drives the nearby surface kinetics.”

The researchers’ results “provide fundamental insights into mechanisms that control both the stability of nanostructures and the formation of nanoscale patterns on surfaces,” Kodambaka said. “We think this spiral growth process is quite general and will be observed in many other materials.”

In addition to Kodambaka and Petrov, the research team included materials science and engineering professor Joseph Greene, electron microscopist Waclaw Swiech and postdoctoral research associates

Sanjay Khare and Kenji Ohmori. The U.S. Department of Energy funded the work.

The original press release can be found here.