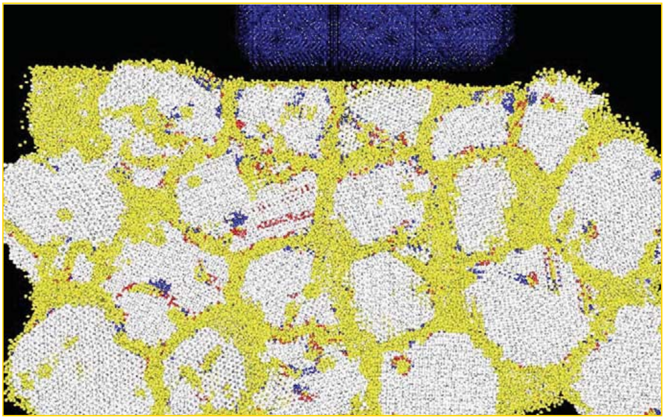
Simulations probe superhard ceramics

MECHANICAL BEHAVIOR



Atomic simulations show the competition between crystallization and disordering in nanocrystalline SiC near the nanoindenter. (Courtesy of Izabela Szlufarska.)

Researchers at the Universities of Wisconsin, Madison and Southern California have used a computer simulation involving nearly 19 million atoms to help understand deformation mechanisms in superhard nanocrystalline ceramics [Szlufarska *et al.*, *Science* (2005) 309, 911].

While normal ceramics are brittle, nanostructured ceramics have been observed to show high hardness, fracture toughness, and superplastic behaviour. These properties could be very useful in applications from automobile engines and high-speed machining tools to medical implants.

The unique mechanical response of nanocrystalline ceramics is believed to result from the large volume of disordered grain boundaries (GBs) in these materials. Indeed, the materials can be thought of as having two coexisting phases: brittle crystalline grains and soft amorphous GBs.

The simulation involved indenting a nanocrystalline SiC substrate with grains averaging 8 nm in diameter using a square indenter 160 x 160 x 72 Å^3 in size. The resulting atomic motions and interactions were observed for different indentation depths. Izabela Szlufarska and colleagues identified a point in the nanoindentation load-displacement curve where the response changed.

"Initially, the grains all move together because the GBs hold them together like glue," explains Szlufarska. Then, at a critical indentation depth, there is a crossover from the cooperative response of coupled grains to the sliding and rotation of individual grains. This happens when the GBs yield plastically. "Because the GBs are flowing, the material is more ductile than normal ceramic would be," says Szlufarska. "As the GBs take part of the deformation, so in essence they protect the grains from breaking."

Two competing mechanisms are operating in the nanocrystalline SiC: crystallization of atoms at the GB edges and disordering of atoms in the grains. There is a clear switch at the crossover point from deformation dominated by crystallization to that dominated by disordering.

The group is able to estimate the hardness of the nanocrystalline SiC from the simulations, gaining a value of 39 GPa. This is in line with experimental values for the material's superhardness of 30-50 GPa for samples with grain sizes of 5-20 nm.

The researchers hope to learn how to control this crossover point to engineer greater hardness without compromising the pliability of nanocrystalline ceramics. This could involve varying the GB volume and grain size, or adding impurities or dopants.

Jonathan Wood

Coatings release corrosion inhibitors on demand

METALS & ALLOYS

One method of corrosion protection is the slow, controlled release of corrosion inhibitors when needed. Chromate conversion coatings have this property, releasing chromate ions when corrosion initiates and stopping when no longer required. While such coatings have been the first line of defense for Al structures in aircraft since before World War II, they are due to be phased out because chromate ions are carcinogenic and highly toxic.

A team at the University of Virginia have invented a family of amorphous Al-Co-Ce alloys that act as multifunctional corrosion protection coatings [Jakab and Scully, *Nat. Mater.* (2005) **4** (9), 667]. The alloys provide a tunable supply of environmentally friendly corrosion inhibitors in response to a pH change, as well as serving as a barrier and a sacrificial anode.

The researchers coated a structural Al alloy with their protective amorphous Al-Co-Ce alloy. A scratch was introduced into the coating and the sample placed in an aqueous solution. The team showed that corrosion of the underlying Al changed the pH of the solution. This prompted dissolution of the amorphous alloy, releasing the corrosion inhibiting ions. The ions migrate to the damage site and suppress the corrosion damage on reaching a critical concentration. When the corrosion stops, the pH of the solution returns to neutral and the dissolution of the Al-Co-Ce alloy returns to a low level.

The researchers found that the new alloy was able to protect Al in the presence of a corrosive, acidic solution. The released inhibitors greatly reduced pitting and decreased pit size. This is very important for prolonging the fatigue life of components.

"In theory, this could be a field-replaceable coating for aircraft fuselage and wing skins, as well as a coating for landing gear, etc." says John Scully. The coating could be applied to damaged or repaired areas using thermal spray methods or laser surface glazing, for example. "Our next step is to try some of these application methods on mimics of real parts and see if it protects against corrosion," says Scully. "Lab results so far have been promising."

Jonathan Wood