A safe reaction

NUCLEAR

Nuclear reactors might one day be constructed using materials that can self-heal following radiation damage, thanks to a materials study by scientists at Los Alamos National Laboratory.

In computer simulations, the LANL scientists have observed a surprising mechanism that allows copper nanocrystalline materials to heal themselves after suffering radiation-induced damage. [Bai *et al.*, *Science* (2010) 327, 1631]. The phenomenon exploits the mix of grains and the grain boundaries between them in such materials.

An important considering in the design, construction and operation of nuclear reactors is the effect of high levels of radiation on the materials from which the reactor is constructed. In addition to constant bombardment, reactor materials might also be exposed to high temperatures, physical stresses, and corrosive conditions. Radiation itself can cause dislocations and interstitial atoms and vacancies to form that insidiously weaken the structure at the nanoscale. The accumulation of defects leads to swelling and hardening leading to brittleness and the potential for catastrophic failure.

Nanocrystalline materials contain a large fraction of grain boundaries, which can absorb and remove defects, and so scientists presumed that such materials might be more radiation tolerant than equivalent materials with larger grain sizes. However, few specific details have been obtained regarding the complex behaviour of such solids under different conditions.

Xian-Ming Bai and colleagues explain that they have now used three atomistic simulation methods to investigated defect-grain boundary interactions in copper on the picosecond to microsecond timescales. They found that grain boundaries have a surprising "loading-unloading" effect in which irradiation leads to interstitials being loaded, or trapped, in the boundary on the short timescale. The loaded boundary then acts as a source unloading, or emitting on the long timescale, interstitials back into the bulk, which eradicates vacancies. The simulations reveal that this recombination mechanism, "has a much lower energy barrier than conventional vacancy diffusion and is efficient for annihilating immobile vacancies in the nearby bulk". The net effect is the surprising self-healing, the efficient annealing, in other words, of material defects caused by radiation exposure.

The team adds that this "loading-unloading" role of grain boundaries might explain the behaviour of irradiated nanocrystalline materials that runs counter to expectations, but more importantly could provide new opportunities for engineering nanocrystalline materials to be self-healing in high-radiation environments.

Team member Blas Pedro Uberuaga told *Materials Today* that the researchers have compared their simulated data with literature experiments, which he says explains very nicely those results. "In terms of more direct validation, we have some experiments in progress on Au and on metal composites (Cu/Nb), that will indirectly connect to these results, but may or may not be able to directly validate these simulation results. So, we have ongoing experimental activities in related areas," he adds.

David Bradley

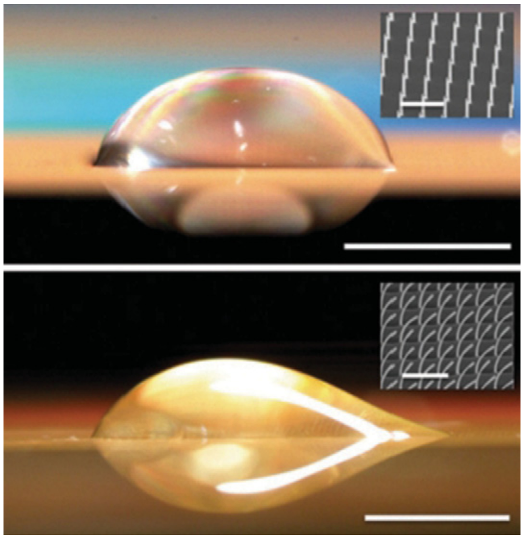
Pushing droplets around

SURFACE SCIENCE

Controlling the way liquids spread across a surface is important for a wide variety of technologies, including DNA microarrays for medical research, inkjet printers and digital lab-on-a-chip systems. But until now, the designers of such devices could only control how much the liquid would spread out over a surface, not which way it would go.

New research from mechanical engineers at MIT has revealed a new approach that, by creating specific kinds of tiny structures on a material's surface, can make a droplet spread only in a single direction [Chu *et al.*, *nature mat.* (2010), doi:10.1038/nmat2726].

The system is completely passive, based on producing a textured surface with tiny pillars shaped in specific ways to propel liquid in one direction and restrict its movement in others. Once the surface is prepared, no mechanical or electrical controls are needed to propel the liquid in the desired direction, and a droplet placed at any point on the surface will always spread the same way.



Symmetrical droplet and, asymmetrical droplet. Courtesy Chu et al.

The chips used for testing were made by etching a silicon wafer surface to produce a grid of tiny pillars, which then were selectively coated with gold on one side to make the pillars bend in one direction. To prove that the effect was caused just by the bent shapes rather than some chemical process involving the silicon and gold, the researchers coated the surface with a thin layer of a polymer so that the water would only come in contact with a single type of material. The pillars are all curved in one direction, and cause the liquid to move in that direction.

The researchers comment, "while this work is still early-stage basic research, in principle such systems could be used for a wide variety of applications. For example, it could provide new ways to manipulate biological molecules on the surface of a chip, for various testing and measurement systems. It might be used in desalination systems to help direct water that condenses on a surface toward a collection system. Or it might allow more precise control of cooling liquids on a microchip, directing the coolant toward specific hotspots rather than letting them spread out over the whole surface".

Jonathan Agbenyega