

# Model simulates atomic processes in nanomaterials

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Researchers from MIT, Georgia Institute of Technology and Ohio State University have developed a new computer modeling approach to study how materials behave under stress at the atomic level, offering insights that could help engineers design materials with an ideal balance between strength and resistance to failure.

When designing materials, there is often a tradeoff between strength and ductility (resistance to breaking)--properties that are critically important to the performance of materials.

Recent advances in nanotechnology have allowed researchers to manipulate a material's nanostructure to make it both strong and ductile. Now, the MIT-related team has figured out why some nano-designed metals behave with that desirable compromise between strength and ductility.

The team, led by Subra Suresh, the Ford Professor of Engineering in the Department of Materials Science and Engineering, developed a simulation method derived from experimental data that allows them to visualize the deformation of materials on a timescale of minutes. Previous methods allowed for only a nanosecond-scale glimpse at the atomic-level processes.

"It's a method to look at mechanical properties at the atomic scale of real experiments without being bogged down by limitations of nanosecond timescales of the simulation methods such as molecular dynamics," said

Suresh, the senior author of a paper on the work that appears as the cover story in the Feb. 27 issue of the *Proceedings of the National Academy of Sciences*.

Using the new method, the researchers found that the ductility and strength of materials are greatly influenced by a special kind of interface known as the twin boundary--an abrupt internal interface each side of which is a precise mirror reflection of atoms of the other side. Twin boundaries can be introduced in various densities, in a controlled manner, inside a nanocrystalline metal.

For many years, engineers have been able to tinker with the structure of metals to make them stronger. Most commonly used metals, including copper, silver, gold and aluminum, are traditionally made from micrometer-scale "building blocks" called grains, which each contain many millions of atoms.

About two decades ago, materials engineers discovered that when they made those grains smaller, typically tens of nanometers in average size, metals become stronger. Known as nanocrystalline metals, they are several times stronger than conventional microcrystalline metals.

However, as nanocrystalline metals become stronger, they also become more brittle (less ductile). For example, copper with a grain size of 10 micrometers may have a ductility of about 50 percent (depending on exact composition), but at a 10 nanometer grain size, the ductility is below 5 percent, according to Suresh.

"In most applications, you need optimum combinations of strength and ductility," Suresh said.

A few years ago, researchers at the Shenyang National Laboratory for Materials Science in China synthesized a novel form of nanostructured

metal, nano-twinned copper. The material was created by introducing controlled concentrations of twin boundaries within very small grains of the metal using a technique known as pulsed electrodeposition.

The Shenyang group, working in collaboration with Suresh's group at MIT, demonstrated in the last two years that nano-twinned copper has many of the same desirable characteristics as nano-grained copper, and in addition resulted in a good combination of strength and ductility. By controlling the thickness and spacing of twin boundaries inside small grains to nanometer-level precision, they were able to produce copper with different "tunable" combinations of strength and ductility.

Internal interfaces such as grain boundaries (which occur between grains) and twin boundaries play a critical role in the strength and ductility of metals.

When there are smaller grains in the metal structure, and hence more grain boundaries for a given volume, there is more interaction between the boundaries and dislocations, or string-like defects in the material that move inside and between grains during mechanical deformation. The larger proportion of these boundaries contributes to the brittleness of the metal.

Adding nano-scale twin boundaries, which effectively subdivide the grains, has a similar strengthening effect, but the twin boundaries do not promote the same level of brittleness as grain boundaries do.

"You can trick the material and optimize both strength and ductility by modifying the interactions between dislocations and these nano-scale twin boundaries inside the grain," said Suresh.

The new study reveals that the ductility of nano-twinned copper can be attributed to changes in the atomic structure of the twin boundaries as

the material is deformed.

Metals with more twin boundaries also maintain their electrical conductivity better than metals with more grain boundaries, making them potentially more useful for applications such as computer chip components. Nanocrystalline metals that are both strong and ductile could also be useful for many wear-resistant thin-film coating applications and MEMS (micro-electro-mechanical systems) devices, Suresh said.

The researchers plan to use their new approach to look at such things as the structures of other materials and other types of boundaries.

Suresh's collaborators on the paper include two former MIT graduate students, Ting Zhu, now an assistant professor at Georgia Tech, and Ju Li, now an assistant professor at Ohio State. Other authors are Amit Samanta and Hyoungh Gyu Kim, both of Ohio State.

Source: MIT

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