Alloy Deformation

Ghazisaeidi studies HCP alloys for theoretical, industrial applications

The compelling need for energy efficiency in the transportation industry provides a strong motivation for the increased use of lightweight engineering materials such as titanium and magnesium alloys that will lead to weight reduction.

A majority of common metals have one of three different crystalline structures, based upon certain attributes of the metal's basic unit cells, which contribute different physical properties to each classification of structure. Some metals are ductile but very soft, others are less ductile but stronger, while still others are very strong but brittle. This last set is known as Hexagonal Close Packed, or HCP, and includes metals such as titanium, magnesium, cobalt, zinc and zirconium. A mixture of different metals, creating an alloy, yields an even different set of properties.

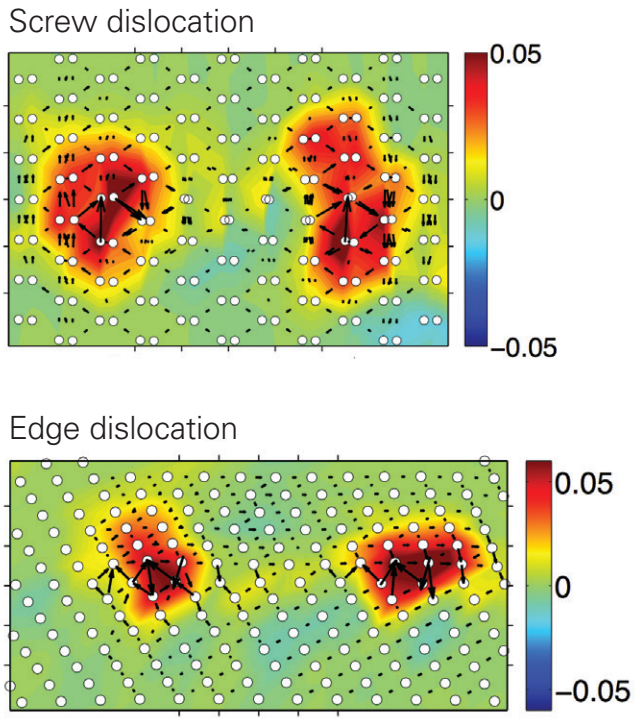
"Increasing both strength and ductility is the ultimate achievement for most structural materials," said Maryam Ghazisaeidi, Ph.D., an assistant professor of Materials Science and Engineering at The Ohio State University, who is leading a study of deformation in HCP alloys. "Traditional methods for strengthening rely on controlled generation of internal defects, and thereby increase strength at the cost of reducing ductility and toughness."

Various levels of ductility are observed in HCP metals and their alloys: from extensive ductility in titanium and zirconium to poor ductility in magnesium, zinc and beryllium. Ghazisaeidi believes understanding the mechanisms behind this divergent behavior is important from both theoretical and industrial application points of view.

"We aim to provide a scientific basis for a quantitative and systematic approach to design the strength and ductility of magnesium and titanium alloys through favorable alloying," she said. "The approach is based on electronic structure calculations of various deformation modes, including slip and twinning with an accurate account for chemistry change due to alloying."

The calculations are being performed on the HP/Intel Oakley Cluster at the Ohio Supercomputer Center by way of the density functional-theory code VASP, short for Vienna Ab initio simulation package. Electronic structure calculations of dislocations typically require large simulation sizes and accurate treatments of boundary conditions.

"Existing approaches to modeling material behavior generally rely on phenomenological constitutive relations that must be calibrated experimentally and therefore lack predictive capability," she explained. "Connecting the accurate atomic-scale study of deformation to the overall mechanical properties will potentially transform alloy design by replacing the trial and error approaches with quantitative predictive models." •



A study led by Maryam Ghazisaeidi, Ph.D., is investigating whether quantitative predictive models could replace existing trial-and-error approaches to modeling material behavior in hexagonal close packed metals and their alloys.

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