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Shattering Intermetallic Conventions

Researchers identify non-brittle intermetallic compounds

Scientists have known for more than 100 years that intermetallic materials — compounds consisting of two or more metals bonded together — possess chemical, physical, electrical, magnetic, and mechanical properties that are often superior to ordinary metals. The problem with these promising materials is that they're quite brittle at room temperature. Until now.

Ames Laboratory researchers have discovered a number of rare-earth intermetallic compounds that are ductile at room temperature. The discovery, announced in an article in the September issue of the journal *Nature Materials,* has the potential to make these promising materials more useful.

Brittle is the rule

"Many intermetallic materials are too brittle to handle," says senior metallurgist Karl Gschneidner, Jr. "If you drop them, they shatter. But you can beat on these new materials with a hammer, and they won't shatter or fracture … they're that ductile."

So far, the Ames Lab research team led by Gschneidner and materials scientist Alan Russell has identified 12 fully ordered, completely stoichiometric intermetallic compounds. In other words, these materials are combined in the proper chemical ratios, and the atoms are properly lined up.

"Intermetallics have been studied for decades," Russell says. "Tens of thousands of them have been identified, and there's a whole menu of 'tricks' that can be used, such as testing them at high temperatures, in zero-humidity, *continued on next page*

The yttrium-silver button shows dents and deformation from repeated hammer blows. The gadoliumium-silicon-germanium material was shattered with a light tap from the hammer.

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or shifting them off stoichiometry, to make them somewhat ductile. The materials we're studying are the first ones that don't need these contrivances."

B2 structure key?

By combining a rare-earth element with certain main group or transition metals, the resulting binary compound has a B2 crystal structure. That alphanumeric designation, developed by crystallographers, means that the compound has a crystal structure like that found in cesium-chloride (CsCl) in which an atom of one element is surrounded by a cubic arrangement of eight atoms of the other element.

The study has focused on yttrium-silver (YAg), yttrium-copper (YCu), and dysprosium-copper (DyCu), but a preliminary examination of other rare-earth compounds showed that cerium-silver (CeAg), erbium-silver (ErAg), erbium-gold (ErAu), erbium-copper (ErCu), erbium-iridium (ErIr), holmium-copper (HoCu), neodymium-silver (NdAg), yttrium-indium (YIn), and yttrium-rhodium (YRh) are also ductile.

In tensile testing, these materials showed remarkable ductility. The YAg stretched nearly 25 percent before it fractured, compared to 1 percent or less for many other intermetallics. In other measurements, the materials showed fracture toughness values comparable with commercial aircraft aluminum alloys.

Why these materials deform while other intermetallics shatter isn't quite clear, but theoretical calculations by former Ames Lab physicist James Morris, now at Oak Ridge National Lab, show that the ductile materials possess much lower unstable stacking-fault energies that exist around defects in the crystal structure of the materials. Because these energies are lower in the ductile materials, it may be easier for them to plastically deform instead of fracturing at the grain boundaries.

"There are particular planes (within the B2 structure) that tend to slip most easily," Russell says, "and particular directions on those planes where deformation slip occurs most easily. However, we have transmission electron micrographs that identify slippage in a direction we didn't see in our single crystal studies, so there are probably other factors at work as well."

Exceptional understanding

While there may be applications for these ductile materials because of their other characteristics, such as high-temperature strength or corrosion resistance, Gschneidner and Russell hope that studying these materials will actually lead to a better understanding of the brittle intermetallics.

"The most exciting thing about them is when they break all the rules like this, it gives you a great opportunity to figure out fundamentally why the others are brittle," Russell says. "To see one that's the exception gives you a new perspective on all the others."

Gschneidner adds, "The exceptions are the ones you want to concentrate on because they can tell you a heck of a lot more than all the ones that obey the rules. It can steer you in a whole new direction and lead to one of those 'eureka' moments."

Since the discovery of these materials evolved from work on another project, it has received only minimal funding. Gschneidner has pursued it as one of his interest areas with the other team members "volunteering" hundreds of hours of their time. In addition to Gschneidner, Russell and Morris, the team includes materials scientists Alexandra Pecharsky and Josh Zhang, senior metallurgist Tom Lograsso, nondestructive evaluation researchers David Hsu and Chester Lo, visiting physicist Ye Yizing, and students David Kesse and Aaron Slager. Physicist and deputy director Bruce Harmon and metallurgist Bulent Biner were also involved in theoretical discussions of the materials.

Overall, Russell calls the amount of knowledge gained per dollar spent "absolutely staggering." However, the group has submitted a funding proposal for further research to DOE and has filed a patent application for the materials. ■

~ Kerry Gibson

Karl Gschneidner demonstrates the ductility of a "button" of yttrium-silver. Unlike most intermetallic materials that are quite brittle at room temperature, Gschneidner and a group of researchers have identified more than a dozen rare earth/main group metal intermetallic compounds that show high levels of ductility and toughness.