# Scientists customize a magnet's performance by strategically replacing key atoms

February 1 2011

Scientists have given us a plethora of new materials – all created by combining individual elements under varying temperatures and other conditions. But to tweak an intermetallic compound even more, in order to give it the attributes you desire, you have to go deeper and re-arrange individual atoms.

It's a process similar to what bioengineers employ when they add and delete genes to create synthetic organisms, and it was the focus of a group of researchers at the U.S. Department of Energy's Ames Laboratory, when they replaced key atoms in a gadolinium-germanium magnetic compound with lutetium and lanthanum atoms.

The group was led by Vitalij Pecharsky, Ames Lab senior scientist and Distinguished Professor of Materials Science and Engineering at Iowa State University, and included his Lab colleagues, Karl Gschneidner Jr., Ames Lab senior metallurgist and Distinguished Professor of MS&E at ISU, and Gordon Miller, Ames Lab senior scientist and ISU professor of chemistry, along with assistant scientists Yaroslav Mudryk and Durga Paudyal. Also participating was Sumohan Misra, research associate at the DOE's SLAC National Accelerator in Menlo Park, Calif., formerly a Ph.D. student of Miller's.

Creating materials by design is no easy task, especially in the case of the complex gadolinium-germanium – $Gd_5Ge_4$ – compound. Making things even more difficult, the compound's structure is highly symmetrical, which is common in intermetallics, so predicting which atoms are key to

changing the material's characteristics would be difficult if not impossible unless some methodology was available to help in the selection process.

The $Gd_5Ge_4$ compound's uniformity results from the fact that like nearly all metallic solids' atoms are arranged in a highly symmetrical crystal structure called a lattice. The more complex the material, the more intricate its lattice. And while the individual elements making up the lattice influence its characteristics, in some cases the location of specific atoms within the lattice can also have a profound influence on such things as its melting point, mechanical strength or – in the case of magnets – ferromagnetic properties.

"Individuality doesn't happen often among the atoms of metallic crystals," Pecharsky explained, "But atoms still are able to 'cooperate' with one another in areas such as magnetic ordering and superconductivity."

By discovering these cooperative relationships, scientists can determine what will happen if they replace one or more of the atoms with those of another element, which is precisely what the team accomplished.

"We revealed that a single site occupied by the Gd atoms is much more active than all of the other Gd sites when it comes to bringing the ferromagnetic order in a complex crystal structure of gadolinium germanide," Pecharsky said.

Pecharsky, Gschneidner and other researchers at the Ames Lab have spent years working with gadolinium alloys, because of the magnetic compound's use in the green, energy-saving field of magnetic refrigeration. However, that was not the main reason the Ames Lab researchers chose $Gd_5Ge_4$ for their work.

As it turns out, "the metal exhibits an impressive combination of intriguing and potentially important properties, the researchers explained in their paper, "Controlling Magnetism of a Complex Metallic System Using Atomic Individualism," published in the August 10, 2010 Physical Review Letters. "The extraordinary responsiveness to relatively weak external stimuli makes $Gd_5Ge_4$ and related compounds a phenomenal playground for condensed matter science."

Besides being unusually responsive, $Gd_5Ge_4$ was an ideal alloy for the work, because any changes in its magnetic properties resulting from the group's manipulations could be easily measured.

In 2008, Pecharsky and members of the same research team had already discovered that adding silicon to the alloy resulted in a magnetostructural transition that occurred without the application of a magnetic field. Chemical pressure alone was able to enhance the material's ferromagnetism.

That earlier finding led the team to experiment with other additions to the alloy. To ferret out precisely which atoms in the lattice were the best candidates for manipulation, the researchers called upon density functional theory, which is a means of studying the electronic structure of solids developed by Nobel Prize winning physicist Walter Kohn.

Kohn's methodology enabled the group to model the effects substituting small amounts of gadolinium atoms within the $Gd_5Ge_4$ solid with the elements lutetium and lanthanum. With the modeled results in hand, the group's next step was to create the actual alloys in the lab, in order to test the accuracy of their computer-based predictions.

In fact, the complex fabrication process confirmed the modeling results. The researchers found if they replaced just a few gadolinium atoms with lutetium, the result would be a severe loss in the alloy's ferromagnetism.

By contrast, substituting an equal number of lanthanum atoms had no significant effect; though substituting greater amounts of lanthanum might have a more pronounced impact on the resulting alloy's ferromagnetism, the researchers speculated.

Going forward, the lessons learned in this experiment could have important far-reaching implications, as materials scientists search for new exotic substances to be used in this and future generations of high-tech products. "Knowing how to identify key atomic positions is similar to understanding the roles specific genes play in an organism's DNA sequence," Pecharsky said. "And that knowledge could ultimately lead to materials by design."

Provided by Ames Laboratory