

Morphing Metals

Texas A&M researcher exploits shape memory alloys to design smart materials for industry



Raymundo Arroyave, assistant professor of mechanical engineering at Texas A&M University.

Imagine a metal that remembers its original shape and can return to that shape when exposed to heat or a magnetic pulse. Discovered in 1931, these metals belong to a class of materials called *shape memory alloys* (SMAs), whose unique atomic make-up allows them to return to their initial form, or to alternate between forms.

SMA's are primarily used in orthopedics, biomedicine, and dentistry; however, many believe these materials will have their greatest impact in the aerospace and automotive industries, where they are expected to significantly improve the performance of motors, wings, and other mechanical parts.

Raymundo Arroyave, at Texas A&M University, used the *Ranger* supercomputer at the Texas Advanced Computing Center to explore a new class of alloy made out of cobalt, nickel, and gallium that operates at high temperatures. He mapped the constitution of the alloy as a function of temperature and composition, establishing a phase diagram of this particular system. In the process, Arroyave discovered that the fundamental dynamics that lead to the alloy's shape change are completely different than other SMAs. They published these findings in the June 2010 edition of the journal, *Acta Materialia*.

Ranger allowed the researchers to do calculations that were impossible a few years ago. For the first time, these virtual experiments approached the level of detail achieved in physical experiments.

"The dream is to design materials atom by atom in near future," said Ibrahim Karaman, Arroyave's collaborator and an expert on SMA's. "This can only be done with computational materials design, starting from an understanding of the electronic structure of these alloys."

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For more information, please contact: Faith Singer-Villalobos, Public Relations, faith@tacc.utexas.edu, 512.232.5771

More at: <http://www.tacc.utexas.edu>