The computational hunt for weird and unusual tech materials

April 20 2016, by Laura Millsaps

Scientists at U.S. Department of Energy's Ames Laboratory are turning to the world of computation to guide their search for the next new material. Their program uses software code developed to map and predict the distinct structural, electronic, magnetic stable and metastable features that are often the source of an advanced material's unique capabilities.

"It's the weird or unusual structure and behaviors of a material that makes it useful for a technological application," said Ames Laboratory Chief Research Officer Duane Johnson. "So the questions become: How do we find those unusual structures and behaviors? How do we understand exactly how they happen? Better yet, how do we control them so we can use them?"

The answer lies in fully understanding what scientists call solid-to-solid phase transformations, changes of a structure of one solid phase into another under stress, heat, magnetic field, or other fields. School kids learn, for example, that water (liquid phase) transforms when heated to steam (gas phase). But a solid, like a metallic alloy, can have various structures exhibiting order or disorder depending on changes in temperature and pressure, still remain a solid, and display key changes in properties like shape memory, magnetism, or energy conversion.

"Those solid-to-solid transformations are behind a lot of the special features we like and want in materials," explained Johnson, who heads up the project, called Mapping and Manipulating Materials Phase

Transformation Pathways. "They are behind things that are already familiar to us, like the expandable stents used in heart surgery and bendable eyeglass frames; but they are also for uses we're still exploring, like energy-harvesting technologies and magnetic cooling."

The computer codes are an advancement and adaptation of new and existing software, led in development by Johnson. One such code, called MECCA (Multiple-scattering Electronic-structure Code for Complex Alloys), is uniquely designed to tackle the complex problem of analyzing and predicting the atomic structural changes and behaviors of solids as they undergo phase transformations, and reveal why they do what they do to permit its control.

The program will assist and inform other ongoing materials research projects at Ames Laboratory, including ones with experimentalists on the hunt for new magnetic and high-entropy alloys, thermoelectrics, rare-earth magnets, and iron-arsenide superconductors.

"This theoretical method will become a key tool to guide the experimentalists to the compositions most likely to have unique capabilities, and to learn how to manipulate and control them for new applications," Johnson said.

Provided by Ames Laboratory