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New Jersey Institute Of Technology Physicist Uncovers New Information About Plutonium

NEWARK — The storage of plutonium has long plagued scientists. “It is a dangerous metal and its long term storage must be done with special care so as not to harm the environment,” said physicist Serguei Savrasov, Ph.D.

Finding a solution to this problem led Savrasov, an associate professor at New Jersey Institute of Technology (NJIT), and a team of researchers at Rutgers University and Los Alamos National Laboratories, to study how this metal reacts to heat, a natural condition of storage over time.

The team’s findings are published in the May 9, 2003 issue of Science.

Using a computer simulation, the researchers employed algorithms, to predict that when plutonium is heated, the volume of the plutonium lattice will change and the precise volume of the metal will collapse five percent. The simulation also predicted that heated plutonium deforms differently in various directions.

Other researchers working on the project were Xi Dai, Gabriel Kotliar and Elihu Abrahams, all of Rutgers University, and Albert Migliori and Hassel Ledbetter of Los Alamos National Laboratories, New Mexico. This simulation was the second part of an effort by this team. The April, 2001 issue of Nature reported the findings of several members of this group (S. Savrasov, G. Kotliar, and E. Abrahams). Their findings explored the anomalous expansion of plutonium.

Support for the project included a National Science Foundation Career



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Development Grant for \$400,000, awarded to Savrasov, and a Department of Energy Division of Basic Energy Sciences grant for \$300,000 awarded to Kotliar, Abrahams and Sasvrasov.

The new computer simulation by members of the same group plus others focused on why the metal shrinks. “There is an exciting and unusual interplay between the electrons and the plutonium lattice dynamic which is responsible for these unusual properties and why the volume collapses,” said Savrasov.

“It is important for the scientists to do the experiment as a simulation because plutonium is a toxic and radioactive element. It is dangerous for scientists to work with it directly,” added Savrasov.

The computer simulation showed the anisotropic elastic properties of plutonium. “Most metals are isotropic which means that the elastic properties are the same when you are stretching them,” Savrasov said. “But plutonium is anisotropic. When you stretch it in some directions, the metal is very soft. But when you pull it in other directions, it behaves like a typical metal, and is hard to stretch.”

The computer simulation done by the researchers modeled the properties of the plutonium lattice. “When you heat plutonium, it shows six structures and you can see it undergo these transitions,” said Savrasov.

The team modeled two of the six high temperature transitions. “When the plutonium is heated, it acts like popcorn in a microwave,” said Savrasov. “It pops up and increases 30 percent of its size and then after you heat it further, the metal collapses. This behavior is very unusual and unexpected for a metal.”

Savrasov said that such information hopefully will aid material scientists and engineers who are responsible for storing the metal. “Of course scientists know what they are doing, but our research helps them understand more about this metal’s basic properties,” Savrasov said.

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