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Scientists Unravel Clues to Behavior of Plutonium
Research may help safety of storing nuclear weapons

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The sometimes-unpredictable behavior of plutonium -- the world's most feared element -- is now considerably more predictable, an achievement that could help ensure the safe maintenance or disposal of nuclear weapons, scientists said yesterday.

Discovered at the University of California at Berkeley early in World War II, plutonium is the key to the U.S. nuclear arsenal: It is the fissionable material that makes most nuclear bombs explode.

Physicists have long been fascinated by plutonium's strange behavior, including its tendency to expand rapidly when heated and its ability to transform into eight "states" -- akin to the solid, liquid and vapor states of water -- more than any other element.

Scientists have tried to develop computer models that accurately predict the rate of plutonium expansion when it is heated. But they have met with frustration and only intermittent success -- until now.

Now, thanks to "a new viewpoint on the physics of plutonium," three physics professors at Rutgers University have developed a computer model that more precisely predicts plutonium's expansion rate, they report in today's issue of Nature.

The achievement could have practical applications. For one thing, it could improve the ability to store and dispose of plutonium from nuclear weapons in the post-Cold War world, say the article's authors, Sergei Y. Savrasov and two colleagues.

Also, experts speculate, the new computer model could be applied to predict the behavior of other elements and create new materials. Such materials might have commercial or military applications, such as microchips that can store far more information.

"It opens a lot of new possibilities for simulating properties of materials, " Savrasov said. He co-authored the paper with Gabriel Kotliar and Elihu Abrahams.

The behavior of plutonium is of special interest nowadays, as world nuclear weapons arsenals rapidly shrink. No new nuclear weapons are being built to replace the old bombs as they age. No one is sure how the aging bombs' spherical plutonium cores will behave as decades pass. The Pentagon fears that if the plutonium cores change their shape in subtle ways, the aged bombs might "fizzle" if used in a future conflict.

Consequently, the Energy Department is funding billons of dollars of research to learn how to predict the long-term behavior of bomb components, including plutonium.

Another concern is how waste plutonium, buried in underground containers in Nevada and New Mexico, will behave over centuries and millennia. Plutonium's sensitivity to temperature changes is a natural concern in those desert locales, which have experienced intermittent volcanic activity over geological time.

The Rutgers team's model better predicts the behavior of plutonium by simulating the interactions of its atomic fabric -- namely, the jillions of plutonium atoms and their accompanying chorus lines of electrons. The "new viewpoint" is based, in part, on a refined understanding of how electrons move as plutonium shifts from one state to another.

A plutonium atom is extraordinarily complex, containing 94 electrons and 244 subatomic particles in two classes -- positively charged particles called protons and neutral particles known as neutrons, said R. C. Albers, who has been a theoretical physicist at Los Alamos for the past 24 years. He authored a commentary on the Savrasov team's work for the same issue of Nature.

Albers compares the plutonium-prediction task to astronomers who predict the behavior of the planetary system. In a "celestial mechanics" model based solely on the gravitational pull of the sun, planetary motions can be predicted with reasonable accuracy well into the future, he notes.

However, if a scientist seeks more precise predictions, he must account not only for the gravitational pull of the sun but of the gravity of each individual planet and its moons. That quickly makes the prediction "very complicated, because you've got nine planets -- and worse, they're all moving simultaneously," Albers said.

A similar problem, Albers continued, faces physicists who try to predict the behavior of plutonium, except they're wrestling not with the sun, planets and moons but with all of the electrons simultaneously moving in the electrical field of the nuclei.

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