

the Exploratory Studies Facility is completed at Yucca Mountain, we will proceed with more extensive integrated tests to validate our models and methods.

Key Words: engineered barrier system (EBS); high-level radioactive waste; spent fuel; Yucca Mountain Project.

References

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Integrated Corrosion Facility

To project effects on candidate metals over a hundred centuries, we need to do laboratory corrosion testing for as long as possible, several years at least. Our new corrosion-testing laboratory at Livermore (Building 435) allows us to investigate modes of degradation in candidate materials for the required times.

This facility contains several dozen large tanks approximately 1 meter square and 2 meters high in which we can simulate conditions that are possible at a repository. Test solutions are varied and controlled for temperature, pH (acidity), solution chemistry, and many other variables. Metal samples are immersed in the aqueous solutions or subjected to the vapor phase to study generalized, localized, and stress-assisted corrosion.

Some samples will be exposed for five years or more, still just a fraction of the time the material must last in the repository. To measure changes in corrosion rates, we will remove samples of candidate materials at six-month intervals for kinetic and mechanistic analysis. Some of our exposure conditions, such as electrochemical polarization, intentionally accelerate the corrosion process. For different exposure conditions, we use computer models to project corrosion effects to much longer times. Thus, the effects we assess can correspond to the vastly longer exposure times in an underground repository.

About the Scientist



WILLIS L. CLARKE received his B.S. in metallurgical engineering from the University of Nevada, Reno, in 1960. He joined the Laboratory's Chemistry and Materials Science Department in 1989 after holding several research and managerial posts, including lengthy service as principal engineer at the Vallecitos Nuclear Center at Pleasanton, California. Since 1991, he has been project leader at Lawrence Livermore for the Yucca Mountain Site Characterization Project, managing a staff of from 40 to 80 researchers

focusing on the design of an engineered barrier system for a permanent nuclear waste repository. He has published more than 80 articles on materials performance, including the effects of radiation, oxidation, and corrosion on metals and alloys.

The Diamond Anvil Cell: Probing the Behavior of Metals under Ultrahigh Pressures

In the absence of nuclear testing, the Laboratory's diamond anvil cell is helping to assure the safety and reliability of our nation's nuclear stockpile. Because it uses very small samples, the diamond anvil cell is a cost effective way to collect accurate, reliable data about the physical and chemical behavior of weapons materials under the ultrahigh pressures encountered in an imploding nuclear weapon without the possibility of radioactive contamination.

HOW materials behave under extreme conditions is of more than scientific interest to Livermore researchers. Issues related to national security are a major motivation. During the implosion of a nuclear weapon, the materials are driven inward, reaching enormously high pressures and temperatures, until they achieve the supercritical state that is necessary for nuclear fission. During the process, the ultrahigh compressions subject the weapon's materials to

continual change in physical properties such as volume, structural state, and density. These changes strongly affect the course of the implosion and therefore the final explosion. Weapon designers need to know exactly what those material properties are and how they change during the implosion process if they are to calculate and reliably predict the performance of a weapon. However, the great violence and brevity of a nuclear event combine to inhibit the collection of precise data.

Until roughly two decades ago, the only alternative to nuclear tests for measuring the properties of materials at ultrahigh pressures and temperatures was shock experiments—shock waves were driven through the material of interest while changes in the material properties during passage of the shock front were measured. However, because shock techniques are dynamic, precise material properties are difficult to measure directly. Instead, the diagnostics were focused on measurements that could be captured in such brief durations; then, using large-scale numerical simulations that incorporated data from the experiments, researchers inferred the properties of interest.

The Diamond Anvil Cell

The diamond anvil cell (DAC) has changed these circumstances because of the pressure and temperature regimes to which a sample can be subjected. It joined shock experiments and tests driven by high explosives as means of providing the experimental data that are important starting points for science-based stockpile stewardship. This apparatus enables Lawrence Livermore researchers to measure many of the properties of interest directly under static pressure conditions (instead of indirectly as in dynamic shock-wave experiments). The use of static pressure means that ultrahigh pressures can be maintained for significantly longer times than in shock experiments, allowing more accurate measurements to be taken directly. Pressures within the diamond anvil cell can approach 350 gigapascals (1 GPa = $\sim 10,000$ atmospheres*) and

temperatures can approach 6,273 kelvin (10,832°F, 6,000°C)—that is, pressure and temperature equal to those at the center of the Earth.

The DAC is also more cost effective than shock-wave experiments. Instead of providing only one volume–density number at a given pressure per experiment, it provides a range of data across the pressure spectrum of the experiment and thus more information for fewer experiments. Another advantage of the DAC is the small sample size needed. Each experiment requires about a microgram of an element, significantly less than in a weapon. The small samples present minimal possibility of radioactive contamination, and containment of the small amount of radiation is assured.

The DAC's capabilities are particularly important for weapons physicists now that the United States is no longer conducting nuclear tests. The safety and reliability of nuclear weapons must now be maintained with indirect experimental techniques and large-scale computations. In particular, the DAC enables direct measurements of changes in volume and density, as a function of changes in the material's crystal structure and of melting under high pressure, that strongly influence the hydrodynamic stability of imploding systems. Fifty years ago, instability was an intractable problem for the designers of the first nuclear weapons. Despite major advances in science and technology, our understanding of instability remains limited because the actual physical state of the material experiencing these changes in volume and density often could not be measured. The DAC now changes this situation. It can provide

some of the data required to accurately predict the yield and performance of nuclear weapons—and thus their safety and reliability—without nuclear weapons tests.

LLNL's physicists also use the DAC data to interpret the data collected from earlier shock-wave experiments. Shock waves passing through a material raise its pressure and temperature simultaneously, making it difficult for researchers to identify with certainty the separate effects of pressure and temperature alone from the data. By statically compressing the same type of material at room temperature in the DAC, we can isolate the effects of pressure on the changing pressure–density relationship (i.e., equation of state) of the material. Physicists then use these data to calculate the temperature component from the shock data and thus derive separate pressure and temperature values for those data. They thus deduce further information about the high-temperature equation of state and phase stabilities useful to weapons physicists in confirming or modifying the complex theoretical calculations upon which weapons computer codes are based.

Figure 1 shows a comparison of DAC data with data from shock experiments recalculated using a theoretical equation-of-state model for uranium. The slight discrepancy between the DAC and theoretical equations of state suggests that the parameters chosen for the theoretical calculations may need further minor modifications that could lead to more accurate predictions of weapon safety and yield. The DAC is thus an important tool that provides weapons

physicists with the experimental data that allow them to improve the calculations upon which weapons codes are based without doing actual nuclear tests.

The Compressing Mechanism

The diamond anvil cell is a small mechanical press that forces the small, flat faces (the culets) of two flawless, brilliant-cut diamonds together on a microgram-size sample to create very high pressures in the sample (see Figure 2).¹ It uses diamonds because, as the hardest known solid, they do not break or deform under the intense pressures of the DAC and are transparent to light and x rays. The mechanism for applying the pressure is a stout lever with a mechanical advantage of 10:1. It is actuated by a heavy screw and Belleville springs at the long end. (Belleville springs are cupped washers stacked back to back around the screw to apply a balanced pressure.) The diamonds, which range from one-eighth to one-third carat each, are in an opposed anvil configuration and mounted over zirconium pads on a pair of tungsten-carbide rockers. These rockers (hemicylinders with their axes at right angles) can be tilted to align the culet faces perfectly parallel. Apertures in the rockers permit x rays and other kinds of radiation to enter and exit through the diamond anvils, thus allowing for diagnostics and heating during experiments.

We customize the surface shapes of the diamonds for the pressures at which we perform experiments. For experiments at pressures below 500,000 atmospheres (50 GPa), each diamond is ground to have a flat face that ranges from 100 μm (micrometers) to 500 μm in diameter; for experiments at still higher

pressures, we use beveled diamonds having a 7- to 8.5-degree bevel on a 300- μm culet with a 30- to 75- μm flat face. (As points of reference, a standard sheet of paper is about 50 μm thick and a human hair is about 100 μm in diameter.)

Once the diamonds are perfectly aligned, we remove the tight-fitting piston that holds one of the two diamonds in place. Between the culets of the anvils, we place a 250- μm thick gasket (a strip or circular metal disc of tool steel or rhenium) and apply a small force to indent or prepress its surface. Then we drill a hole that is 30 to 150 μm in diameter in the center of the indented area. Into that hole we place the sample with a pressure medium—liquid, gas, or solid—which helps to distribute the compressive force of the diamond faces.

To calibrate pressure during the experiment, we add a pressure marker, such as a small ruby chip or platinum powder. Under illumination of a helium–cadmium laser, the ruby chip emits fluorescent light at characteristic frequencies (spectral lines), the

wavelengths of which are calibrated as a function of pressure against a known marker material. The volume of the platinum under pressure can be calculated from the x-ray lattice parameters and compared with the known pressure–volume relationship from shock-wave data in order to ascertain the sample pressure. (The pressure marker acts as a pressure sensor and also indicates when the applied stress becomes nonuniform.) When the pressure is no longer hydrostatic, because, say, a fluid pressure medium has become a solid or has become very viscous, the resulting nonuniform stress broadens the ruby fluorescent peaks.

The Diagnostics

A significant advantage of the DAC is that diamonds are transparent to x rays and visible light. We exploit this feature when we watch the changes in the material as the pressure and temperature are changed. To determine the sample material's crystal structure during an experiment, we collimate the x-ray beam, selecting rays nearly

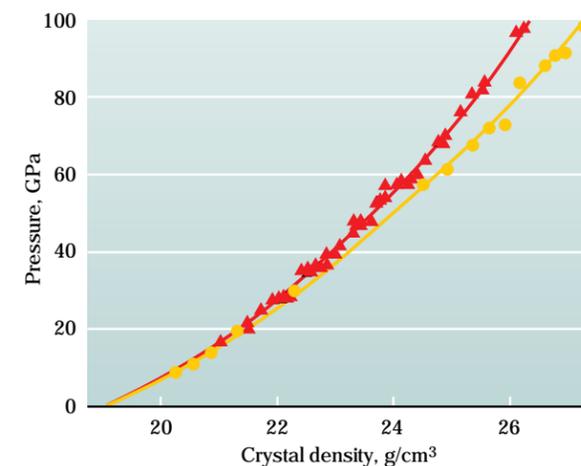


Figure 1. Comparison of diamond anvil cell data (●) with values calculated from a theoretical equation-of-state model for uranium using data from shock experiments (▲). The plot shows that the data derived from theory and shock experiments warrant correction by the data from the diamond anvil cell.

* 1 atmosphere = the ambient air pressure at sea level.

parallel to one another with a slit system.² We pass the well-collimated beam of monochromatic (single-energy) x rays from a rotating anode generator through the sample and both diamonds and record the resulting diffraction pattern on x-ray film (see Figure 3). Efficient computer programs interpret the resulting patterns, which consist of a complex series of concentric arcs or reflections in a spectrum. These x-ray diffraction patterns thus become the

means of “seeing” the changes in the crystal structure of the sample and collecting data about its changing equation of state under the intense pressure of the DAC.

Commonly, phase transformations are thought of as those from a solid to a liquid to a gas. However, there are transformations from one solid to another, and these are the structural transformations generally studied using the DAC. In solid-to-solid structural changes, the atoms of an element rearrange themselves in response to changing pressure, changing temperature, or both to new configurations. The shape of the atomic structural “cages” changes by the rearrangement of the atoms. Structural changes can be accompanied by a sudden volume change. However,

the volume change can be small enough not to be recognized or to be able to be accounted for by a normal margin of experimental error. It can also be smooth and gradual and not exhibit the spikes associated with large, sudden changes. Whether subtle or sharply defined, these are the structural transformations of interest in DAC experiments.

The diagnostic x rays used to record these data in our DAC experiments at ultrahigh pressures are not like those from medical or conventional laboratory x-ray units, which are too weak to yield data in a reasonable time and cannot be collimated sufficiently to collect accurate data. Rather, we use the very bright, highly coherent x rays from a synchrotron source such as the one at the National Synchrotron Light Source

at Brookhaven National Laboratory in New York State and collimate them to 5 to 10 μm in diameter. A combination of high beam intensity and excellent collimation is essential to reduce the time required for data collection (10 to 30 minutes at each pressure, rather than tens of days) as well as to reduce the effects that the pressure gradient across the sample has on the data.

When pressures exceed 40 gigapascals (GPa), we use the apparatus shown schematically in Figure 4 to record the diffraction pattern. First, we use a pair of adjustable slits to collimate the beam from the synchrotron x-ray source to a diameter of less than 10 μm. Then we clamp the DAC, with sample and ruby-chip pressure marker in place, to a four-circle goniometer* in order to align the DAC with respect to

Figure 2. (a) Schematic of the diamond anvil cell. (b) The cell disassembled, showing the major optical and mechanical components. (c) Close-up of the apparatus for holding and compressing the sample.

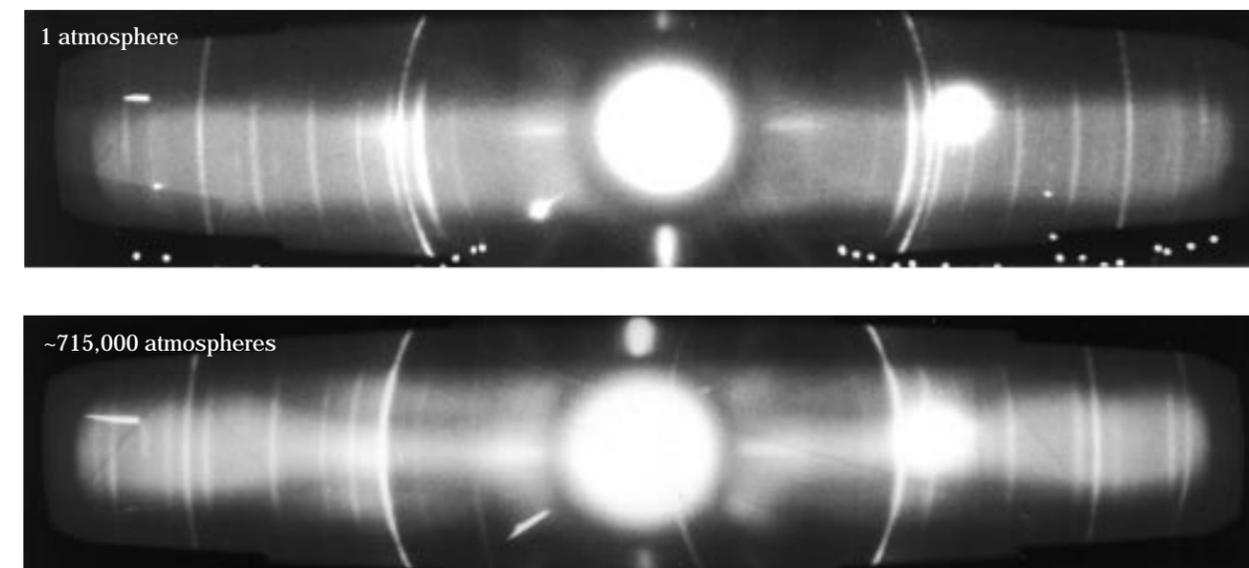
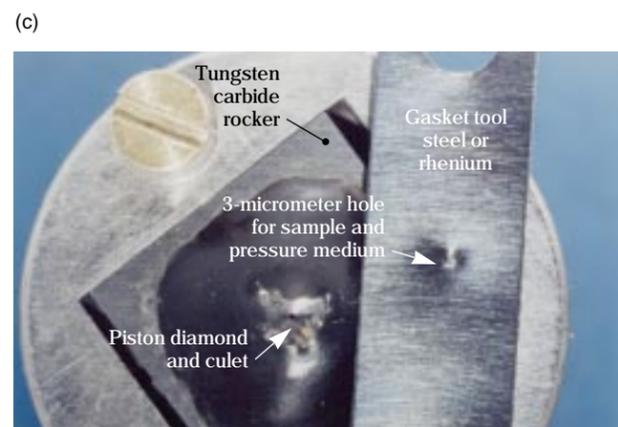
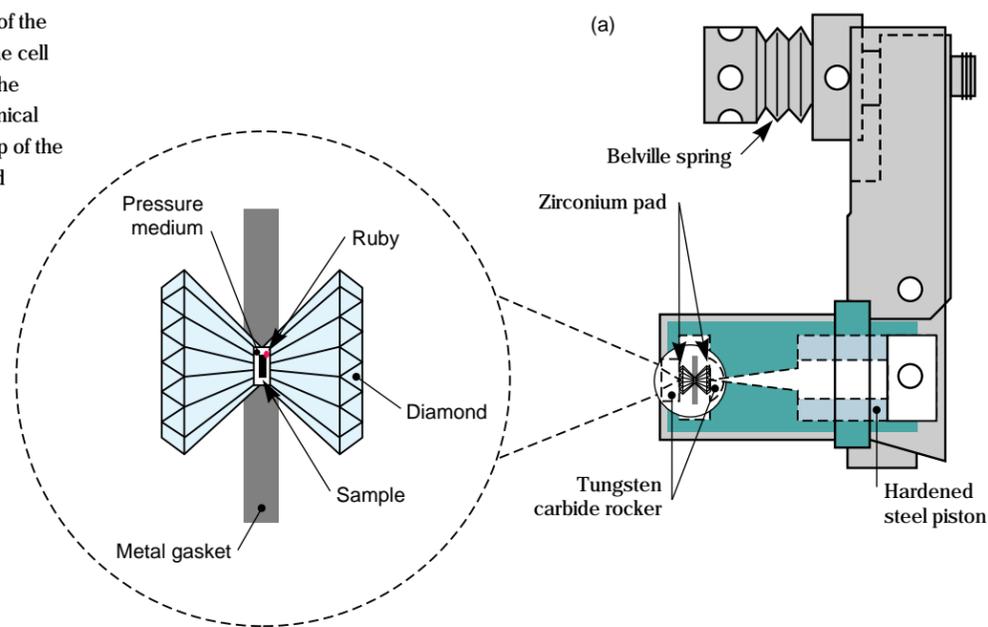


Figure 3. The experimentally interpreted structural sequence for uranium at increasing pressures recorded as an x-ray diffraction pattern by a collimated x-radiation experiment. It is x-ray diffraction patterns like these, but at much higher pressures, that provide the diamond anvil cell data of use to weapons physicists.

* A goniometer is an instrument with a number of degrees of freedom to move a crystal in space and uses x-ray diffraction to measure the angular positions of the axes of a crystal.

the x ray. Aided by the ion chamber, we align the DAC so the 10- μm -diameter x-ray beam probes the center of the sample (the area of greatest pressure and the least pressure gradient). The penta prism is essentially a microscope that directs light so that we can see the sample prior to experiments. The x-ray beam from the synchrotron source passes through the diamonds, diffracts from the sample, and passes through the pinhole collector in the upper part of the apparatus. It then enters the germanium-lithium detector, which records the energy diffraction pattern from the sample, data essential to identify the changing crystal structure. The optical multichannel analyzer in the lower part of the apparatus determines the pressure at which the crystal changes take place by measuring the laser-induced fluorescent light from the ruby-chip pressure marker. Thus, the changing volume and density of the sample are measured as a function of pressure.

Heavy Metals Experiments

As part of our continuing investigation into the high-pressure properties of metals, we have used the diamond anvil cell to determine the pressure-volume relationship and any possible changes in the crystal structure for some actinide and lanthanide metals to approximately 325-GPa pressure at room temperature. **Figure 5** shows the lanthanide and actinide series from the periodic table of the elements; shading highlights those elements we have studied in some depth. The Laboratory is the world leader in the study of lanthanides and actinides under extreme static pressure and temperature conditions.

One purpose of these investigations is to obtain consistent, thorough data of general scientific interest about the properties of these metals under pressure. Another is to study the

behavior of the actinide weapons metals uranium and plutonium under pressures approaching those in imploding nuclear weapons. These purposes, however, are not separate. In theory and reality, there are connections between the high-pressure behavior of elements in both series that are of particular relevance to the high-pressure behavior of the actinide weapons metals uranium and plutonium.³ Representative DAC findings about lanthanides and actinides illustrate how DAC research works in general and how it contributes to weapons safety in the absence of nuclear testing.

Our findings concerning the lanthanides and actinides to date fall into three categories: those concerning the lanthanides, those concerning the heavy actinides (americium through the end of the series), and those concerning the lighter actinides (thorium, uranium, neptunium, and plutonium).^{*} In all

three categories, we are in search of data about the stability—or lack of it—in each crystal structure and the equation of state under ultrahigh pressures. We are looking for structural changes as a function of pressure and temperature, changes in volume (density) due to the structural changes, the ultimate structural form that is stable for these elements, and the similarities between lanthanides and actinides. These are the data that physicists require in combination with shock-wave-derived data to confirm or modify the theory concerning the high pressure behavior of these metals upon which weapons code calculations for uranium and plutonium are based. These DAC data can improve the precision of the

computer codes for the behavior of weapons materials and thereby improve the predictability of their structural behavior in the weapons regime.

The Lanthanides

The lanthanides, or rare-earth series of elements (elements 57 through 71 of the periodic table—lanthanum through lutetium), are nearly indistinguishable in their chemical behavior. Although they all have the same outer electronic shell configuration, each element has one more electron than its next lighter neighbor. This additional electron is located deep within the atom's electron structure. This configuration causes a smooth progression of physical properties across the series but has little

effect on chemical properties. The normal (unpressurized) crystal structures of these elements (**Figure 6a**) show a regular progression across the series.

We studied the lanthanides in the DAC primarily to confirm experimentally the broadly related pattern of the elements' crystal structure across the series predicted by theoreticians.

Our detailed studies of some rare-earth elements have experimentally confirmed the existence of the structural sequence predicted by theoreticians. As pressure increased, the lanthanides transformed to face-centered cubic and a six-layered structure (**Figure 6b**). Under increasing pressure, the lanthanides follow the

Figure 4. The configuration of our static high-pressure experiments using synchrotron radiation, the means of recording accurate diffraction patterns of materials in a reasonable time when pressures exceed 40 gigapascals.

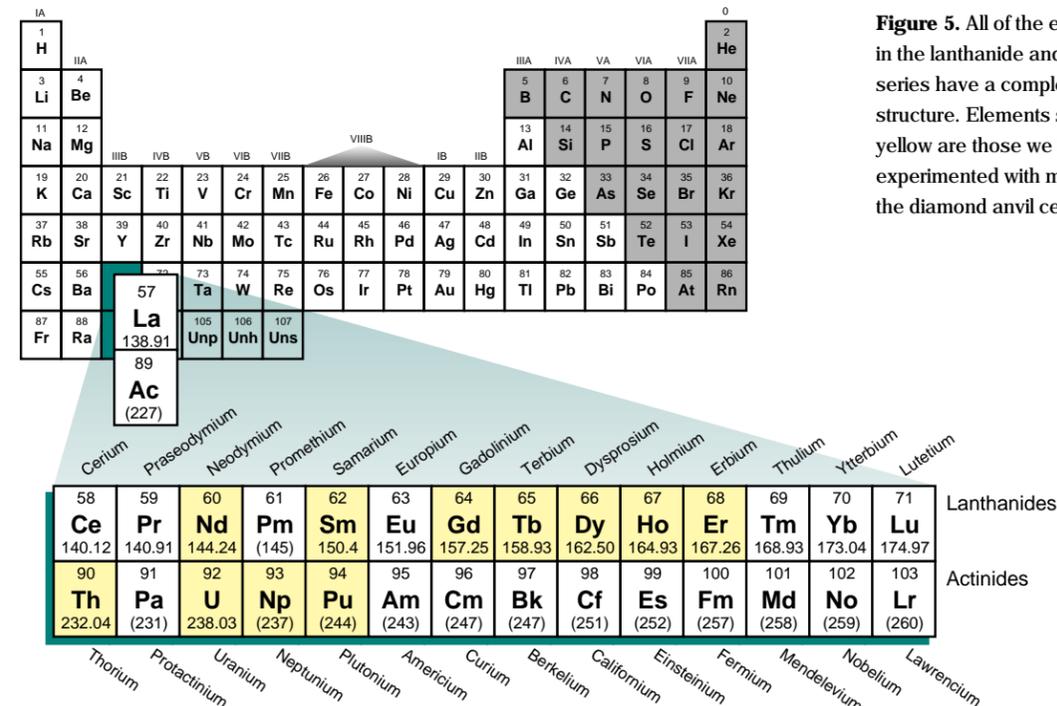
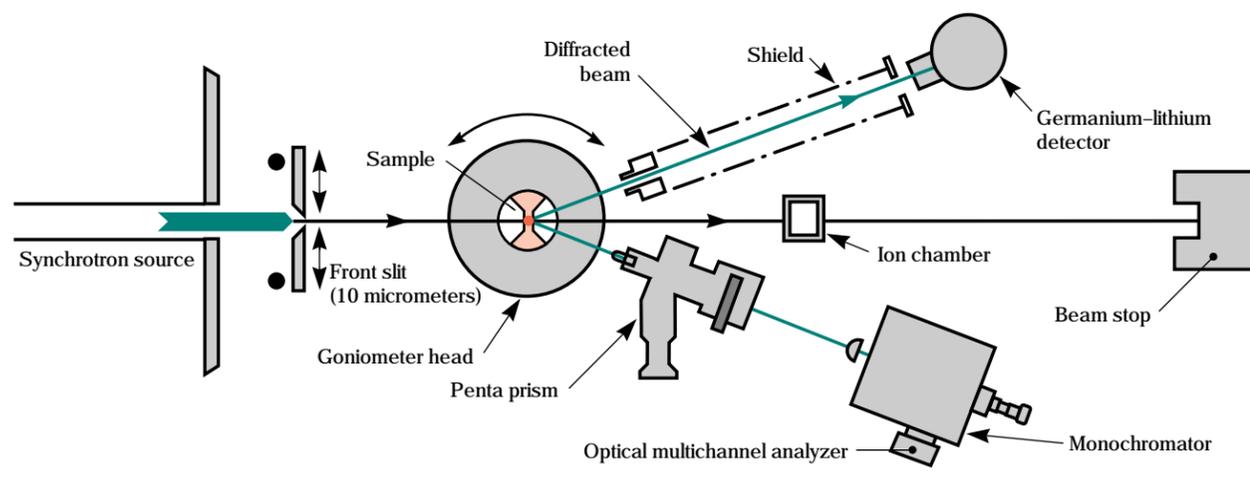


Figure 5. All of the elements in the lanthanide and actinide series have a complex atomic structure. Elements shaded yellow are those we have experimented with most using the diamond anvil cell.

* We have avoided DAC experiments with protactinium because it is too radioactive even in the small quantities needed for our work.

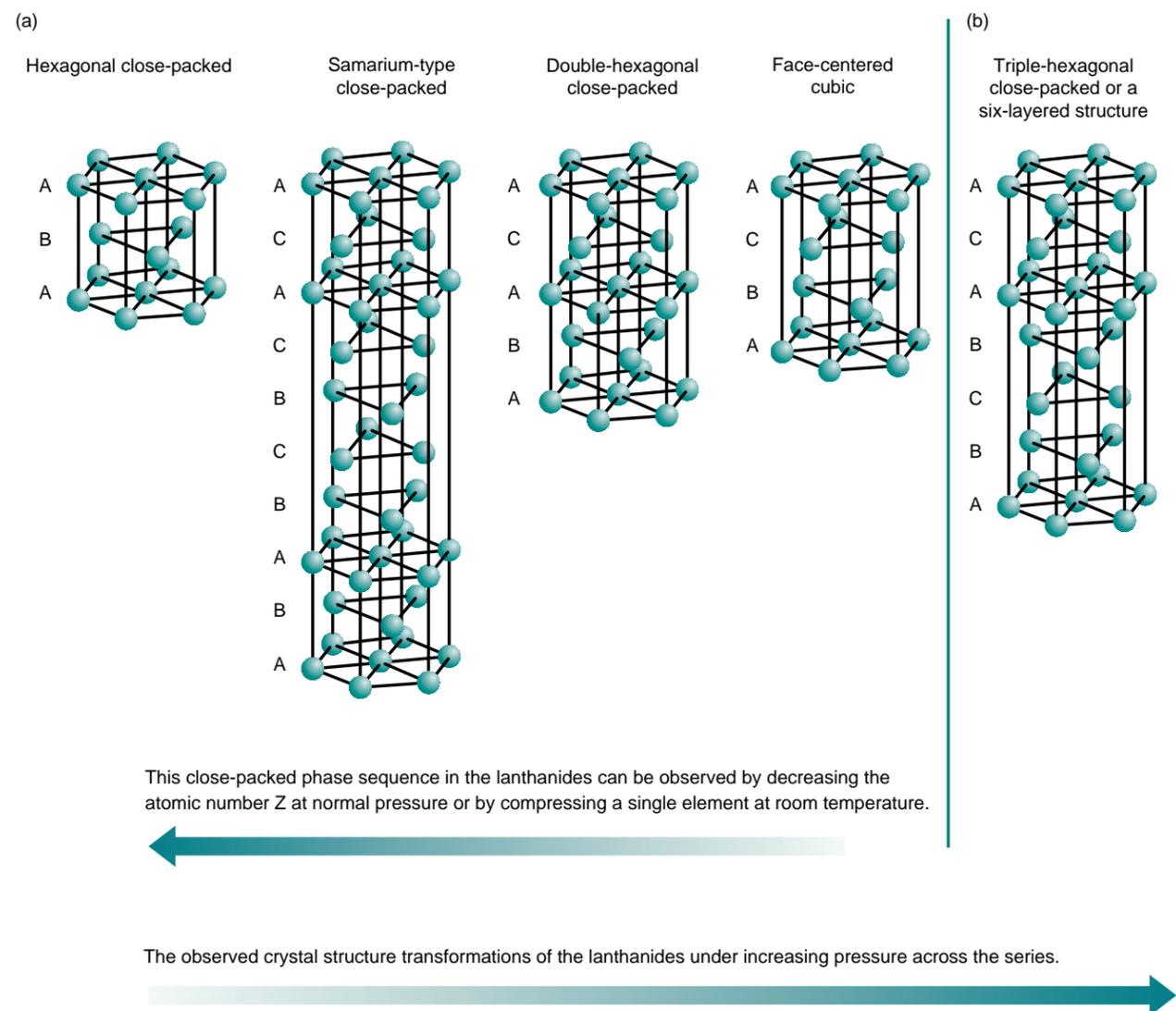


Figure 6. (a) The basic crystal structures found in lanthanide solids at room temperature and normal pressure across the series beginning with the lightest elements and moving to the heaviest. Our diamond anvil cell experiments have confirmed theoretical predictions that under increasing pressures approaching 100 gigapascals (GPa), the crystal lattice structure of the lanthanides follows the reverse of this sequence. In recent experiments, we saw a further transformation to a six-layered structure (b), which transforms to a body-centered tetragonal structure at pressures beyond 100 GPa but without the major volume changes predicted by some researchers. The crystal structures in (a) were first drawn by C. J. Alstetter, *Metals Transactions*, **4**, 2723 (1973).

reverse of the normal, unpressured progression pictured in [Figure 6a](#). When we increased the pressure beyond 100 GPa, we observed that the six-layered structure further transforms to a body-centered tetragonal structure. However, we did not see any big volume changes when the lanthanides transformed from one structure to another as the pressure increased. This behavior is contrary to what other experimenters have conjectured. Thus, our data suggest that the volume of these metals changes rather smoothly as a function of pressure without big, sudden changes.

The Actinides

In theory and in experiments, the actinides, especially the lighter ones early in the series, are less consistent in their behavior at high pressures than the lanthanides. The heavier actinides (americium through the end of the series) are predicted to behave under increasing pressures like trivalent lanthanides such as samarium and gadolinium. Our DAC experiments generally agree with theory for the heavier actinides. Thus at room temperature and pressures to 20 GPa, the trivalent lanthanides and heavy actinides studied exhibit similarities.

On the other hand, the light actinides, which include the weapons metals uranium and plutonium, are believed to behave less symmetrically and predictably under intense pressure than the lanthanides and heavy actinides. We are therefore studying them in the DAC in order to compare the electron behavior deep within them with similar behavior in the lanthanides and other actinides so that we can make critical conclusions about their high-pressure behavior.

Our findings concerning the other early actinides we have studied in depth (thorium and neptunium) illustrate the methodology and potential uses of DAC experiments for the study of uranium⁴ and plutonium.

At room pressure and temperature, thorium has a face-centered cubic structure. In previous experimental studies to pressures below 100 GPa, we studied thorium with gold as a pressure marker. Because of the interference of the thorium and the gold diffraction lines, we did not identify phase changes in these experiments. However, our detailed investigation of thorium to 300 GPa with platinum as an internal pressure marker showed that indeed thorium goes through a structural change from face-centered cubic to a body-centered tetragonal at about 72.6 GPa with no further transformations even up to the highest pressure. Our studies also suggested significant transfer of electrons from outer shells to those deep within the atoms as the pressure increased.

Because thorium has a stable body-centered tetragonal structure even at 300 GPa and similar body-centered tetragonal structures are stable, as we have seen, for some lanthanides, LLNL researchers have asked whether the body-centered tetragonal phase is the ultimate high-pressure stable structure at room temperature for these metals. Answers to such questions are essential if theoreticians are to fine-tune their computer-generated models and code calculations.

Recent studies on the next actinide metal, neptunium, have provided answers to the question. As pressure is

increased, the orthorhombic crystal structure of neptunium at ambient conditions transforms to a body-centered tetragonal structure and then to a body-centered cubic structure that is stable to the highest pressure (see [Figure 7](#)).⁵ This suggests that we might see similar body-centered tetragonal to body-centered cubic structural transformation in the other actinides and rare-earth metals. Thus, the ultimate stable structure of the trivalent lanthanides, the heavy actinides, and some light actinides may be body-centered cubic, not body-centered tetragonal. We also hypothesized from these studies that neptunium should have two body-centered cubic structures, one at low pressures and high temperatures before melting and another at high pressures and low temperatures. Both hypotheses provide new input to theory that can improve the precision of computer weapons code calculations.

Our classified DAC research on the light actinides uranium and plutonium has provided vital information that allows us to revise the computer modeling of the behavior of plutonium during nuclear explosions. In the absence of testing, this data is vital in assuring weapon safety, reliability, and predictability. To a lesser but equally vital extent, our DAC work on the lanthanides and other actinides related to weapons materials has contributed to those refined codes. It allows confirmation or revision of calculations derived from theory and dynamic experiments with accurate data that we can “see” from a high-pressure spectrum captured in static DAC experiments.

Future Directions

The DAC has enabled us to obtain phase stability information that dynamic techniques such as shock-wave methods could not supply and to incorporate that information into our theoretical models. Our scientists constantly endeavor to improve DAC experimental techniques in order to obtain better data and to obtain further information about the physical properties of any material, including weapons-related materials. With the addition of a laser or a resistance heater or with cryogenic cooling, we can also use the DAC to explore the pressure–volume–temperature relationship and the resulting structural changes of any material—its equation of state and phase diagram. Higher pressure and increased temperature may force further structural changes, until the material loses its crystal structure entirely—that is, it melts.

An area of new technology for obtaining high pressure and temperature data using x-ray diagnostics is electrical transport

experiments such as ohmic heating based on resistance to the current. So far, these experiments have been among the most difficult to perform with diamond anvil cells. Special preparation of the sample, anvils, and cell is required, and electrical connections fail easily under the high stresses present in the diamond anvil cell. Consequently, electrical transport experiments have been very difficult to perform beyond several tens of gigapascals. Our scientists have developed techniques to overcome these problems and will embark on further studies of the weapons materials to still higher pressures and temperatures.

In any nuclear weapon, high explosives play a pivotal role at the time of detonation. These energetic materials generally have complex crystal structures with low symmetry and are poor x-ray diffractors. Consequently, properties that are crucial to performance—such as how the behavior of high explosives depends on increased pressure and thus on changes in crystal structure—have

not been thoroughly investigated at elevated pressures and temperatures. The DAC should allow researchers to collect such critical data under static conditions. We recently embarked on an exploratory study of equations of state and structural changes in high explosives using the DAC and synchrotron radiation. These studies will also inform us whether crystal structural changes in a high explosive such as triaminotrinitrobenzene (TATB) under pressure could cause changes in burn rates.

Key Words: actinides, diamond anvil cell, equations of state, lanthanides, science-based stockpile stewardship, shock-wave experiments, x-ray diffraction.

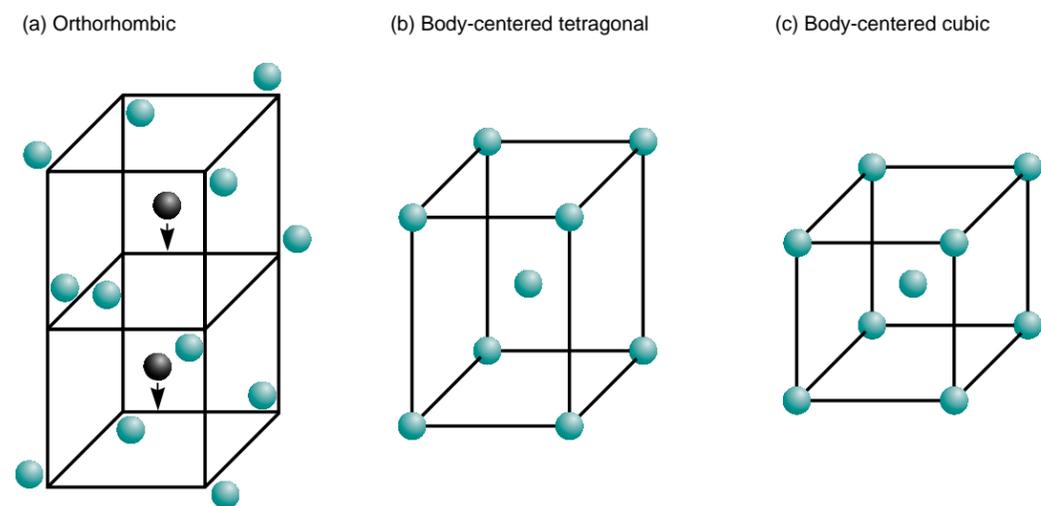
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2. For further information on the use of x-ray diffraction to investigate crystal structure, see "X-Ray Diffraction Applications," *Energy and Technology Review* UCRL-52000-87-11/12 (November/December 1987), pp. 23–28.
3. J. Akella, "Application of Diamond-Anvil-Cell Technique to the Study of *f* Electron Metals and Some Materials Relevant to Planetary Interiors," in *From Mantle to Meteorites*, ed. K. Gopalan, *et al.* for the Indian Academy of Sciences Press (1990), pp. 249–261.
4. Uranium has given us no help answering questions about the ultimate stable crystal structure of the early actinides under high pressure. In our diamond-anvil-cell experiments, it does not go through the phase changes at high pressures and room temperature that its neighboring elements do, and we do not yet know why.

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Figure 7. Schematic of the transformation of (a) orthorhombic neptunium at ambient temperature and pressure to (b) body-centered tetragonal to (c) body-centered cubic. The green circles in (a) represent one type of neptunium atoms, located near the corners of an orthorhombic subcell; the gray circles represent another type located near the centers of two subcells (the arrows indicate they are offset from the centers). Applying pressure moves the atoms to their nearest corner and the center of each subcell and results in (c) a smaller, more symmetric body-centered cubic form.



About the Scientist



JAGANNADHAM (JAGAN) AKELLA, who holds a Ph.D. in geochemistry, is the principal investigator of a Lawrence Livermore project that uses the diamond anvil cell (DAC) to study the *f*-electron metals and related weapons materials under ultrahigh pressures and temperatures.

Akella has successfully used DAC technology in conjunction with synchrotron x-radiation to investigate under controlled laboratory conditions the physical and chemical behavior of highly toxic radioactive samples under ultrahigh pressures and temperatures. These investigations have improved understanding of the fission triggers in nuclear weapons. Akella is also interested in developing new DAC techniques to investigate a wide array of nuclear and nonnuclear materials. Such work is relevant to a better scientific understanding of science-based stockpile stewardship issues as well as geological phenomena.

Akella joined the Laboratory in 1977 and has published more than 80 papers covering geological sciences, condensed matter physics, and materials science. He is an elected fellow of the Mineralogical Society of America and the Indian Mineralogical Association and is one of the recipients of the Department of Energy's 1994 Weapons Recognition of Excellence awards of the nuclear weapons program.