Jose, California. Parker notes that the technique could reduce electrical losses in ITO films used in flat panel displays, and polycrystalline silicon films used in photovoltaic devices, which convert sunlight to electricity.

The strategy works by sweeping away some of the obstacles that slow the passage of electrons through a conducting film. Defects such as impurity atoms or vacancies in the lattice structure slow the passage of electrons through many crystalline materials, but in a polycrystalline film, electrons are also slowed as they pass from one grain to the next, because the grains usually don't line up in nice neat rows—and if they do, their crystalline lattices don't usually align well at the boundary.

The Queens University researchers found that all three of these problems were reduced if they made their films on a substrate that's warmer and colder in alternating strips. But they are still trying to figure out why this occurs. Rauf does have some ideas. The material in films such as ITO, he explains, is typically deposited as a high-temperature vapor of atoms. As hot atoms in a vapor land on a substrate, they initially liquefy and congregate, forming tiny droplets. As the droplets cool, they crystallize, forming the neighboring grains in a polycrystalline film.

Rauf believes that the temperature gradients in the substrate sweep defects to the warmest side of each grain. Within each grain, he explains, the warmer side can dissolve more defects, just as warmer water can dissolve more salt than colder water. As a result, as the drops in the film crystallize, the defects are pushed to one side, creating a defect-free channel for current within each grain. And as the defects migrate within each grain, they force the lattice into a particular alignment, like a comb. Because defects are migrating the same way in neighboring grains, all the lattices end up similarly aligned. Finally, Rauf believes the alternating warm and cool regions also change the energetics between neighboring grains, making it favorable for grains to line up in rows atop regions of equal temperature.

While others found data for improved performance compelling, the explanations are "plausible," says Parker, but need to be proven. Rauf says that he and his colleagues are now working to test their theories by studying the nucleation and growth of their crystals.

Whatever the explanation, Rauf notes that his group has found that the process improves polycrystalline films of copper in addition to ITO. The researchers also used the technique recently to grow a film of the superconducting material yttrium-barium-copper-oxide. It improved grain alignment, and they are now testing the film's electrical properties to see if they can produce a new "Best Performance" nominee.

–Robert F. Service

MATERIALS SCIENCE

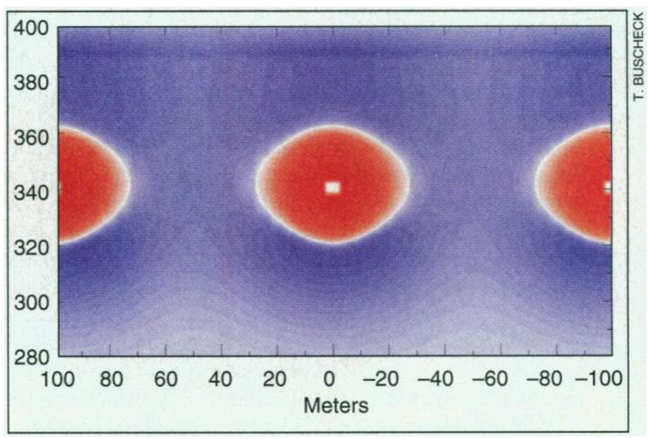
Can Nuclear Waste Keep Yucca Mountain Dry—and Safe?

Disposing of spent nuclear fuel by placing it deep in the earth is a race against time and corrosion—a race the designers of the proposed long-term nuclear waste repository at Yucca Mountain in Nye County, Nevada, know they will eventually lose. The central scientific question in this controversial project isn't whether the waste will leach out of the large metal casks that contain it, but when. In that race, repository designers are looking for every advantage they can get—including the heat generated by the waste's own radioactive decay.

Two weeks ago, at the fall meeting of the Materials Research Society in Boston, geophysicists Thomas Buscheck and John Nitao from Lawrence Livermore National Laboratory, with geologist Lawrence Ramspott of TRW Environmental Safety Systems Inc., proposed some new twists on an old idea: using that heat to boil corrosive moisture out of the surrounding rock. The researchers suggest that blanketing the waste canisters in gravel, then stowing them more densely and in storage tunnels placed farther apart than has been suggested previously, will keep the fuel warm and dry long enough for much of the danger to decay away. The plan, they say, will help keep the canisters intact for at least 10,000 years—the goal set by Environmental Protection Agency regulations, but still long before many of the most dangerous isotopes have decayed away—and perhaps as long as the 1 million years that a National Academy of Sciences (NAS) panel has recommended.

Like nearly every other aspect of this project, such as the viability of such a repository in the first place (*Science*, 30 June, p. 1836), the plan has divided scientific opinion. Some researchers see a great deal of promise. "State of the art," William Murphy, a geochemist at the Southwest Research Institute in San Antonio, Texas, calls it. And officials at the Department of Energy (DOE), which runs the Yucca Mountain project, call the plan "an important input." But critics say that, as with previous plans, prolonged heating could alter the rock's stability and porosity, perhaps allowing corrosive liquid to seep back into the tunnels.

Some 29,000 metric tons of nuclear waste from U.S. civilian reactors—an amount that grows by 1900 tons each year—are waiting for a permanent home, along with high-grade radionuclides, such as cesium, from the nation's nuclear arsenal. That home needs to be as moisture-free as possible, to minimize the chances for canister corrosion (see box on next page). In the major previous plan for storing the waste in the mountain, called "extended dryout," designers left as little as 20 to 40 meters between waste tunnels. The idea was to use the heat coming from the canisters to keep a thick slab of rock above and below the tunnels boiling hot—and thus dry—for thousands of years. But researchers also feared that, as the waste cooled, condensing water might seep through the rock and back down onto the containers, eating through their double skin of steel and alloy and leaching out wastes.



Nuclear space heater. In one plan, widely spaced waste storage tunnels will have a hot, dry zone around them *(red)*, driving moisture into the wetter rock *(purple)*, where it can drain away.

So Buscheck and colleagues used customized computer models, based on known properties of water and heat flow in porous, fractured media such as the Yucca Mountain rock, to test a new approach, dubbed "localized dryout." The scheme would essentially put drains into the rock by spacing the tunnels farther apart. Separating the tunnels by up to 100 meters would keep the zones of boiling-hot rock created by each tunnel from overlapping, allowing the condensate from each zone to drain through the cooler rock in between. With tunnels spaced further apart, waste containers within them could be placed closer to one another, generating a more intense, uniform boiling zone around each tunnel that adds assurance

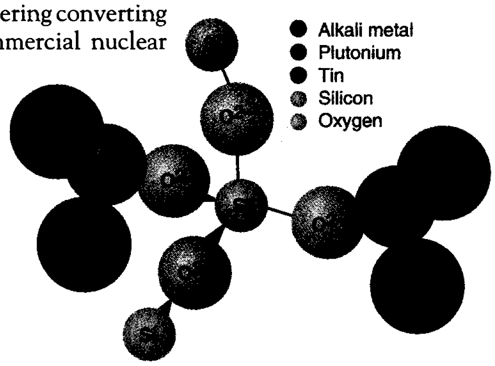
Plutonium Under Glass

Wherever the U.S. decides to put its high-level nuclear waste, planners must also decide how to store a particularly worrisome component: plutonium. There are an estimated 50 tons of the radioactive metal in the U.S. alone, left over from the production of nuclear weapons and their subsequent dismantling under disarmament treaties. Policy-makers are considering converting some of this stockpile into fuel for commercial nuclear reactors. The rest will have to be stored. Now researchers have come up with a new scheme for putting plutonium safely under glass.

Glass has long been considered a good storage medium for nuclear waste because it can be engineered to be stable over thousands of years, resist corrosion, and can easily encapsulate other types of contaminated waste such as incinerator ash. The type of glass traditionally used to entrap nuclear waste has one big drawback, however: It wasn't designed to hold more than a trace amount of plutonium. But at the Materials Research Society meeting in Boston 2 weeks ago, researchers from Argonne National Laboratory reported that a new glass formulation has the potential to incorporate up to 10% plutonium by weight.

Although the new glass, known as alkali-tin-silicate (ATS) glass, must still prove itself under long-term testing, other researchers say these results are welcome news. "If you can't get [plutonium] off the face of the Earth, putting it in that form may be the best option," says Mal McKibben, a chemist at the Department of Energy's Defense Waste Processing Facility in Aiken, South Carolina. Other potential storage materials, such as ceramics, are more expensive and harder to produce. Moreover, ATS glass can be spiked with highly radioactive cesium to deter terrorists from stealing the glass to extract the plutonium for nuclear weapons fuel.

ATS is, of course, far from pure silica glass. Plutonium can't be stored in pure silica glass because the metal atoms tend to congregate—a dangerous prospect, because a large enough cluster could form a critical mass. To prevent this, the Argonne chemists—led by Adam Ellison and John Bates—loaded ATS glass with alkali metals, such as sodium, lithium, and potassium. These positively charged atoms bind to negatively charged oxygens in the glass, creating compounds called nonbridging oxygens (NBOs), which still harbor a slight negative charge. Plutonium atoms carry a strong positive charge, so when they are mixed in the glass each one binds to several NBOs. The NBOs thus form layers around each plutonium atom, dispersing them throughout the glass network.



SOURCE: J. BATES AND A. ELLISON

Glass trap. Alkali metals help bind and disperse plutonium safely throughout a new glass formulation.

In addition to scattering plutonium atoms, the alkalis perform other useful roles, such as lowering the melting temperature of the glass to 1150 degrees Celsius. Unlike "lanthanide-rich glass"—an alternative formulation for high-plutonium-content glass that melts at a higher temperature—that's low enough to incorporate cesium, which vaporizes at around 1200°C, into the matrix.

Loading ATS glass with alkalis does create a problem, however. Alkalis are fickle: Unless they are stabilized by plutonium or a metal with a similar electronic behavior, they will drop their connections to oxygen and leach out of the glass. That would then speed the glass's decay and free the plutonium atoms to assemble in dangerous congregations.

Adding even more plutonium as a stabilizer was ruled out—more than 10% in the glass could make the mixture potentially explosive during processing. So instead, the researchers chose other positively charged metals, including tin and zirconium.

Thus far, the recipe seems a good one. After subjecting an ATS sample loaded with 7% plutonium to 56 days of standard durability tests—including continuous exposure to high temperatures and water vapor—the sample showed no evidence of corrosion or signs that the plutonium was congregating in the material. Says Bates: "The rate of reaction is similar to the natural glass obsidian," which survives intact for millions of years.

–Robert F. Service

that water won't drip back in. This would be impossible with closely spaced tunnels, because the zones would overlap to an even greater degree, eliminating drainage routes. Finally, an insulating blanket of gravel and sand around the containers would help keep the temperature at the canister surfaces higher—and corrosive humidity lower—than in the rock. Even after the waste has cooled for 100,000 years, Buscheck says, these measures will keep the packages dryer than ambient conditions.

But critics such as hydrogeologist Nick Stellevato, Nye County's technical representative at Yucca Mountain, warn that subjecting the mountain's highly fractured interior to above-boiling temperatures for many years could alter its strength and permeability to water. "With a high thermal load, you are going to have localized effects on stability around the tunnels," Stellevato says. Scott Tyler, a hydrologist at the Desert Research Institute in Reno, Nevada, adds that "water has the potential to run back down the fractures," picking up corrosive mineral solutes along the way.

Buscheck agrees that his group's calculations need to be verified, and says his group is planning to do just that by placing large electric heaters in tunnels and measuring temperature and vapor movement behind the tunnel walls. But he points out that under the localized dryout plan, less rock would have to be heated to achieve the same humidity reductions in the tunnels. Even if ground water inundated the tunnels, the temperature difference created by the gravel blanket would keep the waste packages drier than the surrounding rock. And because the blanketing effect strongly reduces humidity at the waste package surface far into the future no matter what the repository's overall thermal output, he adds, officials could take measures such as adjusting the waste packing density, or ventilating excess heat from the tunnels, to limit the period of boiling to as little as 100 years—within the repository's planned observation period.

Still, this and other aspects of the Yucca Mountain plan have a long way to go before the repository gets a green light. A recent NAS report, for example, found deficiencies in DOE's analysis of the potential for surface erosion at the site. The project is a magnet for criticism, and chemist John Bates, head of the nuclear waste office at Argonne National Laboratory, says anything pertaining to safety is relevant: "If you don't have a convincing technical basis for safety, you won't get [Nuclear Regulatory Commission] approval, and I wouldn't expect public approval either."

–Wade Roush