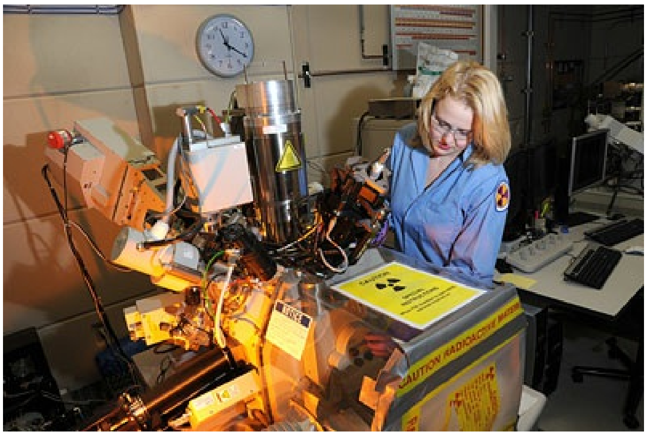


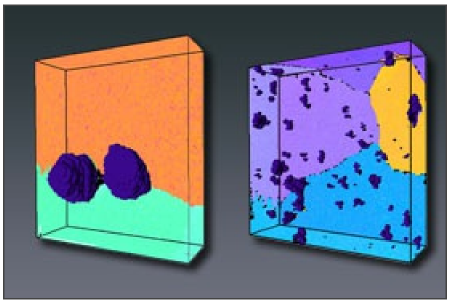
Melissa Teague is an INL materials engineer doing first-of-a-kind microscopic studies on nuclear fuel in the Electron Microscopy lab at INL's Materials and Fuels Complex. She works hand-in-hand with a computational scientist to push the boundaries of what is known about irradiated fuel behavior.

## Junior researchers showing world the way to advanced nuclear fuel design

By Nicole Stricker, *INL Communications & Governmental Affairs*

Two early-career Idaho National Laboratory researchers are earning international attention for their groundbreaking work. They're getting a long-sought look into the 3-D microstructure of irradiated nuclear fuel, then feeding that data into cutting-edge fuel behavior models. Their work will make the design and testing of even safer nuclear fuels more informed and efficient.

The distinctive collaboration stemmed from a fertile environment at the Department of Energy's lead laboratory for nuclear energy research and development. That environment enabled an engineer and a computational scientist to easily work hand-in-hand toward a common goal.



***These reconstructions of high burn-up mixed oxide fuel show size differences between metallic fission product precipitates (purple) in hotter (l) and cooler (r) regions of the fuel.***

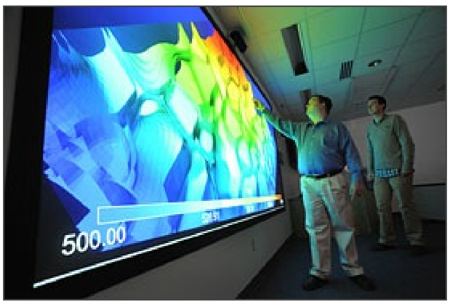
Their collaboration is noteworthy "because computer people and experimental scientists don't tend to interact much," said Michael Tonks.

Tonks is an INL computational materials scientist who built a model of nuclear fuel microstructure. Melissa Teague is an INL materials engineer doing first-of-a-kind microscopic studies on nuclear fuel. Her work is helping refine his models and capturing attention from international scientists.

"We've had people from all over the world coming and asking, 'How do you do this?'" she said.

**Uncommon vision**

The intrigue centers around microscale glimpses of irradiated fuel, which researchers have long pondered but never seen in 3-D. Such information will lead to a more fundamental understanding of how irradiation affects nuclear fuel safety and performance.




***INL computational materials scientist Michael Tonks, left, led development of the MARMOT model to simulate how irradiation changes nuclear fuel on the microscopic level.***

"It's always been kind of a holy grail to understand fuel at the atomic level, but there's never been a way to get this type of data on the small scale," Teague said.

She began her quest for such data through an INL internship while she was a graduate student at the Colorado School of Mines. She knew INL had singular capabilities that could enable her to perform a common microanalysis technique on an uncommon material: irradiated nuclear fuel.

The Electron Backscatter Diffraction (EBSD) technique directs high-energy electrons at the surface of a material sample. Electrons that encounter atoms in the material diffract to form patterns on a detector screen. Skilled crystallographers interpret the patterns to reconstruct the atomic structure and glean insights.

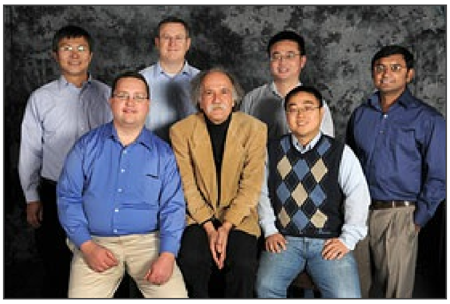
The technique requires sample materials to be highly polished, a feat that had previously been impossible for brittle irradiated nuclear fuel, which must be handled using hydraulic arms inside a hot cell to shield researchers from the radiation. But in 2011, a new sample preparation capability at INL changed all that.

"These were the first 3-D characterizations of irradiated fuel reported anywhere in the world," Teague said. "Before, no one really knew what it looked like in 3-D."

**Replacing assumptions**

Around the time Teague was pioneering advanced microscopy on irradiated fuel, Tonks was developing a new model to simulate how irradiation changes nuclear fuel on the microscopic level. Early versions of his MARMOT code incorporated limited published data about the texture of irradiated fuel, but made many assumptions.

Tonks started looking for research data that could fill in some of those gaps. He quickly learned of the work being done by Teague, whose desk he could walk to in less than a minute. The two applied for Laboratory Directed Research and Development funding and recruited EBSD reconstruction expert Bradley Fromm, who is working on a Ph.D. in materials science and engineering from Washington State University.


***The MARMOT team, left to right, is Xianming (David) Bai, Michael Tonks, Brad Fromm, Bulent Biner, Jianguo Yu, Yongfeng Zhang, Pritam Chakraborty and Daniel Schwen (not pictured).***

The data they collected provided several important insights. First, they proved it was possible to get EBSD information from "really messed up" highly irradiated fuel. The work also revealed how solid particles form, grow and migrate along crystal boundaries inside the fuel during irradiation.

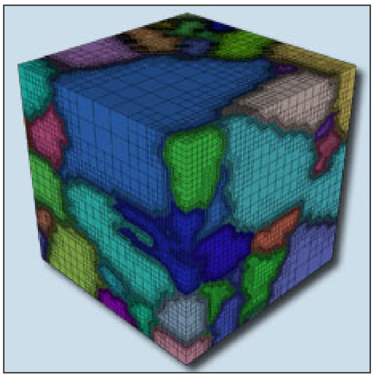
The data enabled Tonks and the MARMOT team of modelers to replace assumptions in the code with real-world information. Teague's experiments also help validate the MARMOT model — simulation outcomes can be compared with real-world data to ensure the model yields accurate predictions.

The refined MARMOT model is now benefiting experimentalists like Teague. It can give researchers a sense of the irradiation duration and conditions required to produce a desired result. For example, MARMOT was able to save one collaborator a lot of waiting time.

"At the temperatures he was going to use, he would have had to watch his experiment for five days and nothing would have happened," Tonks said.

**New possibilities**

Today, both efforts have branched into new areas. Tonks and the MARMOT team won funding from DOE's Nuclear Energy Advanced Modeling and Simulation program. They continue to refine and validate MARMOT with data from Teague, Los Alamos National Laboratory, Arizona State University and others.


***This MARMOT reconstruction of a nickel alloy sample shows the boundaries where one continuous crystal ends and another begins.***

Teague's initial results laid the groundwork to begin investigating other types of nuclear fuel. A Nuclear Energy Enabling Technology grant and funding from DOE's Fuel Cycle Research & Development program now support the research.

And laboratories around the world are asking Teague's team to help set up similar capabilities. The Swedish company Studsvik has succeeded, and labs in England, Germany and France are working toward advanced nuclear microscopy, Teague said.

Such atomic-scale data is sought after because it can help inform the development of nuclear fuel with enhanced safety and performance. The information can reveal how and why certain materials perform better than others. It can also make testing and validation more efficient by cutting down the number of time-consuming irradiation experiments required to qualify a new material.

"Before, those experiments had been a big black box," said Teague. "If we can make truly fundamental, physics-based models, we could get to the point where you could model material performance and then design a more targeted irradiation campaign."

*(Posted Aug. 18, 2014)*

Feature Archive