Understanding and predicting materials behavior

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One of the great challenges in the world of nuclear engineering is the behavior of materials under extraordinarily harsh conditions. Over time, the intense radiation, high temperatures and stresses, and corrosive environments in fission and fusion reactors alter material properties and behavior; understanding these changes is central to effective reactor design and operation.

“Strategic planning in the nuclear science and engineering department is leading us to a greater emphasis on materials in extreme environments, in both education and research,” explains nuclear science and engineering (NSE) associate professor Bilge Yildiz, who has taught the department’s class on nuclear materials since 2008. “Experimentally and computationally, understanding and predicting how materials evolve as they age in nuclear environments is essential.”

Close coupling of computer simulations with experiments is an important approach for developing new knowledge of nuclear materials. For this reason, undergraduates and graduate students who take the nuclear materials class must complete an end-of-term computation or experimental project on a subject of their choice, with input from guest lecturers.

“It’s a great opportunity for our students,” Yildiz says. “Not just for nuclear materials, but for the whole range of nuclear work, where computational modeling and simulation is increasingly important.” This importance is exemplified by Professor Ju Li’s subject in Computational Nuclear Science and Engineering, which teaches programming, algorithms and modeling.

On the experimental side, a number of NSE faculty are working to develop in-situ techniques for probing material behavior under functional conditions similar to those found in reactor chambers, both to validate simulations and gain new insights. “You can do a post-mortem, but it’s important to be able to see what’s going on in real time, the dynamic evolution of the materials, because mechanisms of structural evolution cannot be captured post-mortem,” Yildiz notes.

NSE Professor Dennis Whyte is using this approach to explore plasma-surface interactions, a central issue in fusion reactor design, while Li is developing better understanding of charge/discharge mechanisms in battery materials. Yildiz is probing structure-reactivity-stability relations on surfaces in fuel cells, and corrosion at elevated temperatures.

Materials work at NSE is also increasingly engaged with the Institute’s materials science and engineering and mechanical engineering departments, developing interdisciplinary knowledge through several broad initiatives. These include the Department of Energy-sponsored Consortium for Advanced Modeling of Light-Water Reactors, which is focused primarily on nuclear fuel-related challenges, including fuel rod cladding — the slender tubes that hold fuel pellets while they are in use in

fission reactors.

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