Surface dynamics studies yield resilient materials for applications in high-intensity environments

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Bilge Yildiz. Credit: David Sella

Solid core material is almost a given for technology. But just because the guts are right doesn't guarantee success. The surface layer, in fact, can hold the key in some applications. Yet its importance is still easy to overlook. This area is where Bilge Yildiz keeps her focus. The associate professor of nuclear science and engineering and principal investigator of the Laboratory for Electrochemical Interfaces looks at a surface and how it acts in harsh environments.

High temperatures, reactive fluids, and mechanical stresses all conspire to alter material behavior, and, with it, performance. When it comes to something such as clean fuel production and energy conversion, bad surfaces slow down reactions and lower output. In nuclear power plant or oil pipelines, this leads to faster rates of corrosion. Yildiz wants to reverse those processes. Through lab and computational work, her research group have been making inroads by studying the interaction of material and environment on the atomic and nanoscale, and ultimately making better, more resilient materials for energy technology.

Looking at the outside

The key to mitigating the corrosion of materials is to understand the passive outer layer of film that natively forms and serves to protect the base material. If that can be done, the layer can be engineered to last longer. And while it sounds obvious, industry testing and predictive models on corrosion have been rudimentary, relying mostly on empirical data rather than solid physical mechanisms, Yildiz says. One obstacle has been the difficulty of probing these very surfaces in inhospitable environments that are difficult to access. In answer to that, Yildiz has designed a specialized instrument—a scanning tunneling microscope—which works in situ, in temperatures up to 600 degrees Celsius, and which offers a new way of visualization at the nanometer and atomic scales.

She's used the device to study pyrite, which has brought an essential finding. The mineral is insulating in bulk, and relying on that information—which essentially has been the standard course—leads people to believe that the corrosive process would be slow. But by looking at pyrite's surface, Yildiz found that it easily transfers electrons, forms defects, and can accelerate corrosion. This gap exists, and, by knowing this, smarter choices can now be made. "It's very important input in designing and developing models to predict the rates at which these materials would corrode and ultimately degrade and fracture," she says.

Blowing off hydrogen

A side product of metal corrosion caused by water is that the water splits and releases hydrogen. One of two things then happens. The hydrogen can leave the surface or it becomes incorporated into the bulk of the material and degrades the load-bearing properties via hydrogen embrittlement. The former is desirable; the latter isn't. "Hydrogen in the bulk of the materials has been studied for a long time, but the key may be to just not let it enter through the surface," Yildiz says. Again, it's a confined interface in a harsh environment, but those qualities make understanding the hydrogen entry process, and the potential to control it, even more necessary.

Yildiz has performed computational work on how hydrogen absorption and transport can take place through this surface layer from the environment into the bulk metal. Surveying different compositions that could be used to alter the physical properties of the passive surface film, the results predicted physical descriptors that are tunable by composition to stop or minimize the entry of hydrogen through this critical interface. While this work was performed for zirconium alloys, it can now be extended to a wide range of metals that suffer from hydrogen embrittlement. Yildiz is collaborating with industrial partners to implement the new materials. "The aim is to make materials that are more durable by stopping hydrogen at the surface and avoid its entry into the metal," she says.

Boosting energy

Yildiz also works on electrochemical energy conversion in high-temperature fuel cells and electrolytic cells. In this field, she's looking at the same properties as with metallic interfaces, namely how the oxide surface chemistry affects either efficiency or degradation. For fuel cells, the goal is to enable clean and sustainable electricity generation. With electrolyzers, the goal is to connect them to nuclear reactors or concentrated solar plants in order to provide the necessary heat to electrolyze steam and carbon dioxide, and generate hydrogen or synthetic gas. Such potential would be of interest to the nuclear industry, she says, because it's one means to expand the applicability of nuclear energy to making fuels that would work for something like transportation.

Furthermore, these systems can run reversibly—as a fuel cell and electrolyzer—meaning large-scale energy storage capabilities, in conjunction with renewable and nuclear energies. Currently, U.S. nuclear plants run with a base load that can't respond to fluctuations in demand. The cell would not only generate electricity, but also store energy in the form of produced fuel. Add that to the plant's existing electricity, and peaking behavior in the demand curve can be addressed and supplied, she says.

Again, it comes down to understanding the material surfaces—in this instance, for improving the productivity and durability of the device. It is desirable to have faster reaction and conversion rates for these technologies to produce electricity and fuels. But without knowing what's on the surface of the material, since that's where reactions occur, the rates can't be accelerated. Through her work, Yildiz has been able to identify the surface behavior and design materials to accelerate reaction rates for better performance and increased life. This means that the technology can be made more efficient, more durable, and more economical when coupled with other energy sources, such as nuclear, solar, and wind.

"While this is a new technology," Yildiz says, "it can become a game-changer in large-scale energy storage."

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