The **Advanced Photon Source**

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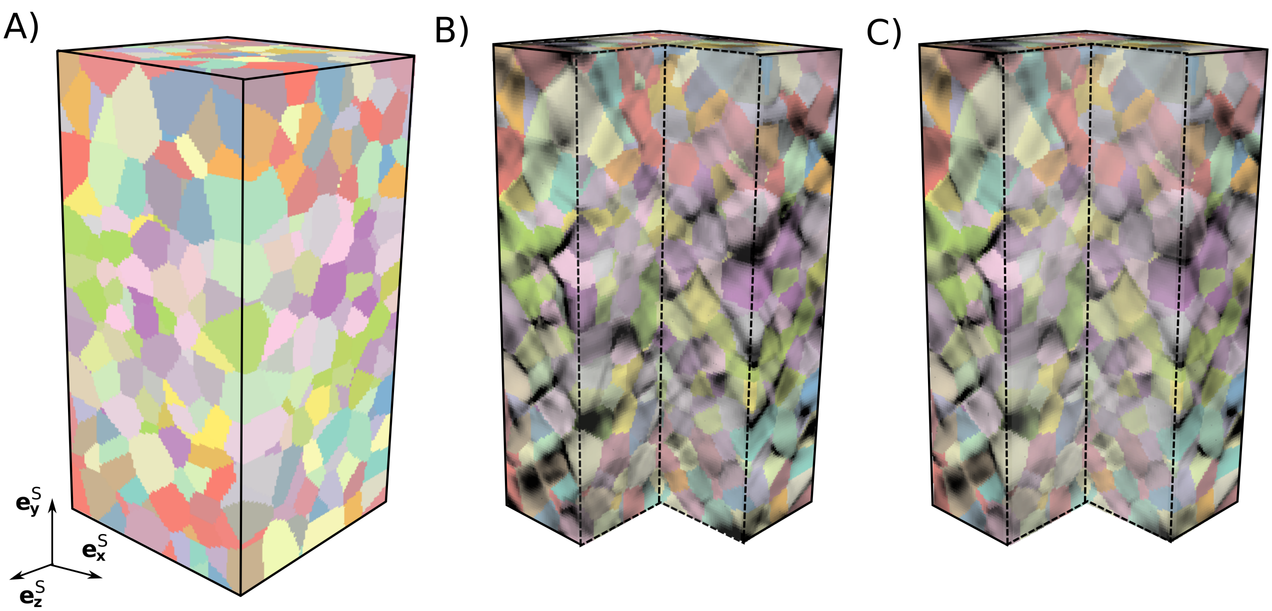
Stressing Over New Materials



Titanium is a workhorse metal of the modern age. Alloyed with small amounts of aluminum and vanadium, it is used in aircraft, premium sports equipment, race cars, space craft, high-end bicycles, and medical devices because of its light weight, ability to withstand extreme temperatures, and excellent corrosion resistance. But titanium is also expensive. Metallurgists would love to understand exactly what makes it so strong so that they could design other materials with similarly desirable properties out of more common, less expensive elements. Now, researchers utilizing the U.S. Department of Energy's Advanced Photon Source (APS) have used high-intensity x-rays to show how titanium alloy responds to stress in its (until now) hidden interior. Eventually, the researchers believe they will be able to predict how strong a titanium part such as an aircraft engine will be, just by knowing how the crystals are arranged inside of it. And materials scientists may be able to use such a computational model to swap in atoms from different metals to see how their crystalline structures compare to that of titanium.

Previous work on titanium's physical qualities required materials scientists to grow a macroscopic crystal large enough to see. But researchers from Lawrence Livermore National Laboratory, Carnegie Mellon University, and the U.S. Air Force Research Laboratory wanted to see how a typical titanium alloy made up of crystals of realistic size — tens of microns or so across — reacted to stress in its natural environment inside a larger block of titanium, just as a titanium crystal inside a bicycle frame or artificial hip might react. They took a chunk of titanium alloyed with 7% aluminum and, working with colleagues from Argonne National Laboratory, exposed it to the high-energy x-rays at the X-ray Science Division 1-ID-E beamline at the APS, which is an Office of Science user facility at Argonne. The titanium-aluminum alloy is similar to titanium-aluminum-vanadium but simpler to model. The 1-ID-E beamline delivers a high flux of x-rays energetic enough to penetrate a full centimeter into solid metal. There are only five facilities in the world capable of producing brilliant x-rays of such high energies.

The researchers carefully aligned a titanium specimen inside a custom built apparatus that could exert various forces on it — pulling in this case – while still allowing the sample to rotate which enabled thee-dimensional measurements. When the high-brightness and high-energy x-rays illuminated the mm-thick titanium sample, most of them were transmitted while a fraction of them were absorbed and another fraction interfered with the atoms comprising the metals crystalline lattice. The absorbed x-rays could be used to form a radiographic image of the specimen, just like in medical and dental applications. The interference led to tell-tale diffraction patterns which reveal the type of crystalline lattice and its corresponding atomic spacing. As the researchers pulled on the titanium block, the crystals inside were stressed and their atoms shifted slightly, changing the lengths of the bonds between them. The changes in the bond lengths reflected the stress the bonds were under. The x-ray diffraction patterns changed as the atoms shifted, revealing how the stress on the atoms increased as the load on the titanium block grew.

Surprisingly, as the load grew so large that the crystals began to permanently deform, the stress on some of the individual atomic bonds and even on entire crystal faces began to drop. In other places the stress grew to compensate (Fig. 1). The researchers did not expect this, and it puts a wrinkle into their theories as to why the titanium alloy is as strong as it is. Permanently deformed areas represent "hot spots" where cracks and other damage are likely to start.

The researchers used the data they gathered at the APS to build a new computational model of titanium at the molecular level. In future experiments they hope to gather more data in more complex environments that are closer to real life situations that titanium parts would encounter. This includes very high or low temperatures, as well as repeatedly stressing and then relaxing the metal to simulate fatigue that happens during actual use. — Kim Krieger

See: Darren C. Pagan[1*‡], Paul A. Shade[2], Nathan R. Barton[1], Jun-Sang Park[3], Peter Kenesei[3], David B. Menasche[4], and Joel V. Bernier[1], "Modeling slip system strength evolution in Ti-7Al informed by in-situ grain stress measurements," Acta Mater. **128**, 406 (2017). DOI:

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Author affiliations: [1]Lawrence Livermore National Laboratory, [2]Air Force Research Laboratory, [3]Argonne National Laboratory, [4]Carnegie Mellon University [‡]Present address: Cornell University

Correspondence: * dcp99@cornell.edu

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