UC San Diego

UC San Diego News Center

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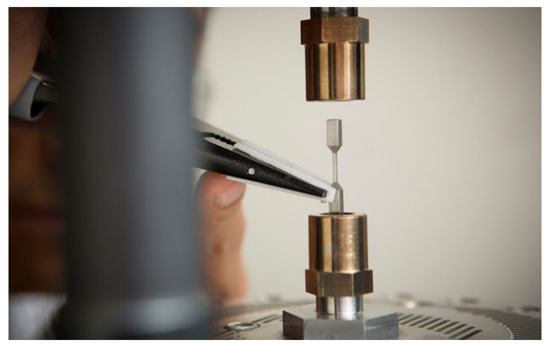
San Diego Supercomputer Center to Help Create Science Gateway for New Materials Discovery

UC San Diego part of a multi-university collaboration funded by the National Science Foundation

Developing predictive computational tools for the design, development, and manufacture of next-generation devices and materials is a grand challenge problem in material sciences. A first step in reaching this long-term goal is conducting detailed studies of how existing materials behave at the atomic level under a wide variety of conditions.



Merging the data taken from samples at CHESS at Cornell University with the most current generation of structural material models can change the way new alloys and new engineering components are constructed and designed. Image: Cornell University

The National Science Foundation (NSF) recently awarded a $1 million Research Advanced by Interdisciplinary Science and Engineering (RAISE) grant to a multidisciplinary team of researchers at the San Diego Supercomputer Center (SDSC) at the University of California San Diego, the University of Minnesota, Carnegie Mellon University, and Cornell University to create the X-ray Imaging of Microstructures Gateway (XIMG), a science gateway designed to make it possible for global material sciences researchers to study the behavior of new and existing materials using X-ray diffraction.

The XIMG Science Gateway will be an online resource that provides researchers everywhere with tools to examine high energy X-ray data collected from beamlines at the Cornell High Energy Synchrotron Source (CHESS) as well as other synchrotrons around the world. A single experiment at CHESS using high energy x-rays generates Terabytes of high-fidelity scattering data and XIMG (*pronounced X-image*) will provide tools to examine these large datasets in the presence of software and compute power available through the NSF-funded *Expanse* and *Comet* supercomputers at SDSC. This will allow scientists and engineers to analyze data that are currently difficult or impossible to access on-line.

Science gateways make it possible to run available applications on supercomputers such as SDSC's *Comet* system, allowing researchers to focus on their scientific problems without having to learn the details of how supercomputers work.

Over the past decade, CHESS and several other high-energy synchrotrons around the world have developed cutting edge techniques to use spatially resolved X-ray diffraction to characterize important structural materials. These materials, such as steel, titanium, and aluminum alloys, are used in almost every important load-bearing application. When analyzed by high-performance supercomputers, the large X-ray diffraction data sets collected at high intensity x-ray sources reveal how the three-dimensional microstructure of complex materials behaves under stress, where reliability, sustainability, and durability are key. Ultimately, the data gathered and analyzed using XIMG will make it possible to predict the properties of next-generation devices and materials using computer-aided design.

The XIMG will be developed by a multi-institutional team led by Principal Investigator (PI) Jorge Vinals of the University of Minnesota, Professor Matthew Miller at Cornell University, Professor Robert Suter of Carnegie Mellon University, and Dr. Mark Miller, a biologist at SDSC and PI of the NSF-funded CyberInfrastructure for Phylogenetic RESearch (CIPRES) gateway. The project will include domain colleagues and software developers from all four institutions.

"Merging this high-fidelity X-ray data from CHESS with the most current generation of structural material models can change the way new alloys and new engineering components are constructed and designed with those alloys," said co-PI Matt Miller at Cornell. "We are excited for the accessibility this will create for researchers in the broader materials science community."

"The XIMG will be the first of its kind for the materials science community where toolkits are available for visualization, modeling, and simulation at mesoscale and nanoscale levels," said Mark Miller. "Providing public access to these resources will not only make it easier to use existing tools to analyze synchrotron data, it will also make it easier to develop and benchmark new tools, and distribute and test new tools within the community."

The NSF RAISE program supports lines of research that promise transformational advances through prospective discoveries that reside at the interfaces of disciplinary boundaries and can be outside the scope of a single NSF program, according to the federal agency. The XIMG award, (NSF OAC 2037773), runs from August 1, 2020 through July 31, 2022 (estimated). The award abstract can be found here.

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