LDRD@SNL

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Sandia National Laboratories
Laboratory Directed Research and Development

We welcome your questions, comments, and ideas for future LDRD projects to feature! Email your feedback to Marie Arrowsmith, mdarrow@sandia.gov

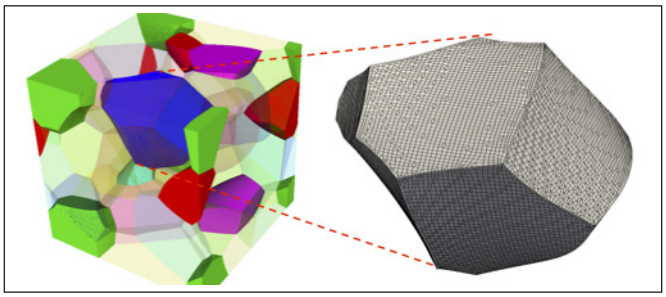
Creating Physically-Based 3D Microstructures: Bridging Phase Field and Crystal Plasticity Models

Corbett Battaile (PI), Hojun Lim, Fadi Abdeljawad, Sandia's Cubit team

LDRD-developed capability for constructing realistic finite element models of materials microstructures provides first-ever technology for mechanics analysis of fully realistic 3D microstructure models.

Understanding microscale behavior of materials used in engineering applications is critical for ensuring performance and reliability, particularly for miniaturized components. Simulating material behavior at the microscale (e.g., individual grains) depends on models of 3D structures that realistically depict material properties, such as grain size and shape, texture, and orientation. Existing finite element polycrystalline models and 3D models derived from experiments fail to adequately represent real microstructures. In this Exploratory Express LDRD (short-term and formulated to answer a key research question), Sandia researchers successfully developed a technique to create physically based 3D microstructures, to be used as input into codes for simulating and analyzing mechanical behavior at the microscale.

The team used phase field and crystal plasticity modeling (used to study interfacial problems by considering thermodynamic and mechanical behaviors) to develop 3D microstructure models using a newly developed finite element meshing technique. By using hexahedral finite elements, these realistic polycrystalline meshes simulate smooth grain interfaces and realistic grain boundaries. This capability provides the first-ever technology for mechanics analysis of fully realistic 3D microstructure models, and has wide-ranging applicability to microstructure-based finite-element analysis.



Conformal meshing finite element representation of a three dimensional polycrystalline microstructure, constructed from

Radiography Signature Science of Homemade Explosives

John Parmeter (PI), Vicki Garcia, Ed Jimenez, Burke Kernen, Jason Phillips, Kyle Thompson

Sandia researchers are investigating the X-ray attenuation properties of key types of homemade explosives both experimentally and theoretically, and developing novel algorithms for the analysis of X-ray radiography data.

The ability to accurately screen baggage for explosive materials is critical to aviation security. Detection of explosives based on the differential attenuation of X-rays at different energies is currently used to attempt to identify explosives at airport checkpoints. While considerable research in this area has focused on the detection of traditional explosives, research on the X-ray radiography of homemade explosives (HME) has received less attention. In this LDRD, Sandia researchers used multi-energy computed tomography (CT) measurements and theoretical calculations to investigate the X-ray attenuation properties of various liquid and powder HME, demonstrating excellent agreement between experiment and theory in many cases. Work was also carried out in the development of novel algorithms for the analysis of raw radiography data. The LDRD concluded in September 2015, and the project team will continue research on the X-ray radiography of various explosives as part of the Open Threat Assessment Platform (OTAP) project, funded by the Transportation Security Administration.

LDRD Participants Recognized

Carol Adkins was named a distinguished alumna by the University of New Mexico's School of Engineering.

Dan Sinars was elected a Fellow of the American Physical Society through its Division of Plasma Physics. The distinction is awarded to no more than 0.5 percent of the society's membership.

The American Institute of Aeronautics and Astronautics (AIAA) has recognized Sandia researchers **Joe Oefelein** and **Guilhem Lacaze** with a best paper award for their work on scramjet engine simulations.

LDRD PROJECTED BUDGET AND STATUS

FY16 Q1 $155 MILLION 319 PROJECTS *FUNDED AT* $141.7 MILLION

Upcoming Events

Nov 4/5 - HAANA Grand Challenge External Advisory Board
Nov 13 - Deadline to submit R&D100 one-page applications (for corporate sponsorship)
SAVE THE DATE! Jan 28 - FY2017 LDRD Program Town Hall

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