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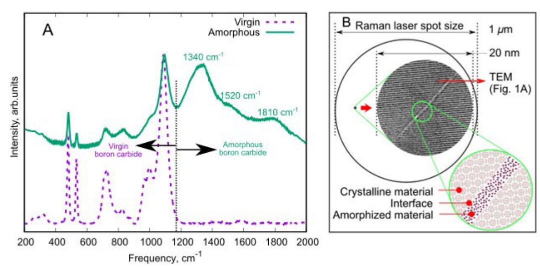
SDSC Supercomputer Simulations Aid in Solving Boron Carbide Mystery

Novel research findings assist in advancing future military armor

Boron carbide is one of the hardest materials on earth yet also very lightweight, which explains why it has been used in making vehicle armor and body protection for soldiers during the last 50 years or so. Building upon decades of research on how to make boron carbide even more efficient, an engineering team at the University of Florida (UF) has been conducting supercomputer simulations to better understand the nanoscale level of this important material.



A: The longstanding mystery: Raman spectrum of amorphized boron carbide contains unexplained new peaks (green). B: A multi-scale model showing layout of proposed mechanistic rationale and length scales of TEM (transmission electron microscopy) and Raman laser-size. Credit: High-Pressure Deformation and Amorphization in Boron Carbide in the Journal of Applied Physics (2019) (DOI:10.1063/1.5091795)

The research, which primarily used the *Comet* supercomputer at the San Diego Supercomputer Center (SDSC) at UC San Diego along with the *Stampede* and *Stampede2* systems at the Texas Advanced Computing Center (TACC), may ultimately provide the military with more protective mechanisms for vehicle and soldier armor after further testing and development are done.

The study, using fundamental physics principles including quantum mechanics, was published earlier this year in an article called High-Pressure Deformation and Amorphization in Boron Carbide in the *Journal of Applied Physics.* Access to *Comet* was provided by a grant from the National Science Foundation's Extreme Science and Engineering Discovery Environment, or XSEDE.

“Our research provided new insights and an excellent way of analyzing the root cause of catastrophic failure at high pressure induced by high-velocity impacts,” said UF Professor of Mechanical and Aerospace Engineering Ghatu Subhash. “Although boron carbide has several desirable properties, under high-velocity projectile impacts it suffers from a deleterious phenomenon called amorphization, where its crystal structure collapses in nanometer-sized regions within the materials.”

Amorphization is the precursor for cracks in the armor, which may cause eventual catastrophic failure.

Researchers were able to do large-scale and multi-scale modeling of icosahedral-boron rich solids, the class of crystallographic structure to which boron carbide belongs. “Our simulations ran over three times faster per core when we switched from local work stations to *Comet*, and today our knowledge pertaining to material behavior of icosahedral ceramics has been elevated to a level that is second to none,” said Subhash.

MEDIA CONTACT

Jan Zverina, 858-534-5111, jzverina@sdsc.edu
Kimberly Mann Bruch, 858-822-3622, kbruch@ucsd.edu