

May 18, 2020 | By Kimberly Mann Bruch

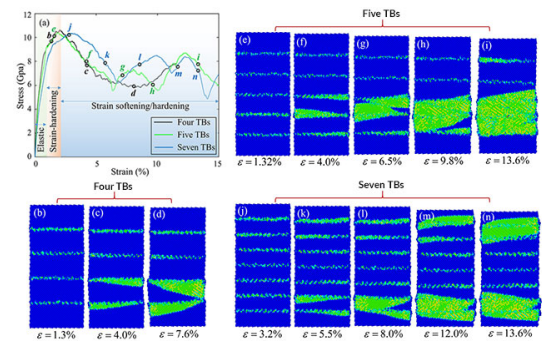
Supercomputers Reveal True Strengths of Some Zirconia Ceramics

Simulations suggest applications ranging from prosthetics to aerospace engines

For thousands of years, humans have produced ceramics by simply combining specific minerals with water or other solvents to create ceramic slurries that cure at room temperature and become some of the hardest known materials. In more recent times, zirconia-based ceramics have been useful for an array of applications ranging from dental implants and artificial joints to jet engine parts.

Researchers from the Colorado School of Mines have been using multiple supercomputers – *Comet* at the San Diego Supercomputer Center ([SDSC](#)), *Stampede2* at the Texas Advanced Computing Center ([TACC](#)), and *Bridges* at the Pittsburgh Supercomputing Center ([PSC](#)) – to study certain characteristics of zirconia. The team recently published their findings in the *Journal of the European Ceramic Society*.

According to corresponding author Mohsen Asle Zaeem, a mechanical engineering professor at the Colorado School of Mines, the study focused on creating supercomputer simulations that show zirconia-based ceramic's ability to withstand harsh conditions as well as the extreme limits of fracture and fatigue.



The findings provided significant insight into the behavior of twin boundaries and pre-existing defects in shape memory ceramics. These simulations illustrate: (a) Stress-strain relations of four-, five- and seven-twin boundaries (TB) YSTZ nanopillars. The elastic, strain-hardening, and strain softening/hardening regions of four- and five-TB pillars are denoted by shadows with different colors. The seven-TB pillar regions shift at about 1% strain to the right. Snapshots in (b–n) correspond to strain points b–n (a). Atoms in b–n are colored by coordination number (CN). Blue and green atoms represent tetragonal and monoclinic phases, respectively. Atoms with other colors stand for disarranged structures. Credit: N. Zhang and M. Asle Zaeem, Colorado School of Mines

“By using large-scale atomistic simulations, these simulations revealed to us how specific type nanoscale structures, twin boundaries, and pre-existing defects control the mechanical behavior and the corresponding plastic deformation of an advanced shape memory ceramic called yttria-stabilized tetragonal zirconia or YSTZ,” explained Asle Zaeem. “Some important applications, such as jet engines, require advanced materials that can perform reliably at extreme conditions. Shape memory ceramics have shown superior properties at those higher temperatures such as high strength and excellent oxidation/corrosion resistance. Addressing their deformation, fracture, and fatigue limitations will open the door for creating the next generation of high-temperature materials.”

This research was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, (DE-SC0019279).

MEDIA CONTACT

Jan Zverina, 858-534-5111, jzverina@sdsc.edu

UC San Diego’s [Studio Ten 300](#) offers radio and television connections for media interviews with our faculty, which can be coordinated via studio@ucsd.edu. To connect with a UC San Diego faculty expert on relevant issues and trending news stories, visit <https://ucsdnews.ucsd.edu/media-resources/faculty-experts>.