MM 6: Invited Talk: David Rodney

Time: Monday 15:00–15:30 Location: SCH/A251

Invited Talk MM 6.1 Mon 15:00 SCH/A251

Transformation-induced plasticity in zirconia ceramics: simulations and experiments — •David Rodney — Insitut Lumière Matière, University of Lyon, France

Similar to steels, zirconia ceramics display transformation-induced plasticity (TRIP) through an stress-induced tetragonal-to-monoclinic phase transformation. However, the conditions under which TRIP occurs remain unclear, owing to the intrinsic complexity of the transformation, which involves multiple variants and intermediate phases, and to experimental and computational limitations. Experimentally, the transformation is difficult to track in situ and classical interatomic potentials do not capture zirconia's polymorphism.

We present a combined experimental and numerical study addressing these challenges. Experimentally, we perform in situ Laue microdiffraction on ceria-doped zirconia micropillars compressed along different crystallographic directions. We replicate the same loading conditions in atomistic simulations using a neural-network interatomic potential (NNIP) trained on extensive DFT data and capable of describing the phase behavior of pure and ceria-stabilized zirconia.

Comparison between experiments, NNIP simulations, and DFT calculations provides new insights into the transformation mechanisms. The results clarify the origin of tetragonal stabilization by ceria and show that TRIP proceeds through a complex sequence of stable and metastable phases, including multiple monoclinic and orthorhombic structures, revealing a richer transformation landscape than previously recognized.