MM 25: Invited Talk: D. Rodney

Time: Thursday 9:30–10:00 Location: H10

Invited Talk MM 25.1 Thu 9:30 H10

Transformation-induced plasticity in zirconia ceramics: neural network simulations and in-situ experiments — •David Rodney — Institut Lumière Matière, Université de Lyon, France

Brittleness limits the structural use of ceramics, but zirconia stands out due to transformation-induced plasticity (TRIP) between tetragonal and monoclinic phases. This stress-driven transformation enables up to 7% plastic deformation in single-crystalline ceria-doped zirconia, offering potential for high ductility. However, understanding the TRIP effect remains incomplete.

To address this, we combined in situ Laue micro-diffraction experiments at synchrotron facilities with atomistic simulations. Existing interatomic potentials fail to capture zirconia's complex polymorphism. We thus developed neural network interatomic potentials (NNIP) using DeepMD-kit for pure and ceria-doped zirconia. These NNIPs align well with ab initio data on thermodynamic, mechanical, and dynamical properties, accurately modeling phase stability, elastic properties, and energy barriers.

Using the NNIPs, we simulated the uniaxial compression of tetragonal ceramics, exploring stress-strain behavior, phase transformations, and deformation mechanisms across various compression directions. Simulations are confronted with the in situ experiments and the phenomenological theory of martensitic transformation. Key factors, including size, temperature, strain rate, and pre-existing defects, are critically analyzed, providing a comprehensive understanding of stress-induced phase transformations in zirconia ceramics.