Transformation-induced plasticity in ceria-doped zirconia ceramics: atomic-scale insights using a deep neural network potential

Jin-Yu Zhang, Gaël Huynh, Tristan Albaret, David Rodney

Institut Lumière Matière - Université Claude Bernard Lyon 1, 69622 Villeurbanne, France

Abstract

Zirconia (ZrO_2) ceramics exhibit remarkable mechanical properties, namely transformation-induced plasticity (TRIP), shape memory, and superelasticity. However, understanding the complex atomic-scale processes controlling these phenomena is challenging. Here, we introduce a deep neural network interatomic potential to accurately predict phase transformations in both pure and CeO_2-doped ZrO_2 ceramics. Through molecular dynamics simulations, we examine the mechanical responses of tetragonal CeO_2-ZrO_2 single crystals and polycrystals under uniaxial loading. At odds with the traditional understanding of the TRIP effect in zirconia ceramics, our simulations reveal that the classical stress-induced tetragonal-to-monoclinic phase transformation often involves an intermediate phase, which can either be a tetragonal phase resulting from ferroelastic switching or an orthorhombic $Pbc2_1$ phase. Consequently, the TRIP effect may be hindered if the applied compression is unfavorable for the intermediate phase, even if the final martensite phase has a high Schmid factor. Our findings on polycrystalline compression underscore the importance of grain boundaries as nucleation sites. Combined with the complex internal stress distribution, this leads to the formation of all three monoclinic lattice correspondences through complex pathways that are analyzed in detail.

Links to the recent papers:

https://doi.org/10.1016/j.actamat.2024.120661

https://doi.org/10.1016/j.jeurceramsoc.2024.01.007