TRIP effect in Zirconia: atomistic simulations and in-situ experiments

Gaël Huynh[1], Jin-Yu Zhang , Marcelo Demetrio De Magalhaes[2], Tristan Albaret , and David Rodney*†

[1]Institut Lumière Matière [Villeurbanne] – Université Claude Bernard Lyon 1, Centre National de la Recherche Scientifique – France

[2]Université de Lyon, INSA-Lyon, UMR CNRS 5510 MATEIS, 69621 Villeurbanne Cedex, France (MATEIS) – MATEIS, UMR 5510 CNRS, 69621 Villeurbanne Cedex – 345 Av. Gaston Berger, 69100 Villeurbanne, France

Abstract

Like steels, zirconia ceramics exhibit transformation-induced plasticity (TRIP) due to a transformation between a tetragonal and a monoclinic phase. This unique feature allows zirconia ceramics to undergo substantial plastic deformation, reaching a remarkable 7% plastic strain. However, this effect is far from fully understood, hindering the development of ceramics with macroscopic deformability exceeding 1%. Additionally, the lack of interatomic potentials capable of accurately describing zirconia complex polymorphism and phase transformations makes understanding the TRIP effect at the atomic scale difficult.

In this work, we combine in-situ Laue diffraction on micropillars and atomic-scale simulations to obtain microscopic information on transformation conditions. Specifically, we explore how compression direction influences the transformation. The simulations required the development of a neural network-based interatomic potential to accurately describe zirconia polymorphism. We characterize the deformation processes, critical stress-strain states, and phase transformations both experimentally and numerically across various compression directions, spanning the entire standard triangle.

Our simulations challenge the prevailing notion that a limited number of variants govern the TRIP in zirconia. Furthermore, we observe through simulations a complex interplay between competing stable and metastable phases, some of which have not been documented experimentally. An interesting question, which remains to be explored, is why these phases have not been reported experimentally so far: an effect of size, temperature, or strain rate, a lack of realism of the NNP, or have these phases been overlooked experimentally in the past?

*Speaker

†Corresponding author: david.rodney@univ-lyon1.fr