Role of the electron irradiation on the plasticity of a-Al2O3: atomistic simulations meet experiments

Giuliana Materzanini[*†1], Andrey Orehkov[‡2], Paul Baral[3], Erkka J. Frankberg[4], Gian-Marco Rignanese[1,5], Thomas Pardoen[1], and Hosni Idrissi[§1]

[1]Université Catholique de Louvain – Belgium
[2]University of Antwerp – Belgium
[3]Ecole Nationale Supérieure des Mines de Saint-Étienne – Ecole Nationale Supérieure des Mines de Saint-Etienne, Ecole Nationale Superieure des Mines de Saint Etienne – France
[4]Tampere University – Finland
[5]Northwestern Polytechnical University – China

Abstract

Investigating the response of amorphous oxides to stress is crucial for applications such as wear-resistant coatings, catalysis, and microelectronic devices. The current experimental setup includes a push-to-pull deformation device for tensile testing and a transmission electron microscope (TEM) for imaging the evolving microstructure. However, during TEM experiments, the electron beam (e-beam) can alter the specimen, affecting its elastic and plastic properties and leading to structural rejuvenation of the amorphous material. In this study, we combine in situ quantitative tensile testing of amorphous alumina (a-Al2O3) in the TEM with large-scale molecular dynamics simulations (∼900,000 atoms) using classical force fields to simulate tensile strain. The e-beam effect is modeled as one-time kinetic energy excitations applied to a small fraction of selected atoms at regular intervals. Both experimental and computational stress-strain curves reveal that the presence of the e-beam reduces stress, enhances plasticity, and increases strain-rate sensitivity in a-Al2O3. Furthermore, analysis of the coordination number and local nonaffine displacement evolution under strain shows that the e-beam promotes bond switching, which relaxes local stresses and favors plasticity. These findings provide new insights into the local structural modifications and rejuvenation of amorphous oxides under electron irradiation.

*Speaker
†Corresponding author: Giuliana.materzanini@uclouvain.be
‡Corresponding author: andrey.orekhov@uantwerpen.be
§Corresponding author: hosni.idrissi@uclouvain.be