Numerical simulation of the UO2 viscoplasticity at the polycrystal scale : microscopic validation

Luc Portelette, Bruno Michel, Étienne Castelier, Marcelle Ibrahim, Mariem Saada, Xavière Iltis, Philippe Garcia

Numerical simulation of the UO2 viscoplasticity at the polycrystal scale : microscopic validation

Luc Portelette * [1], Bruno Michel [1], Etienne Castelier [1], Marcelle Ibrahim [1], Mariem Ben Saada [2], Xavière Iltis [2], Philippe Garcia [2]

[1] French Alternative Energies and Atomic Energy Commission, Fuel Study Department, Fuel Simulation Laboratory (CEA/DEN/DEC/SESC/LSC) – Centre de recherche du Commissariat à l'Energie Atomique - CEA Cadarache (Saint Paul-lez-Durance, France) – France
[2] French Alternative Energies and Atomic Energy Commission, Fuel Study Department, Fuel Behavior Laboratory (CEA/DEN/DEC/SFER/LCU) – Centre de recherche du Commissariat à l'Energie Atomique - CEA Cadarache (Saint Paul-lez-Durance, France) – France

A model based on dislocation glide in a single crystal has been developed in order to simulate uranium dioxide (UO2) viscoplastic behavior during reactor operation of PWRs (pressurized water reactors). This model is then implemented through a 3D finite element formulation to simulate the polycrystal behavior in the volume element application (VER) of the PLEIADES nuclear fuel behavior software environment [1]. With this full field computation, the strain incompatibility induced by the disorientation at grain boundaries is computed along with associated stress and strain heterogeneities. In order to assess the grain size effect, the geometrically necessary dislocation densities are also computed from the viscoplastic strain field. The main objective of this study is to propose a validation methodology at the microscopic scale, in order to check that the computed stress-strain heterogeneity is in good agreement with experimental results. The experimental data used for this validation are based on 2D SEM-EBSD characterizations of polished sections of UO2 pellets, with as-fabricated grains in the 10 μm size range, following to uniaxial compressive creep tests [2]. EBSD provides quantitative micronscale information relating to the crystal lattice orientation, which is strongly correlated to the local viscoplastic strain induced during the mechanical test. Regarding simulation results, the crystal lattice orientation is derived from the elastic rotation computed through a finite strain formulation of the elastoviscoplastic transformation.
First a qualitative comparison between experiment and simulation is proposed which enables us to analyze the spatial variation of orientations within the original grains. Simulation results show that polycrystal viscoplasticity induces a non-uniform crystal lattice orientation as is observed from EBSD measurements. However the experimental spatial variation is discontinuous, as sub-grain boundaries appear, whereas our model describes a continuous variation in grain orientation. Statistical comparisons are provided of the orientation changes within the grains. In order to avoid grain size sensitivity and 2D-3D corrections, a variogram function is defined. According to these first results, it appears that the spatial statistical distribution is consistent with experimental results. However, the magnitude of the orientation variation is greater in the simulation, which suggests that the strain incompatibility is overestimated. Applying this methodology provides a more robust means of both analyzing basic deformation mechanisms and identifying the appropriate intragranular model to describe viscoplastic strains in uranium dioxide polycrystal.

[1] B. Michel, C. Nonon, J. Sercombe, F. Michel, V. Marelle, *Simulation of the Pellet Cladding Interaction phenomenon with the PLEIADES fuel performance software environment*, Nuclear Technology 182 (2), 124-137, 2013.
[2]. M. Ben Saada, N. Gey, B. Beausir, X. Iltis, H. Mansous, N. Maloufi, *Sub-boundaries induced by dislocational creep in uranium dioxide analyzed by advanced diffraction and channeling electron microscopy,* accepted in " Materials Characterization ".

*Speaker

Keywords: UO2, uranium dioxide, ceramic, viscoplasticity, model, polycristal, variogram, disorientation