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Multiscale modelling of polycrystalline UO_2 : full-field simulations (FFT) and model reduction technique (NTFA).

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Uranium dioxide (UO_2) is a polycrystalline ceramic used as nuclear fuel within Pressurised Water Reactors (PWR). To account for the behaviour of this material during a Reactivity Initiated Accident (RIA) characterised by strain rates $\dot{\epsilon} \in [0.1, 10.] [s]^{-1}$ and temperatures $T \in [500, 2400] [^\circ C]$, a micro-mechanical approach is adopted. In this numerical study, UO_2 is studied above a temperature ($T > 1000 [^\circ C]$), which the material exhibits an elasto-visco-plastic behaviour with strain hardening. Assumption is made that the visco-plastic strain is entirely induced by the sliding of dislocation lines overcoming the Peierls barrier energy. An empirical thermally activated plasticity law is adopted to model this behaviour[3]. Validated at the single crystal scale[2], the numerical results differ from the experimental results[4] on a polycrystalline VER. In response, to obtain a better agreement with the experimental results at the polycrystal scale[4] an inverse calibration is performed taking into account the strain hardening and the sensitivities to the loading parameters ($T, \dot{\epsilon}$). Once validated at the polycrystalline scale on uniaxial compressive strain tests[4], the full field FFT numerical simulations are taken as reference to develop and validate a reduce order model.

In the perspective of using this law in an industrial code, implying reasonable simulation times, it appeared necessary to use a model reduction technique to replace the full field resolution. In particular, the Non Transformation Field Analysis (NTFA)[1] is used. The agreements between NTFA model and full-fields simulations (FFT) are checked on the macroscopic and local fields.

It is first verified on few uniaxial loadings that the numerical results from the NTFA Tangent Second Order (TSO)[1] model applied to the problem at hand match the Full-Field simulations. Then work is done to address the difference in behaviour covered by the different loading parameters specific to the RIA while keeping the number of internal variables as low as possible. In particular, interpolation functions are used to make the modes of the NTFA model temperature dependent ($\mu_{vp}(T_0)$). Next a method is used to achieve the dependence of the strain rate ($T_0 = f_{|\dot{\epsilon}_0}(T, \dot{\epsilon})$). It is checked that the numerical results are not deteriorated either macroscopically or locally. Finally, a comparison is made between the strain hardening taken as constant per grain and the decomposition of this internal variable, like the visco-plastic strain, on modes.

References

- [1] Michel, J.-C., Suquet, P., “A model-reduction approach to the micromechanical analysis of polycrystalline materials”, *Computational Mechanics*, 57.3, pages 483-508 (2016).
- [2] Mordike, B.L., “Yield and flow of single crystals of uranium dioxide”, *Journal of Nuclear Materials*, 60.2, pages 223-226 (1976).
- [3] Portelette, et al., “Crystal viscoplastic modeling of UO_2 single crystal”, *Journal of Nuclear Materials*, 510, pages 635-643 (2018).
- [4] Salvo, M., et al., “Experimental characterization and modeling of UO_2 grain boundary crack- ing at high temperatures and high strain rates”, *Journal of Nuclear Materials* (2015).