Multiscale - atomistic/mesoscopic approach for the determination of fracture criterion in uranium dioxyde - UO_2

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For the thermomechanical modeling of the global evolution of the nuclear fuel (UO_2) during a hypothetical accident situation such as RIA (Reactivity Initiated Accidents) [1], it is necessary to establish a reliable UO_2 grain boundaries fracture threshold, whether it be in terms of stress or energy of the grain boundaries. At present, the fracture thresholds used in nuclear fuel simulation codes need to be consolidated by experience and theory. The aim of this study is to obtain, by calculations at two scales (atomistic/mesoscopic), mechanical and fracture parameters of grain boundaries.

Our approach consists of feeding a mesoscopic model with data from simulations at the atomic scale. The atomistic simulations are of the molecular dynamics type and use a variable charges semi-empirical potential (SMTB-Q [2]) to describe the interactions between atoms. These calculations, carried out using the LAMMPS software, are performed on three grain boundary nanoscale structures representative of UO_2 at different temperatures. The atomistic simulations allow to obtain elastic properties and local fracture parameters (maximum stress and fracture energy) characteristic of the grain boundaries studied.

The results from atomistic calculations are then used as input data in cohesive zone models to perform simulations at the scale of the uranium dioxide grains which is that of the micron. At this scale, cohesive-volumetric approach using the concepts of Frictional Cohesive Zone Model (FCZM) in a multibody systems framework based on the Non-Smooth Contact Dynamics (NSCD) is employed [3]. The impact of the presence of intergranular bubbles of different sizes is studied. A plastic model is used in the volume to consider possible dislocation movement in the system. The associated calculation code, called XPER, allows to analyze cracking induced by grain boundaries. The results are compared with the experiment to validate the approach.

In the end, we propose, based on results of the present study, a failure criterion that can be used in macroscopic simulation codes of nuclear fuel.

References

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