

Multiscale Phase-Field Modelling of Shape Effects on Crack Initiation from Complex Pressurized Bubbles.

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Paper ID: 84

[Symposium S8: Fracture, and damage of materials](#)

Abstract

Spent nuclear fuels exhibit restructured microstructures and porosities of varying complex geometries [1], [2], [3]. The latter are pressurised by rare gases [4], and may act as singularities from which, in storage conditions, cracks may onset [5], [6]. Understanding the influence of these bubble shapes on fracture behaviour is essential for predicting spent fuel behaviour and assessing its structural integrity in long-term storage. In that regard, this study presents a multiscale phase-field modelling approach [7], [8] to investigate how bubble shape impacts crack initiation under internal pressure loading. The framework intends to capture the coupling between geometric features, stress concentration, and fracture initiation across multiple length scales on the one hand, and to propose an engineering model to predict crack initiation from arbitrarily shaped pressurised bubbles on the other hand. A hierarchical micromechanical modelling strategy is thus employed, combining microscale phase-field simulations with macroscale stress analyses to resolve the onset of cracking. Various bubble geometries, based on Scanning Electron Microscopy (SEM) examinations of irradiated fuel [9], are systematically analysed to quantify their influence on local stress singularities, damage distributions, and critical fracture pressure thresholds. Phase-field results show deviations in comparison with non-singular geometries (through carefully chosen shape parameters)

and enable the construction of a learning database for a simplified engineering model devoted to crack initiation assessment. The main improvements enable the engineering model to account for the bubble size effect on crack initiation pressure and to include an uncertainty assessment associated with the random distribution of real bubble shapes. For this second aspect, the learning database provides the sensitivity analysis to the selected shape parameters used for geometrical description. The proposed multiscale framework thus serves as a versatile engineering tool for predicting crack initiation and understanding the mechanistic role of geometric features in brittle fracture processes.

Keywords:

Irradiated nuclear fuel behavior Crack initiation Phase field modelling Coupled criterion Pressurized bubbles Complex shapes

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