Coupling Crystal Plasticity with Phase Field Fracture for Creep Damage Formation Analysis in Austenitic and Ferritic Steels

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Abstract
Accurate modelling and prediction of both statistical trends in damage formation and damage site initiation is critical in both the design, microstructure optimization and lifetime management of components and welded joints for nuclear power stations. This paper presents a coupling between a strain-gradient based crystal plasticity formulation and a phase field fracture model to predict damage initiation sites, damage propagation and void initiation statistics that match electron microscopy experimental results for grain boundary damage from a 316H stainless steel creep test specimen. The interplay between the grain misorientation and the presence of carbides at the grain boundaries is investigated. A range of novel variations are incorporated into this approach that can isolate damage from varying mechanisms, including slip, creep, and contributions from plastic or elastic deformation within the simulated microstructure. The local effect of carbides, forming on specific grain boundary types, on void cavitation is included by using a misorientation-dependent critical energy release rate. The direct comparison with electron backscatter diffraction experiments clarifies what the most important damage mechanisms are and the quantitative fracture energy reduction as a function of carbide density. The extension of this model to ferritic steel microstructures is also explored.

1. Introduction
A significant limiting factor for the economics of nuclear fission reactor power stations is the safe operating lifetime. In-service testing and monitoring and maintenance techniques have enabled operators to determine and alleviate faults to extend plant lifetime, but the next generation of reactors will incorporate predictive computational modelling techniques to better understand how component performance degrades over time and target maintenance with fewer costly stoppages in operation as testing, monitoring, and maintenance is carried out. Components are subject to high temperatures and pressures, meaning that creep induced damage is a key focus of modelling efforts.

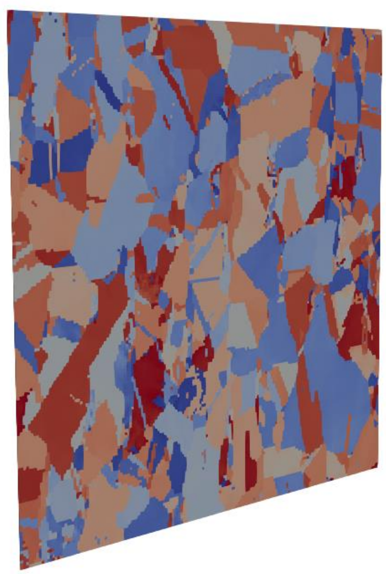
Crystal plasticity modelling approaches have been employed in conjunction with phase field fracture to model various types of material degradation on the microstructural level. Work has been done modelling the nucleation and propagation of twin boundaries, with a coupled model. These coupled models have also been used to model damage surrounding existing voids within a microstructure when subjected to tensile loading.

Investigated in this paper are attempts to pull these concepts together, in order to produce a coupling between crystal plasticity and phase field fracture. A comprehensive model capable of simulating early and late stages of damage and fracture on the material microscale, predicting the statistical trends and damage initiation in fracture, is a new approach.

Austenitic and ferritic steel structures are considered for this work. The model was developed with less complex austenitic microstructures, before applying the model to more inhomogeneous phase structures seen in ferritic steels commonly used in nuclear reactor pressure vessel components.

2. Methodology and Results
A crystal plasticity model was coupled with an energy-based model for phase field fracture and was applied to experimentally determined grain microstructures found using electron backscatter diffraction (EBSD) on

a uniaxial creep specimen. The phase field damage distribution in the crystal plasticity model was compared with experimentally determined voids in the same grain microstructure along grain boundaries. Correlations relating to the statistical distribution of damage across the simulated microstructure were made that match those determined experimentally.



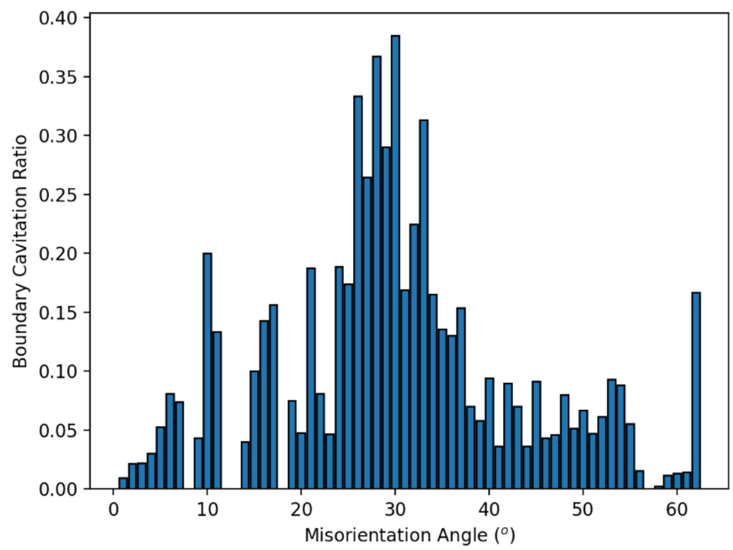


Fig.1 (left) – The polycrystal microstructure simulated from EBSD data of austenitic 316H stainless steel

Fig.2 (right) – The ratio of grain boundaries of specific misorientation angles that exhibit cavitation damage as a function of scalar intergranular misorientation angle in 316H stainless steel

Ferritic steel structures were recreated virtually through EBSD measurements and modelled to determine damage initiation and fracture propagation statistics.

3. Conclusions

The application of a crystal plasticity finite element approach coupled with a phase field fracture model when applied to the grain microstructure of a notched uniaxial creep specimen shows agreement with experimental results when comparing the statistical trends in damage initiation with grain microstructural geometry and creep damage initiation sites in both austenitic and ferritic steels.

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