### PREDICTING MICROSTRUCTURALLY SENSITIVE FATIGUE-CRACK PATH IN WE43 MAGNESIUM USING HIGH-FIDELITY NUMERICAL MODELING AND THREE-DIMENSIONAL EXPERIMENTAL CHARACTERIZATION

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# Abstract

Microstructurally small fatigue-crack growth in polycrystalline materials is highly three-dimensional due to sensitivity to local microstructural features (e.g., grains). One requirement for modeling microstructurally sensitive crack propagation is establishing the criteria that govern crack evolution, including crack deflection. Here, a high-fidelity finite-element modeling framework is used to assess the performance and validity of various crack-growth criteria, including slip-based metrics (e.g., fatigue-indicator parameters), as potential criteria for predicting three-dimensional crack paths in polycrystalline materials. The modeling framework represents cracks as geometrically explicit discontinuities and involves voxel-based remeshing, mesh-gradation control, and a crystal-plasticity constitutive model. The predictions are compared to experimental measurements of WE43 magnesium samples subject to fatigue loading, for which three-dimensional grain structures and fatigue-crack surfaces were measured post-mortem using near-field high-energy X-ray diffraction microscopy and X-ray computed tomography. Findings from this work are expected to improve the predictive capabilities of numerical simulations involving microstructurally small fatigue-crack growth in polycrystalline materials.

#### 1. Introduction

The critical assessment of potential crack-deflection criteria for short cracks requires both experimental observations of crack growth in three-dimensional microstructures and a numerical toolset capable of of quantifying micromechanical fields ahead microstructurally short cracks. For the latter, the authors developed a voxel-based previously remeshing framework and mesh-gradation tool to represent and propagate complex three-dimensional cracks through polycrystalline materials. For the former requirement, four experimental datasets are used to investigate potential crack-deflection (i.e., kink angle) criteria based on the numerical simulations. Grain structure and crack surfaces from three underaged magnesium WE43 thin-foil samples are reproduced directly in numerical simulations to make preliminary assessments of candidate criteria and to establish proposed modifications to the criteria. The criteria include the maximum tangential stress criterion, a Fatemi and Socie-based fatigue indicator parameter, and

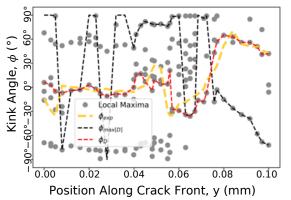


Fig.1 –Predicted kink angles in a thin-foil simulation informed by taking the maximum Fatemi-Socie value ahead of the crack front  $(\phi_{\max[D]})$  and after application of graph-based modification  $(\phi_D)$ . Experimentally observed kink angle is  $\phi_{exp}$ .

the spatial gradient of the aforementioned fatigue indicator parameter. The predictive capabilities of the modified criteria are then tested by performing blind predictions of three-dimensional crack growth in an experimentally characterized underaged magnesium WE43 polycrystal extracted from a cylindrical fatigue sample.

### 2. Results

In the preliminary analysis of the crack-deflection criteria with the three thin-foil samples, it was found that the angle where the maximum value of the Fatemi-Socie parameter (and spatial gradient) occurs does not

correlate with the experimentally observed kink angle, illustrated in Fig. 1 as  $\phi_{\max[D]}$ . However, it can be seen that there exist local maxima that clearly correlate with the experimental kink angle. A graph-based approach is proposed, in which the peaks of the fatigue indicator parameters are represented with a graph structure, and the shortest path through the graph (after applying edge weighting) is used to select the kink angles along the crack front. Predicted kink-angles after the graph-based operation is applied are shown to be more reasonable compared to the experimental kink angle, as illustrated in Fig. 1.

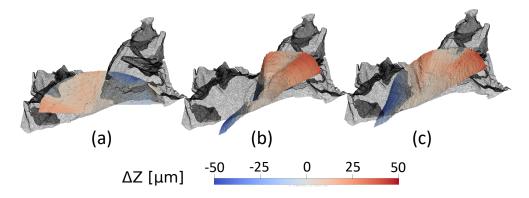


Fig. 2 – Preliminary three-dimensional crack surfaces informed by three potential crackdeflection criteria, colored by elevation error relative to the experimental crack surface ( $\Delta Z$ ); the experimental crack surface is shown as a black wire frame: (a) maximum tangential stress, (b) Fatemi-Socie, (c) spatial gradient of Fatemi-Socie parameter.

Crack-deflection criteria are benchmarked in a blind prediction of three-dimensional crack growth in a polycrystal. Fig. 2 shows preliminary crack-surface predictions informed by the maximum tangential stress (a), Fatemi-Socie (b), and the spatial gradient of the Fatemi-Socie (c) criteria, colored by the elevation error  $(\Delta Z)$ , which is the difference between the predicted and observed elevation of the crack surface at a given location. The experimental crack surface is shown as a black wire frame.

# 3. Conclusions

A recently developed high-fidelity crack-simulation framework was used to model three-dimensional crack growth in experimentally measured microstructures of underaged magnesium WE43. Experimentally measured crack surfaces in three thin-foil samples were directly replicated to study candidate crack-deflection criteria by evaluating micromechanical fields ahead of the crack fronts at different times during the crack histories. Criteria based on the maximum tangential stress, a slip-based fatigue indicator parameter (FIP), and the spatial gradient of the slip-based FIP were considered. Because the slip-based criteria pose multiple possible deflection angles at a given crack-front point, a graph-based approach was implemented to aid in predicting kink angles along the three-dimensional crack fronts. The candidate crack-deflection criteria were then assessed by making blind predictions of three-dimensional crack propagation in an experimentally measured polycrystal extracted from a cylindrical fatigue specimen. The predicted crack surfaces were then compared to the experimentally measured crack surface to quantify relative performance among the candidate crack-deflection criteria.

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