ADVANCING MICROSTRUCTURE-SENSITIVE FATIGUE SELECTION AND DESIGN VIA COMPUTATION AND DATA SCIENCE

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Abstract
This work pursues computational micromechanics approaches that define and compute mesoscopic Fatigue Indicator Parameters (FIPs) which serve as surrogate measures of driving forces for fatigue crack formation and microstructurally small crack growth. Attention is focused on constructing the extreme value distributions of FIPs as a function of microstructure to facilitate relative rank-ordering of fatigue resistance of microstructures as a function of thermomechanical process-history for a given alloy composition. Data science correlations are considered as a means to reduce uncertainty associated with model forms and parameters and to accelerate assessment of hot spot FIP distributions used to rank order microstructures. Further extensions in fusing information obtained from such computational strategies with *in situ* measurements of microstructurally small cracks and AI-enhanced crack detection methods for high cycle fatigue (HCF) are explored.

1. Introduction

The formation and early growth of HCF fatigue cracks in structural alloys is a challenging rare-event problem that is closely related to the statistical distributions of microstructure features or attributes. At the scale of individual grains or phases, fundamental processes such as slip band structures and associated slip irreversibility lead to formation and growth of microstructurally small cracks. Bottom-up models for early mesoscopic fatigue crack "nucleation" processes are complicated by details of material composition, environment, and defect structures, and are largely inaccessible to predictive atomistic and discrete modeling methods. Moreover, supporting experimental results are limited and have significant uncertainty. On the other hand, top-down experimental correlations based on some decomposition of fatigue crack initiation and propagation have large uncertainty associated with microstructure effects and sample size of observations, along with limitations on scale-appropriate fatigue crack growth relations. This work pursues top-down computational micromechanics using physically-based crystal plasticity models to compute FIP distributions across a statistically relevant volume of each microstructure of interest.

2. Results

Figure 1 presents the overarching strategy for using microstructure-sensitive simulations to support screening/relative ranking of candidate microstructures for a given alloy system with regard to fatigue crack formation and early growth resistance. The approach consists of several key steps:

1. Generate a sufficient number of statistical volume elements (SVEs) to represent target microstructure statistics obtained experimentally and from process-structure simulations as appropriate. Enough SVEs must be generated to obtain representative statistical distributions of fatigue responses for each microstructure, which are of course of extreme value nature in the HCF regime.
2. Conduct simulations using physically-based models supported by experimental observations to evaluate extreme value (EV) FIPs for each SVE.
3. Populate EV distributions (Gumbel or generalized EV) for each microstructure and loading condition of interest over the entire set of SVEs.
4. Evaluate marked correlation functions at FIP hot spots within the microstructure SVEs to discern spatial correlations of any dominant features that affect extreme value FIPs.
5. Rank order microstructures in terms of resistance to fatigue crack formation and early growth, i.e., lowest EV FIPs.
6. Modify composition or thermomechanical process path to improve responses (materials design) in another iterative loop of steps 1-6 or select highest ranked candidate microstructures for further experimental evaluation.

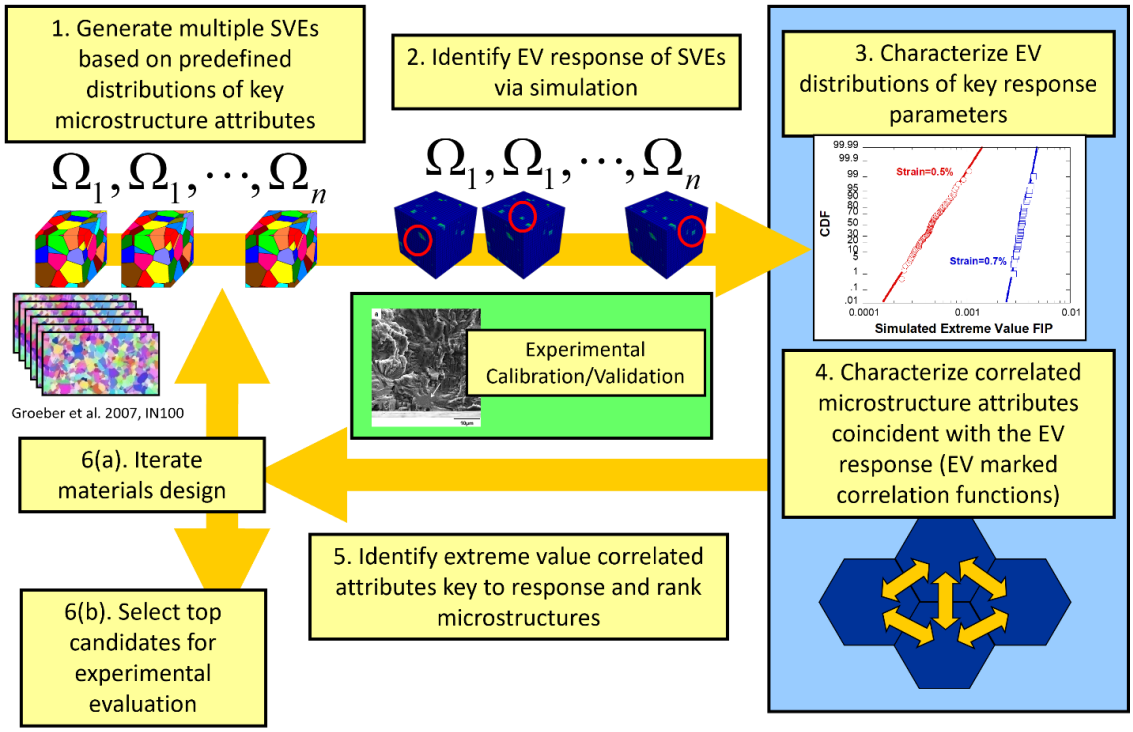

Fig.1 – Flow of information in microstructure-sensitive fatigue simulation for extreme value fatigue response to inform decision-making in alloy selection and design (Przybyla and McDowell, Int. J. Plasticity 26(3) 2010; 27(12) 2011).

We have employed a grain-scale version of the Fatemi-Socie FIP (FFEMS 11(3) 1998) that serves as a representative surrogate for the cyclic crack tip displacement in the finite process zone of a crystallographic crack in the matrix or at the slip band-matrix interface (Castelluccio and McDowell, Int. J. Fracture 176(1) 2012) in fcc alloys such Ni-base superalloys, α–β Ti alloys, and precipitate-strengthened Al alloys (Stopka and McDowell, Int. J. Fatigue 133 2020). The algorithm has been extended to microstructurally small crack growth across the first 10-20 grains (Castelluccio and McDowell, Mater. Sci. Eng. A 598(26) 2014, and recently implemented in an open source, massively parallel solution engine, PRISMS-Fatigue (Yaghoobi et al., npj:Computational Materials 7(38) 2021).

3. Conclusions

An algorithm has been introduced for conducting parametric simulations of statistical volume elements of realistic microstructures of candidate alloys to screen and rank-order in terms of resistance to fatigue crack formation and early growth. This strategy can be updated continuously with experiments, can be leveraged and extended using data science methods, and supports decision-making for accelerated insertion of improved materials and development of new materials which typically have sparse available fatigue data.

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