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Data-driven reduced-order models for rank-ordering the high cycle fatigue performance of polycrystalline microstructures

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Abstract

Computationally efficient estimation of the fatigue response of polycrystalline materials is critical for the development of next generation materials in application domains such as transportation, health, security, and energy industries. This is non-trivial for fatigue of polycrystalline metals since the initiation and growth of fatigue cracks depends strongly on attributes of the microstructure, such as the sizes, shapes, orientations, and neighbors of individual grains. Furthermore, regions of microstructure most likely to initiate cracks correspond to the tails of the distributions of the microstructure features. This requires the execution of large numbers of experiments or simulations to capture the response of the material in a statistically meaningful manner. In this work, a linkage is described to connect polycrystalline microstructures to the statistically signified driving forces controlling the high cycle fatigue (HCF) responses. This is achieved through protocols that quantify these microstructures using 2-pt spatial correlations and represent them in a reduced-dimensional space using principal component analysis. Reduced-order relationships are then constructed to link microstructures to performance characteristics related to their HCF responses. These protocols are demonstrated for α -titanium, which exhibits heterogeneous microstructure features along with significant elastic and inelastic anisotropies at both the microscale and the macroscale.

Keywords: 2-point correlations, extreme value statistics, structure-property relationship, crystal plasticity, fatigue

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