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Multiscale modeling of transgranular short crack growth during fatigue in polycrystalline metals

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Key words: short cracks; polycrystalline materials; N-R model; multiscale; molecular dynamics.

Abstract

An atomistics-informed multiscale modeling approach was proposed to quantify the transgranular short crack growth during fatigue in polycrystalline metals. The approach solved the two scale inconsistency problems of the classical N-R model, replacing the arbitrary materials strength parameter by the atomistically determined ideal shear strength in the evaluation of both the fatigue crack growth (FCG) rate and the corresponding range of short-crack-featured fluctuations, and incorporating atomistically simulated Peierls stress into the discrete dislocation formulation to quantify the microscopic threshold of FCG through explicitly modeling the interactions between dislocations and grain boundaries. The model-predicted FCG results were compared with the experimental FCG data of GH4169 Ni-based superalloy, demonstrating improved predictive capability than the classical N-R

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