Dislocation dynamics in Ni-based superalloys: parameterising edge dislocation trajectories with uncertainty quantification

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Abstract

The extraordinary strength exhibited by Ni-based superalloys at high temperatures is attributed to the presence of nanoscale precipitates in their microstructure, which hinder dislocation motion. In our work, we study edge dislocation-precipitate interactions using Molecular Dynamics (MD) simulations with classical effective potentials. The motion of a pair of edge dislocations moving under shear between pure Face-Centred Cubic (FCC) Ni into Ni3Al with an L12 structure was simulated using MD, where Ni is used to represent an idealised γ solid solution phase and Ni3Al for the γ' precipitate phase. The obtained trajectories are parameterised using a model developed by extending an equation of motion (1) to account for dislocation-dislocation and dislocation-precipitate interactions. Differential Evolution Monte Carlo (DE-MC) within a Bayesian framework is used to determine parameter distributions and the correlations between them. These distributions are then used to quantify the uncertainty in the model outputs, namely the dislocations' positions and velocities. Parameterising dislocation dynamics in this way yields physically meaningful parameters. Accordingly, the present approach offers a means of extracting quantitative information from the atomistic scale that can be used to inform larger length scale simulations of dislocations such as Discrete Dislocation Dynamics (DDD). Using DE-MC as a sampling approach also means that parameter uncertainties can be propagated through a hierarchy of multiscale models. We illustrate how such uncertainty propagation can be achieved by considering a dislocation mobility law with quantified uncertainties. This work is part of a wider study aiming to develop a more comprehensive surrogate model to describe the deformation behaviour of Ni-based superalloys with a focus on propagating and quantifying uncertainties (2).

References:

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