

Dislocation dynamics in Ni-based superalloys: parametrising edge dislocation trajectories
from atomistic simulations with uncertainty quantification

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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, Molecular Dynamics (MD) simulations are used to study the motion of edge dislocations in Ni-Ni₃Al with a coherent interface to represent idealised γ solid solution and γ' precipitate phases. A reduced model is developed to parametrise the obtained dislocation trajectories by extending an equation of motion to account for dislocation interactions with the Ni-Ni₃Al interface. The developed model describes the major features of the dislocation trajectories observed and can capture a range of qualitatively different behaviour within the system studied. The model parameter distributions are determined using Differential Evolution Monte Carlo (DE-MC) as a sampling approach and a Gaussian process surrogate model. The present approach offers a means of extracting quantitative information from the atomistic scale, which can be used to inform larger length scale simulations of dislocations such as Discrete Dislocation Dynamics (DDD). Using DE-MC as a sampling approach 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 in pure Ni. This work is part of a wider study aiming to model the deformation behaviour of Ni-based superalloys with a focus on quantifying and propagating uncertainties.