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Predicting the strength of superalloys by 3D dislocation dynamics

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ABSTRACT

Single crystals of nickel-base γ/γ' superalloys exhibit excellent mechanical properties, specifically at high temperatures. They consist of two coherent phases, the FCC γ phase and the ordered $L1_2$ γ' phase. The cubicodal geometry and high volume fraction of the latter create narrow channels of γ matrix through which dislocations accomodate the deformation. At certain temperatures, the dislocations bow around the γ' precipitates, whereas at other temperatures they are sheared by the dislocations. Dissociation of superdislocations in these precipitates creates a flow stress anomaly. Due to the complex interplay between these factors, the mechanical reponse under different loading directions, velocities and temperatures is particularly difficult to predict. The design of a constitutive model for the deformation and life prediction of superalloys is a longstanding problem, even though interesting models exist in the literature, e.g. [1].

Three-dimensional dislocation dynamics may well be the tool delivering a better understanding of the relation between local slip activity and the macroscopic stress-strain behavior. In the past, 2D simulations [2], and 3D simulations on one incoming slip system [3] have been carried out in order to understand elementary deformation mechanisms, such as the interaction with misfit dislocations. In this work, two different formalisms of carrying out dislocation dynamics simulations ("classical" DD and the Discrete-Continuum Method (DCM), see for instance [4]), are applied to the γ/γ' system at a wide range of temperatures and loading cases.

In order to carry out simulations for different loading directions and temperatures, several essential microscopic mechanisms have been added to the dislocation dynamics code. First, a novel criterion for pairing superpartials and their associated anti-phase boundary upon entering the ordered precipitate is introduced, similar but possibly simpler than other criteria in the literature [3]. Also, the mobility of the superdislocation is modified in the temperature range between 300 and 800 K according to the model of Demura [5]. With these additions, both formalisms are then compared in terms of results and performance, and underlying deformation mechanisms for specific loading cases are presented.

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