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Ronghai Wu, Stefan Sandfeld

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A dislocation dynamics-assisted phase field model for Nickel-based superalloys: the role of initial dislocation density and external stress during creep

Ronghai Wu[a,*], Stefan Sandfeld[a,b]

[a]*Department of Materials Science and Engineering, Institute of Materials Simulation, Friedrich-Alexander Universität Erlangen-Nürnberg, Dr.-Mack-Str. 77, 90762 Fürth, Germany*
[b]*Institute of Mechanics and Fluid Dynamics, Chair of Micromechanical Materials Modelling, Technische Universität Bergakademie Freiberg, 09596 Freiberg, Germany*

Abstract

The effect of initial dislocation density and external stress on primary creep of Nickel-based superalloys are studied by a combined continuum dislocation dynamics/phase-field model. This model can simultaneously predict the dislocation motion as well as the γ/γ' evolution and yields macroscopic creep properties as a natural outcome – all of which are supported by experimental data. The rafting simulation results show that the initial dislocation density as well as the external stress can dramatically influence the aspect ratio of the γ' precipitates and the interface dislocation density at the γ/γ' interfaces. In contrast, the plastic strain towards the end of primary creep is not sensitive to the initial dislocation density due to a seeming "strain rate inversion" during creep, and it is dependent on the applied external stress.

Keywords: superalloy; creep; phase-field model; dislocation dynamics; microstructure

1. Introduction

Nickel-based superalloys are engineered materials with a number of key properties relevant for high temperature service, such as excellent creep resistance and corrosion resistance [1, 2]. Development of superalloys is divided into distinct "generation": a class of superalloys is considered a new generation if there is an increment of about 30 °C in the upper limit of their service temperatures. Although several generations of Nickel-based superalloys have been developed during the past decades, the demand for more efficient engines is still pushing the design of new generations of Nickel-based superalloys, which consequently requires deeper understanding of the microstructural mechanisms present in the materials. Traditional superalloy development often relied on experimental trial-and-error approaches, whereas, nowadays heuristic investigations are largely assisted by modern modeling and simulation methods [3–6]. The phase-field method is one of the most commonly used simulation method for predicting the phase microstructure evolution. It is a method that does not require explicit interface tracking and is also becoming increasingly popular for simulations of Nickel-based superalloys in multi-scale frameworks. On the nano-scale, the atomic configurations can be described by occupation probability functions of atoms [7–9]. These models are especially suitable for investigating the γ' pre-precipitation including the effect of temperature, elastic strain and additive elements, to name but a few. Another type of atomic phase-field model is the phase-field crystal (PFC) method in which atoms are represented by atomic densities, and their evolution is governed by the Cahn-Hilliard equation [10–12]. Microstructures such as dislocation configurations, grain boundaries and cracks can be naturally rec-

*Corresponding author
Email address: ronghai.wu@fau.de (Ronghai Wu)