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Influence of misfit stresses on dislocation glide in single crystal superalloys: A three-dimensional discrete dislocation dynamics study

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ABSTRACT

In the characteristic γ/γ' microstructure of single crystal superalloys, misfit stresses occur due to a significant lattice mismatch of those two phases. The magnitude of this lattice mismatch depends on the chemical composition of both phases as well as on temperature. Furthermore, the lattice mismatch of γ and γ' phases can be either positive or negative in sign. The internal stresses caused by such lattice mismatch play a decisive role for the micromechanical processes that lead to the observed macroscopic athermal deformation behavior of these high-temperature alloys. Three-dimensional discrete dislocation dynamics (DDD) simulations are applied to investigate dislocation glide in γ matrix channels and shearing of γ' precipitates by superdislocations under externally applied uniaxial stresses, by fully taking into account internal misfit stresses. Misfit stress fields are calculated by the fast Fourier transformation (FFT) method and hybridized with DDD simulations. For external loading along the crystallographic [001] direction of the single crystal, it was found that the different internal stress states for negative and positive lattice mismatch result in non-uniform dislocation movement and different dislocation patterns in horizontal and vertical γ matrix channels. Furthermore, positive lattice mismatch produces a lower deformation rate than negative lattice mismatch under the same tensile loading, but for an increasing magnitude of lattice mismatch, the deformation resistance always diminishes. Hence, the best deformation performance is expected to result from alloys with either small positive, or even better, vanishing lattice mismatch between γ and γ' phase.

1. Introduction

Ni-base single crystal superalloys possess an outstanding creep deformation resistance and are mainly applied as turbine blades in the hottest regions of gas turbines. Their extraordinary creep resistance is caused by a characteristic microstructure in which the face centered cubic (fcc) solid solution strengthened γ matrix is further hardened by a high volume fraction (60–70%) of coherent cuboidal precipitates of ordered γ' phase with a $L1_2$ structure. The typical edge length of a γ' precipitate is ~0.5 μm and the narrow γ matrix channel between the precipitates has a typical width of only 0.05–0.1 μm (Reed, 2008).

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The creep mechanisms of single crystal superalloys for different temperature and stress conditions have been studied extensively. It was reported in the literature that the creep behavior is closely related to conservative and non-conservative dislocation motion, as well as dislocation self-interaction and dislocation interaction with coherent precipitates, see for example Leverant and Kear (1970), Feller-Kniepmeier and Link (1989), Pollock and Argon (1992), Sass et al. (1996), Reed et al. (1999), Rae and Reed (2007), Agudo Jácome et al. (2013). In the heat treated state, single crystal superalloys contain low dislocation densities in the γ matrix and γ' precipitates are essentially dislocation-free. During primary creep, dislocations with different Burgers vectors are produced and interpenetrate into horizontal and vertical γ matrix channels, depositing dislocation segments on γ/γ' interfaces. This filling of γ channels with interfacial dislocation segments renders the motion of mobile channeling dislocations increasingly difficult and thus increases the creep resistance of the single crystal. In the secondary creep regime, a stable interfacial dislocation network forms associated with dislocation climb and diffusion, which leads to a low and constant creep rate. The directional coarsening (rafting) of γ' precipitates accompanied by dislocation evolution occurs at elevated temperatures (Pollock and Argon, 1984; Kamaraj, 2003). High local stresses and interactions of interfacial dislocations may result in the shearing of γ' precipitates creating either an anti-phase boundary (APB) or superlattice stacking fault (SSF) ribbons (Chiba and Hanada, 1994; Coujou et al., 1997; Chen and Knowles, 2003; Raujol et al., 2006).

On top of the applied stress, the misfit stress, which is a consequence of the lattice mismatch between γ and γ' phases, is an important driving force for dislocation motion. The lattice mismatch is negative in all currently used Ni-base superalloys and becomes more negative with increasing temperature. However, recently developed Co-base superalloys with a similar γ/γ' microstructure and promising high temperature properties possess a positive lattice mismatch that decreases at higher temperatures (Nathal et al., 1985; Biermann et al., 1996; Sato et al., 2006; Biermann et al., 2013; Mughrabi, 2014). The experimental study by Zhang et al. (2005) shows that the lattice mismatch influences the effective force for dislocations to overcome the Orowan resistance and the evolution of γ/γ' interfacial dislocation networks. It is difficult to clarify the effect of lattice mismatch on the strength of superalloys experimentally, because lattice mismatch can only be changed by different alloying contents which also modifies a number of other alloy properties at the same time (Mughrabi and Tetzlaff, 2000). Hence, it is essential to study the influence of lattice mismatch and the resulting internal stresses by microstructural models. Svoboda and Lukáš (1997, 1998) have developed a continuum level creep model of Ni-base single crystal superalloys taking into account many important mechanisms of dislocation motion and precipitate morphological evolution to investigate lattice mismatch effects on the creep performance. Other authors have estimated the misfit stress field by the finite element method (FEM) adopting isotropic or anisotropic elastic properties for the matrix and the precipitate (Pollock and Argon, 1992; Müller et al., 1992, 1993). Besides, Fedelich (2002) combines some advantages of previous approaches to implement a constitutive law in a FEM code for the microstructural deformation analysis, considering the misfit stress as a part of internal stresses.

In order to describe dislocation behavior precisely and to obtain the corresponding plastic deformation directly, three-dimensional (3D) discrete dislocation dynamics (DDD) modeling has been advanced to become a mature method during the last decades, based on different treatments of dislocation lines (Kubin et al., 1992; Fivel et al., 1996; Verdier et al., 1998; Kubin and Devincre, 1999; Ghoniem et al., 2000; Zbib and Diaz de la Rubia, 2002; Bulatov and Cai, 2006). Through modeling dislocation slip, climb (Mordehai et al., 2008; Gao et al., 2011), evolution of dislocation patterns (Madec et al., 2002) and interactions with precipitates (Shin et al., 2003), DDD simulations have been used in many fields. In particular we name here studies of Ni-base single crystal superalloys (Yashiro et al., 2006; Vattré et al., 2009, 2010; Huang et al., 2012; Yang et al., 2013; Hafez Haghighat et al., 2013). Most of these DDD studies focus on the cutting of precipitates by superdislocations, the hardening contribution of precipitates, and evolution of interfacial dislocation networks. Only a few of them insert the misfit stress field into DDD simulations (Vattré et al., 2010; Huang et al., 2012), but they lack systematic studies for the influence of different lattice mismatch on the global deformation resistance.

The aim of this work is to combine the complex misfit stress field with DDD simulations and to apply this new model to investigate dislocation movement in γ matrix channels and γ' precipitates as well as to study the effect of sign and magnitude of lattice mismatch on the deformation behavior of single crystal superalloys under constant external uniaxial load. This work focuses exclusively on athermal dislocation glide and takes into account all dislocation interaction mechanisms and the shearing of γ' precipitates by pairs of perfect matrix dislocations including the generation of an APB by the leading dislocation and its healing by the trailing one. Neglecting diffusion, dislocation cross slip and climb in the current model, we are not able to capture temperature effects or to predict true creep behavior. Nevertheless, this model well captures the fundamental deformation mechanisms influenced by misfit stresses in a γ/γ' microstructure of single crystal superalloys.

2. Simulation method

2.1. DDD simulation theory

The DDD code based on the discretization of dislocations into alternating sequences of pure edge and screw segments *Tridis* developed at the Laboratoire de Science et Ingénierie des Matériaux et Procédés (SIMaP) of Grenoble Institute of Technology(Grenoble INP) in France is used in this paper (Verdier et al., 1998; Fivel and Canova, 1999; Shin, 2004). The motion of each segment is governed by the effective shear stress acting on the center of the segment. The effective shear