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The strength and dislocation microstructure evolution in superalloy microcrystals

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ABSTRACT

In this work, the evolution of the dislocations microstructure in single crystal two-phase superalloy microcrystals under monotonic loading has been studied using the three-dimensional discrete dislocation dynamics (DDD) method. The DDD framework has been extended to properly handle the collective behavior of dislocations and their interactions with large collections of arbitrary shaped precipitates. Few constraints are imposed on the initial distribution of the dislocations or the precipitates, and the extended DDD framework can support experimentally-obtained precipitate geometries. Full tracking of the creation and destruction of anti-phase boundaries (APB) is accounted for. The effects of the precipitate volume fraction, APB energy, precipitate size, and crystal size on the deformation of superalloy microcrystals have been quantified. Correlations between the precipitate microstructure and the dominant deformation features, such as dislocation looping versus precipitate shearing, are also discussed. It is shown that the mechanical strength is independent of the crystal size, increases linearly with increasing the volume fraction, follows a near square-root relationship with the APB energy and an inverse square-root relationship with the precipitate size. Finally, the flow strength in simulations having initial dislocation pair sources show a flow strength that is about one half of that predicted from simulations starting with single dislocation sources. The method developed can be used, with minimal extensions, to simulate dislocation microstructure evolution in general multiphase materials.

1. Introduction

Thanks to their unique balance of structural, thermodynamic and kinetic properties as well as their excellent creep resistance properties, Ni-base superalloys are the state of the art materials used in the most demanding sections of gas turbine engines, which are subject to high temperature and stress levels (Reed, 2006). Embedded in the base Ni crystal (the γ phase) is a distribution of secondary phase $Ni_3(Al, Ti)$ precipitates (the γ' phase) that have an $L1_2$ crystal structure. Unlike most metallic materials, the yield strength of Ni-base superalloys does not decrease with temperature up to 750–850 °C (Westbrook, 1957; Davies and Thornton, 1977; Veyssiere and Saada, 1996). On the other hand, Co-based superalloys typically exhibit a higher melting temperature and

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exhibit superior single-crystal solidification characteristics while maintaining compressive flow stresses comparable to their Ni-based counterparts (Eggeler et al., 2014). Similar to the Ni-based superalloys, the strengthening in these Co-based superalloys arises from the presence of $Co_3(Al,W)$ secondary phase precipitates (γ' phase having an $L1_2$ structure, embedded in the Co matrix (γ phase) (Sato et al., 2006). As such, Co-based superalloys could potentially be of use for applications requiring higher operating temperatures than that accessible by Ni-based superalloys.

The shearing of γ' precipitates by the glide of dislocations in the γ phase is one of the dominant deformation mechanisms of Ni-based and Co-based superalloys at room temperature (Reed, 2006). A typical $\frac{1}{2}\langle 110\rangle$ dislocation gliding into the γ' phase would disturb its local ordering forming an Anti-Phase Boundary (APB) surface that leads to an increase in the precipitate's energy. Thus, γ' phase shearing is always resisted by a force proportional to the precipitate's APB energy, which for Ni-based superalloys is typically in the range of 0.12–0.4 J/m^2 (Sun et al., 1999; Rao et al., 2004). On the other hand, a $\frac{1}{2}\langle 110\rangle$ dislocation gliding on an already formed APB region would restore the local ordering back to the minimum energy state, hence, its glide is assisted by an APB force of the same magnitude and opposite direction of that during the APB formation. This alternation between resisting dislocation shearing and assisting it, makes the force acting on a dislocation in superalloys history dependent. A pair of identical dislocations gliding together on the same plane (i.e a superdislocation having twice the typical FCC Burgers vector $\frac{1}{2}\langle 110\rangle$) has no net effect on the local ordering of γ'. Thus, In the absence of coherency strains, the pair would experience no resistance as it approaches the precipitate surface locally compared to the case of a single dislocation approaching a precipitate in the absence of coherency strains. This is not to be confused with the global picture of a dislocation pair shearing through a distribution of precipitates where there is always a resisting force regardless of the presence of coherency strains. Pollock and Argon (1992) suggested that precipitate shearing by superdislocations requires the blockage of a leading dislocation at its surface until a two-dislocation pile-up forms. When Γ_{APB} is too high and the formation of superdislocations is difficult, dislocations can glide in the narrower γ-channels when the resolved shear stresses are high enough, leading to the formation of loops around the precipitate. Alternatively, at high temperatures dislocations can overcome the precipitates by cross-slip and/or climb (Picasso et al., 1997). Finally, it should be noted that the shearing of a γ' precipitate by a single $\frac{1}{2}\langle 110\rangle$ dislocation has not been observed in Ni- or Co-based superalloys, however, the predominant cutting process in Co-based superalloys containing 30–39 at% Ni is by a single $\frac{1}{2}\langle 110\rangle$ dislocation, leaving behind APBs with the same displacement (Eggeler et al., 2014).

Numerical simulations of the plastic response of superalloys can greatly facilitate the quantification of the underlying deformation mechanisms that affect their macroscopic mechanical properties, as well as expedite the design of the superalloy microstructure to achieve optimal strength and creep resistance. One suitable computational method that can handle all the physical dislocation-precipitate interactions with minimal ad-hoc assumptions is Discrete Dislocation Dynamics (DDD) (Kubin et al., 1992; Ghoniem et al., 2000; Verdier et al., 1998; Zbib et al., 2002; Weygand et al., 2002; Benzerga et al., 2004; Zhou et al., 2010). In this method, dislocations are explicitly modeled and their time evolution is calculated. Both two-dimensional (2D) (Rao et al., 2004, 2006; Devincre et al., 1999; , 2012) and three-dimensional (3D) (Devincre et al., 1997; Mohles et al., 1999; Mohles, 2001a, 2001b, 2004; Mohles and Nembach, 2001; Shin et al., 2001, 2003, 2005, 2007; Yashiro et al., 2006; Vattré et al., 2009, 2010; Huang et al., 2012; Haghighat et al., 2013; Liu et al., 2014; Yang et al., 2014; Gao et al., 2015) DDD simulations have been used in the past to study the behavior of Ni-base superalloys. However, most of these DDD studies have used simplified precipitate geometries (cubic or spherical) arrangements (a single precipitate or a regular array of precipitates), and simple precipitate shearing rules where the precipitate can either be unshearable or shearable only by superdislocations. A realistic superalloy simulation requires the capability of handling precipitates of geometries and distributions similar to those found in experiments. In addition, the formation of superdislocations in the simulation should take place only if the local stresses and precipitate resistance allow it to happen. This has been challenging for the DDD community in the past due to the geometric complexity of the problem.

To address these limitations, the target of the current study is to extend the DDD framework to model more realistic dislocation-precipitate interactions in small crystals. The paper is organized as follows, in Section 2, the necessary extensions to the 3D-DDD framework to model dislocation-precipitate interactions in superalloys are described. In Section 3, the parameters for the numerical simulations conducted are summarized. In Section 4, the results of the simulations are discussed and comparisons with analytical predictions and experimental observations. Finally, a summary and a conclusion of the work are given in Section 5.

2. Computational method

All simulations performed here are conducted using an in-house, modified version of the 3D-DDD open source code ParaDiS (Tang et al., 2007) that guarantees that all dislocation reactions are planar, and incorporates a set of atomistically-informed, physics-based cross-slip mechanisms, the details of which are described in Hussein et al. (2015). In addition, ParaDis naturally accounts for dislocation reactions such as the formation of Lomer, Hirth and glide locks. The code was then extended as described below to model superalloys. Unlike pure single phase metals, the additional APB forces acting on dislocation segments in an $L1_2$ crystal structure depend on the history of the dislocation glide activity. The APB force per unit length is equal to $f_{APB} = \frac{-\Gamma_{APB}}{b}$ if the dislocation is gliding on an unsheared plane in the γ' phase (the negative sign indicates a repulsive force), or $f_{APB} = \frac{\Gamma_{APB}}{b}$ if it is gliding on a sheared plane in the γ phase. Since superdislocations do not create or destroy APB regions, no APB forces act on them. In order to handle the most general case, the state of being sheared or unsheared should be tracked for every point in the γ' regions. This process amounts to tracking the APB fault regions as they are created and destroyed. The APB representation and tracking will be discussed next, however, an important prerequisite for APB tracking is a flexible precipitate geometry representation.