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Interfacial dislocation motion and interactions in single-crystal superalloys

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Abstract

The early stage of high-temperature low-stress creep in single-crystal superalloys is characterized by the rapid development of interfacial dislocation networks. Although interfacial motion and dynamic recovery of these dislocation networks have long been expected to control the subsequent creep behavior, direct observation and hence in-depth understanding of such processes has not been achieved. Incorporating recent developments of discrete dislocation dynamics models, we simulate interfacial dislocation motion in the channel structures of single-crystal superalloys, and investigate how interfacial dislocation motion and dynamic recovery are affected by interfacial dislocation interactions and lattice misfit. Different types of dislocation interactions are considered: self, collinear, coplanar, Lomer junction, glissile junction, and Hirth junction. The simulation results show that strong dynamic recovery occurs due to the short-range reactions of collinear annihilation and Lomer junction formation. The misfit stress is found to induce and accelerate dynamic recovery of interfacial dislocation networks involving self-interaction and Hirth junction formation, but slow down the steady interfacial motion of coplanar and glissile junction forming dislocation networks. The insights gained from these simulations on high-temperature low-stress creep of single-crystal superalloys are also discussed.

Keywords: Dislocation dynamics; Superalloys; High-temperature low-stress creep; Interfacial dislocation motion; Dislocation interactions

1. Introduction

Single-crystal superalloys are used as turbine blade materials because of their excellent creep resistance during the operation of gas turbines in aircraft and power-generation engines. The microstructure of these alloys consists of γ matrix (face-centered cubic) containing a high volume fraction of cuboidal γ' particles ($L1_2$ lattice). Creep deformation in these structures exhibits three regimes: a low-temperature and high-stress regime (e.g. 750 °C, 750 MPa), where plastic strain is accumulated by $\langle 1\,1\,2\rangle$ dislocation ribbons cutting the γ' precipitates [1,2]; an intermediate-temperature and -stress regime (e.g. 900 °C, 450 MPa), where plastic deformation occurs by Orowan bypassing of 1/2 $\langle 0\,1\,1\rangle$ dislocations through the γ matrix channels [3,4]; and a high-temperature and low-stress regime (e.g. 1100 °C, 137 MPa), where plastic deformation initializes easily as the grown-in 1/2 $\langle 0\,1\,1\rangle$ dislocations glide in the horizontal channels [5–7], proceeds slowly by the motion of 1/2 $\langle 0\,1\,1\rangle$ dislocations along the interfaces [8–10], and eventually accelerates via $\langle 1\,0\,0\rangle$ superdislocations cutting the γ' precipitates [11,12].

Interfacial dislocation motion and interactions occur in the high-temperature and low-stress regime. These interfacial dislocations are generated by the glide of grown-in dislocations driven jointly by the applied stress and misfit

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stress in the horizontal channels [13–15]. As more dislocations are deposited on the interface, the internal stresses associated with the interfacial dislocation networks soon become high enough to prevent the further propagation of the grown-in dislocations, and thus end primary creep [5,16,17]. Interfacial dislocation motion, by a combination of glide and climb, becomes the main deformation process during secondary creep that constitutes the majority of the superalloy's creep life [9,10,18,19].

The objective of this work is to investigate how interfacial dislocation motion in the γ/γ' structure is affected by long-range and short-range dislocation interactions in interfacial dislocation networks using discrete dislocation dynamics (DDD) simulations. Three-dimensional DDD models [20–25] are robust tools to study elementary dislocation interactions [26–28], and the strengthening effect of dislocation interactions in nanoscale metallic multilayered composites [29], microscale plasticity [30–32] and coarse-grained crystals at low-angle grain boundaries [33,34]. The present work is focused on the role of interfacial dislocation interactions during high-temperature creep of single-crystal superalloys. In previous studies [26–29,31–34], dislocation interactions were generally found to contribute to material strength and cause strain hardening. In this work, we show that interfacial dislocation interactions may also induce dynamic recovery, which relieves internal stress and leads to creep softening. Although dynamic recovery has long been assumed to occur during secondary creep of single-crystal superalloys [5,9,10,18,19], direct observation and hence in-depth understanding of such processes has not been reached. In the γ phase matrix channels, positive and negative dislocations are forced by the external stresses onto opposite interfaces, so that dynamic recovery does not proceed as in pure metals where dislocations of opposite signs directly meet and annihilate. Our simulations of interfacial dislocation motion and interactions will cast light on the recovery mechanisms during high-temperature low-stress creep in these channel structures.

We will first introduce our model to simulate interfacial dislocation motion and interactions in the γ/γ' structure, which includes model modifications that enable dislocation climb driven by mechanical and chemical forces, incorporates the antiphase boundary back-driving force in the precipitates, and considers the biaxial misfit stresses in the matrix channels. The simulations of interfacial dislocation motion during creep are then presented, which consider different initial configurations, namely mixed dislocations, edge dislocations and dislocation networks involving different types of dislocation interactions (self, collinear, coplanar, Lomer junction, glissile junction, and Hirth junction). In each case, the role of the misfit stress is also investigated by running two separate simulations with the misfit stress in the model being switched on and off, respectively. The insights gained from these simulations on high-temperature low-stress creep in single-crystal superalloys will be finally discussed and summarized.

2. Simulation method

Dislocations climb through emission and adsorption of vacancies at jogs. Under the condition of high temperature and low stress, the jog density is high enough that each point along the dislocation line may act as a source or sink of vacancies, and the vacancy concentration is approximately uniform along the dislocation core [35]. The velocity of dislocation climb is then controlled by vacancy diffusion [35–42]:

$$V_c = \frac{2\pi\Omega D_v c_0 F_c}{b^2 \ln(R/b) k_B T}, \tag{1}$$

where D_v is the vacancy diffusion coefficient, c_0 is the equilibrium vacancy concentration, F_c is the climb force, Ω is the atomic volume, b is the magnitude of the Burgers vector, R is a distance from the dislocation core over which the vacancy concentration reaches its average value in the sample, k_B is Boltzmann's constant, and T is the absolute temperature.

A drag relation between the climb force and velocity can be derived from Eq. (1):

$$V_c = \frac{F_c}{B_c}, \quad B_c = \frac{b^2 \ln(R/b) k_B T}{2\pi\Omega D_v c_0}, \tag{2}$$

where the drag coefficient B_c is a function of the vacancy diffusion coefficient D_v, the equilibrium vacancy concentration c_0, and the temperature T. It is worth mentioning that a similar climb force–velocity drag relation has also been derived in the case of low jog density (source/sink-controlled climb) [43].

The climb motion of dislocations can be described in a drag-type relation similar to the glide motion, which allows dislocation dynamics models to handle dislocation glide and climb in the same framework [25,39,41,43–45].

We use the ParaDiS DDD code [25], which defines the nodal force and velocity in a drag-type relation:

$$\boldsymbol{F}_i = \frac{1}{2}\sum_j \|\boldsymbol{l}_{ij}\| \boldsymbol{B}_{ij} \boldsymbol{V}_i, \tag{3}$$

where $\boldsymbol{F}_i$ is the force on node i, j is a node connected to i through a line segment $\boldsymbol{l}_{ij}$, $\boldsymbol{B}_{ij}$ is the drag tensor (inverted mobility tensor) for segment $\boldsymbol{l}_{ij}$, and $\boldsymbol{V}_i$ is the calculated nodal velocity. The drag tensor $\boldsymbol{B}$ enforces spatial constraints on the dislocation motion in face-centered cubic (fcc) crystals according to:

$$\boldsymbol{B} = \begin{cases} B_g(\boldsymbol{m}\otimes\boldsymbol{m}) + B_c(\boldsymbol{n}\otimes\boldsymbol{n}) + B_l(\boldsymbol{t}\otimes\boldsymbol{t}) & \boldsymbol{n}\|\langle 111\rangle \\ B_c\boldsymbol{I} + (B_l - B_c)(\boldsymbol{t}\otimes\boldsymbol{t}) & \boldsymbol{n}\nparallel\langle 111\rangle \end{cases} \tag{4}$$

where the drag coefficient B_g controls dislocation glide on the glide plane and perpendicular to the dislocation line, B_c defines dislocation climb along the glide plane normal $\boldsymbol{n}$, and B_l is the drag coefficient associated with moving a node along its line direction $\boldsymbol{t}$.