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Atom probe informed simulations of dislocation–precipitate interactions reveal the importance of local interface curvature

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Abstract—The interaction of dislocations with precipitates is an essential strengthening mechanism in metals, as exemplified by the superior high-temperature strength of Ni-base superalloys. Here we use atomistic simulation samples generated from atom probe tomography data of a single crystal superalloy to study the interactions of matrix dislocations with a γ' precipitate in molecular dynamics simulations. It is shown that the precipitate morphology, in particular its local curvature, and the local chemical composition significantly alter both, the misfit dislocation network which forms at the precipitate interface, and the core structure of the misfit dislocations. Simulated tensile tests reveal the atomic scale details of many experimentally observed dislocation–precipitate interaction mechanisms, which cannot be reproduced by idealized simulation setups with planar interfaces. We thus demonstrate the need to include interface curvature in the study of semicoherent precipitates and introduce as an enabling method atom probe tomography-informed atomistic simulations.

Keywords: Ni-base superalloys; Precipitation hardening; Misfit dislocation network; Atomistic simulation; Atom probe tomography (APT)

1. Introduction

Ni-base superalloys are key materials for single crystal turbine blades in gas turbines of aero-engines and power plants [1,2]. Their ability to withstand mechanical loads at high temperatures is mostly due to their γ/γ' microstructure, consisting of about 70 vol.% cuboidal precipitates of the ordered $L1_2$ γ' phase embedded in a face-centered cubic (fcc) solid solution matrix. The increased strength of these two-phase superalloys, compared to the individual phases, is a direct result of the coherent γ/γ' interfaces [3]. During the initial stages of high temperature, low stress creep, the lattice misfit between the two phases is relieved by the deposition of dislocation segments at the $\{100\}$-γ/γ' interfaces by dislocations gliding in the γ-channels between the precipitates [4–6]. These dislocation segments react with each other and locally rearrange to form an interfacial misfit dislocation network [7–10]. This process is usually accompanied by a change of the precipitate shape from cuboidal to a lamellar structure (rafting) [11,12]. This rafted microstructure determines the creep of single crystalline superalloys by effectively hindering the annihilation of dislocations of opposite sign by climb processes [13,14]. The interfacial dislocation network plays a key role in protecting the γ' precipitate by preventing dislocations from the γ channels to cut into the γ' phase [15,10].

The present knowledge of dislocation–precipitate interactions is based almost exclusively on post-mortem transmission electron microscopy (TEM) studies of dislocation "relics" from which the underling formation processes can only be inferred. These critical dynamic interaction processes can on the other hand be directly explored through large-scale atomistic simulations, which can capture the interaction mechanisms at the dislocation core level. However, only very few such simulations have been reported in the literature [16–22], and almost all of them make use of highly idealized simulation setups with perfectly planar interphase boundaries (IPB) and periodic boundary conditions (PBC) [17–22]. In particular, the

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interaction of matrix dislocations with the interfacial dislocation network only recently became the focus of an atomistic study: Zhu et al. [22] studied the interaction of infinite, straight screw dislocations with a misfit dislocation network on a planar IPB in a quasi-2D setup at 0 K.

The use of highly idealized, quasi-2D simulation scenarios is typical for atomistic simulations. While simplified, highly controlled setups are often necessary to quantitatively determine material properties, overly simplified setups might artificially suppress important mechanisms. Examples include the use of PBC along the crack front in nearly all studies on fracture which suppresses kink formation and crack front curvature effects [23,24], neglecting surface roughness in the study of nanowires where it was shown to significantly influence dislocation nucleation and the overall deformation behavior [25], and the nearly ubiquitous use of Voronoi tessellation in simulations of nanocrystalline metals resulting in perfectly planar grain boundaries (GBs) which fail to represent the GB network topology of real materials [26].

Ideally, one would like to be able to perform simulations on samples which are atom-by-atom reproductions of the experimental specimens. Atom probe tomography (APT), which combines time of flight spectroscopy on individual ions that are sequentially evaporated from a sharp tip with a position-sensitive detector [27,28] (Fig. 1a), could provide exactly this kind of 3D information on the position and chemical species of atoms within a needle-shaped specimen. APT measurements are therefore increasingly used in conjunction with atomistic simulations. APT data were used to construct representative idealized models, e.g. for (kinetic) Monte Carlo [29,30] and Molecular Dynamics (MD) [31] simulations, or density functional theory (DFT) calculations [32–35]. The simulation results were subsequently either compared to experiments or used to evaluate the experimental findings. Only rarely, APT data have been directly used for constructing the actual atomistic simulation samples [35]. This is due to the partial loss of evaporated ions (detection efficiency is 37–80% depending on the equipment) and field evaporation artefacts affecting the accuracy of reconstructed atomic positions. Recently, new approaches were proposed to create complete atomistic samples based on APT data [35–37]. Here, a key element is the reconstruction of the lattice configuration of the original sample (lattice rectification), which requires real-space spatial distribution maps [37] or the use of Fourier transformations [36]. The lattice rectification replaces the missing atoms, but without reproducing the correct short-range order (SRO). Statistical analysis of the original APT data in combination with a Monte Carlo algorithm to interchange atoms can then be used to match the real SRO [35,38].

In the present work, we suggest a simpler alternative approach to generate APT-informed atomistic simulation samples and use it to obtain a real γ/γ' microstructure directly from a reconstructed APT sample of the alloy ERBO/1 [39]. By comparing the simulation results using this microstructure with the results of simulations on typical idealized simulation setups with planar IPBs, we show that the misfit dislocation network, and in particular the core structure of the misfit dislocations, depend on the precipitate morphology and play a crucial role in determining the possible interaction mechanisms between matrix dislocations and the misfit dislocation network.

2. Methods

2.1. Experiments

The key idea of the present study lies in conducting APT-informed atomistic simulations. For this purpose, as a first step APT characterization was conducted on a single crystal Ni-base superalloy ERBO/1 with a composition close to the commercial CMSX-4 alloy [39]. In a second step atomistic starting configurations for subsequent MD simulations were generated from the APT data set as outlined in the ensuing section. The master melt was provided by Cannon-Muskegon and cast into a single crystal plate with $\langle 0\,0\,1\rangle$ orientation along the solidification direction by Doncasters Precision Casting, Bochum. The cast plate was homogenized at 1300 °C for 6 h to minimize elemental segregation at the dendrite scale. The homogenized plate was then aged in two steps, 1140 °C for 4 h and subsequently at 870 °C for 16 h, to form a common γ/γ' superalloy microstructure. The alloy was cooled in air after each step of heat treatment process. The actual chemical composition of the alloy after heat treatment was determined by inductive-coupled plasma atomic emission spectroscopy (ICP-AES) and is presented in Table 1.

Specimens for APT analyses were prepared with their $\langle 0\,0\,1\rangle$ crystallographic orientation parallel to the specimen axis using a dual-beam focused-ion-beam (FIB) system (FEI Helios Nanolab 600). A conventional lift-out method described in [40] was applied. To eliminate the subvolume damaged by Ga ions during preparation, final shaping of the APT tips was performed using low-energy (5 keV) ions. APT measurements were performed using a reflectron-equipped local electrode atom probe (LEAP 3000X HR, Cameca Instruments) in pulsed voltage mode with pulse rate of 200 kHz and pulse fraction of 15%. The specimen base temperature of 60 K and detection rate of 0.005 ions per pulse were maintained throughout the analysis. Reconstruction, visualization and analysis of APT data sets were performed using the commercial software IVAS 3.6.6 (Cameca Instruments). From the initial APT data set obtained from the experiment about 1 million ions were discarded to eliminate the outer Ga contaminated regions.

2.2. Atomistic sample generation from APT data

To construct APT-informed atomistic simulation samples we suggest here a simpler alternative to the approaches currently found in the literature [35–37]. The fundamental step is to obtain information on the IPB from the APT data. The γ and γ' phases have different chemical compositions, and hence the IPB position can be defined by the isodensity surfaces of any ion which partitions strongly into either γ matrix or the γ' precipitate, see Figs. 1(b) and (c). Once the precipitate shape is determined, it can be filled with atoms arranged according to the crystallographic structure and orientation of the lattice of the precipitate phase which – in case it cannot be determined from the APT dataset itself – has to be determined by complementary experiments, e.g. by correlative TEM, electron backscatter diffraction (EBSD) or X-ray diffraction [41]. The remainder of the sample is filled with atoms on lattice positions of the matrix phase. The approach of using complementary information on the crystallography renders the lattice rectification step [36,37] in the sample reconstruction