Materials Science & Engineering A 616 (2014) 275–280

Contents lists available at ScienceDirect

Materials Science & Engineering A

journal homepage: www.elsevier.com/locate/msea

Parametric dislocation dynamics simulation of precipitation hardening in a Ni-based superalloy

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ARTICLE INFO

Article history:
Received 13 June 2014
Received in revised form
1 August 2014
Accepted 4 August 2014
Available online 11 August 2014

Keywords:
Ni-based superalloys
Precipitation hardening
Critical resolved shear stress
Dislocation dynamics

ABSTRACT

The precipitation hardening in Ni-based superalloys, which contain up to 73% volume fraction of cubic coherent γ' precipitates in γ matrix, has been investigated by three-dimensional parametric dislocation dynamics. Dislocations glide under external stress on a (111) slip plane intersected by cubic γ' precipitates. The critical resolved shear stress (CRSS), the stress to drive dislocations through precipitates, is evaluated for variations in various microstructural parameters: γ' volume fraction, anti-phase boundary (APB) energy and γ channel width (i.e., precipitate/particle spacing). It is shown that the CRSS depends on the square root of the APB energy while being linearly proportional to the volume fraction of γ'. A microstructure with a non-uniform size distribution of γ' has a CRSS that is 20–30% smaller than that of a microstructure with a uniform γ' size of the same value as the average γ' size in the non-uniform microstructure. This is due to some local channel widths larger than the average channel width, and larger channel widths allow easier bending of the dislocation line. Our results indicate that the channel width plays an important role in determining the CRSS in addition to the γ' size. For channels narrower than 20 nm, the CRSS is found to increase with decreasing channel width but to depend only weakly on γ' size.

1. Introduction

Ni-based superalloys are widely used as advanced structural materials for high temperature applications, such as in jet engines and high performance turbine engines for aerospace and power generation industries. Their superior mechanical properties are derived from a unique two-phase microstructure with both γ' precipitates and γ matrix. Plastic deformation in crystalline metals is primarily due to the movement of a collection of dislocations. Second phases in these alloys, such as precipitates, can hinder dislocation motion and contribute to the strengthening/hardening of materials. Thus, study of the interaction between dislocations and γ' precipitates can provide crucial understanding of the plastic deformation mechanisms in superalloys, and help design the size, shape and distribution of precipitates in these alloys to achieve better properties for extreme working conditions.

The point obstacle model has been widely used to study precipitation hardening. In this model, a dislocation is treated as a flexible line with line tension, while point obstacles are randomly distributed on the glide plane. The dislocation can move under external applied stresses. Studies applying this model have been dedicated to predict the critical resolved shear stress (CRSS) for the dislocation to glide through a population of identical obstacles or two different (weak and strong) obstacles. Classical analysis done by Friedel [1] showed that the critical stress scales with weak obstacle strength with a power of 3/2, while with strong obstacles with a power of 1 from the Orowan equation [2]. This model was further developed by Morris and Klahn [3], Hanson and Morris [4], Labusch [5] and others. Since last 70s, two dimensional (2D) dislocation dynamics computer simulations [6,7] have appeared to study problems in plastic deformation. Recently, a 2D thermally activated point obstacle model [8,9] was used to study the CRSS and strain rate sensitivity of metallic alloys with a field of single, two and many different kinds of obstacles in the glide plane. Their results show good agreement with analytical superposition law [10] and simulation results from Foreman and Makin [11].

A proper understanding of plasticity in superalloys involves summing up the properties of individual dislocations over a volume large enough to represent bulk materials as well as considering the size, shape and morphology of precipitates beyond the simple point obstacle models. In recent years, three dimensional (3D) dislocations dynamics methods have been developed to directly simulate the behavior of dislocations, and the technique

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http://dx.doi.org/10.1016/j.msea.2014.08.011
0921-5093/

has been envisioned as the link between single dislocation behavior and the plasticity of a single crystal. In dislocation dynamics, dislocations are discretized into small segments. Equations of motion are constructed for segments subjected to internal and external forces. Several 3D dislocation dynamics (DD) methods [12–19] have emerged with the ability of simulating dislocations and their interactions with finite size obstacles, including precipitates in Ni-based superalloys. While these studies are still explorative, they have shown that the DD methods are becoming more capable in understanding dislocation-based deformation mechanisms in heterogeneous materials.

In this article, a parametric dislocation dynamics (PDD) method [20–22] will be used to extend these efforts to more complex precipitate microstructures, which have smaller channel widths and non-uniform γ' size distributions. A superdislocation model with consideration of the anti-phase boundary (APB) force has been implemented for dislocation interactions with coherent γ' precipitates. The critical resolved shear stress is investigated for variations in microstructural parameters: γ' volume fraction, APB energy and γ channel width. The purpose of the present investigation is firstly to validate our PDD code for further massive 3D DD simulations of γ/γ' superalloys, and secondly to investigate the effect of microstructural parameters on the mechanical properties of superalloys and provide valuable guidelines for superalloy design. Section 2 will discuss the model and simulation setups. Section 3 will present simulation results and discussions followed by concluding remarks in Section 4.

2. Model and simulation procedure

2.1. Precipitate distribution

Two types of precipitate distributions are studied in this work: uniform and non-uniform distributions. Fig. 1(a) shows a 3D view of precipitate arrays, while Fig. 1(b) and (c) shows uniform and non-uniform distributions. For a uniform distribution of precipitates, where each precipitate has the same size, the centers of precipitates are placed at regular grid points. The distance L between centers of two closest precipitates is estimated from the volume fraction f, and precipitate size l, as

$$L = \frac{l}{\sqrt[3]{f}} \quad (1)$$

The γ channel width is $w = L - l$, which is the spacing between precipitates.

For a non-uniform distribution of precipitates, the sizes of precipitates are not equal. But the centers of precipitates are still placed at regular grid points according to Eq. (1), where l is replaced with the average size of precipitates as l_{ave}. This

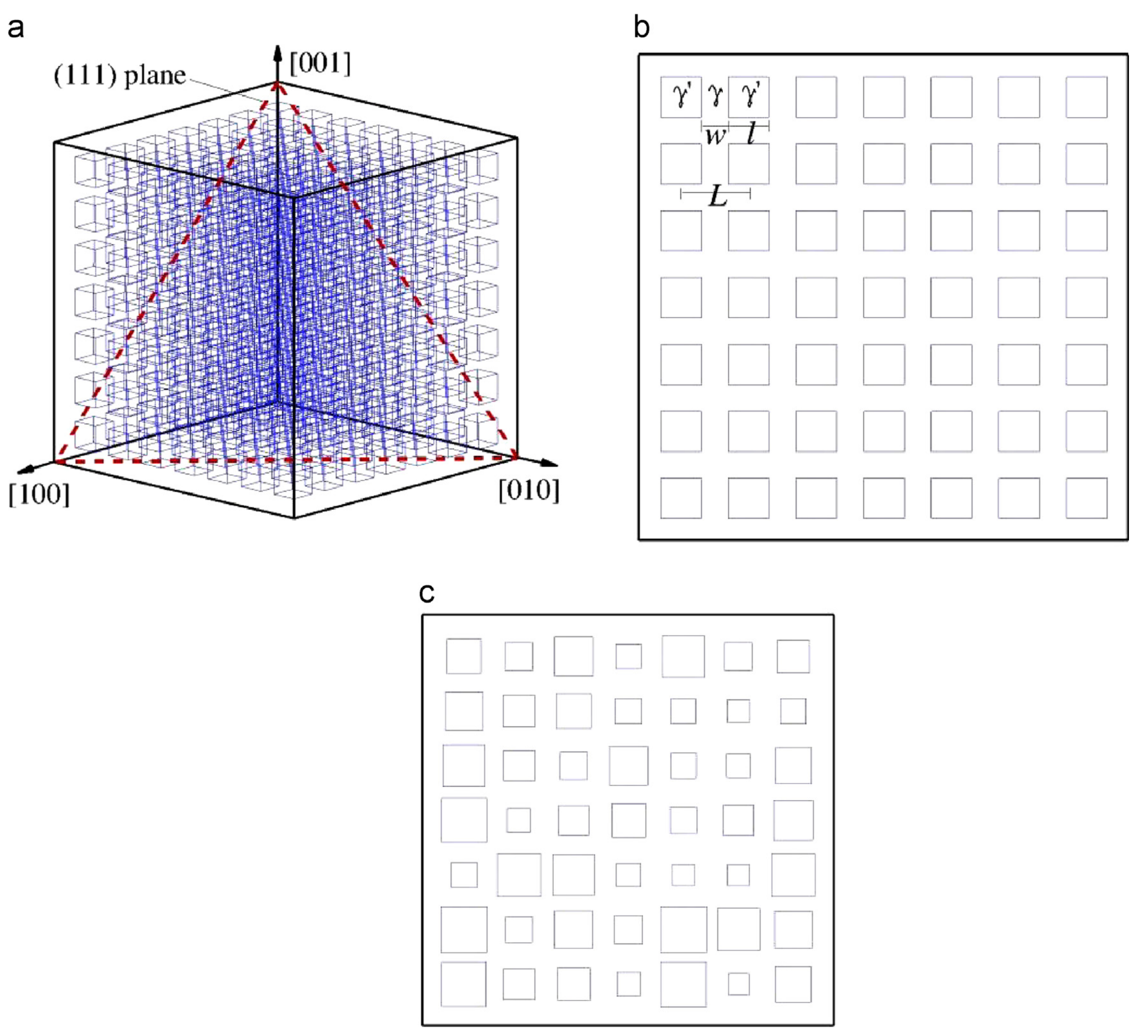

Fig. 1. (a) Arrays of cubic precipitates in a volume with crystallographic orientations and a (111) slip plane also shown; (b) [100] view of a uniform distribution of precipitates; (c) [100] view of a non-uniform distribution of precipitates (only one front layer is shown).