Journal of Physics and Chemistry of Solids 98 (2016) 220–232

Contents lists available at ScienceDirect

Journal of Physics and Chemistry of Solids

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

Orientation dependence of void growth at triple junction of grain boundaries in nanoscale tricrystal nickel film subjected to uniaxial tensile loading

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ARTICLE INFO

Article history:
Received 10 May 2016
Received in revised form
13 July 2016
Accepted 18 July 2016
Available online 19 July 2016

Keywords:
A. Metals
A. Nanostructures
A. Thin films
D. Defects
D. Fracture

ABSTRACT

Molecular dynamics simulation was performed in order to investigate the dependence of void growth on crystallographic orientation at the triple junction of grain boundaries in nanoscale tricrystal nickel film subjected to uniaxial tensile loading. The nucleation, the emission and the transmission of Shockley partial dislocations play a predominant role in the growth of void at the triple junction of grain boundaries. The orientation factors of various slip systems are calculated according to Schmid law. The slip systems activated in a grain of tricrystal nickel film basically conform to Schmid law which is completely suitable for a single crystal. The activated slip systems play an important role in plastic deformation of nanoscale tricrystal nickel film subjected to uniaxial tensile loading. The slip directions exhibit great difference among the activated slip systems such that the void is caused to be subjected to various stress conditions, which further leads to the difference in void growth among the tricrystal nickel films with different orientation distributions. It can be concluded that the grain orientation distribution has a significant influence on void growth at the triple junction of grain boundaries.

1. Introduction

Classical dimpled fracture is the main failure pattern of ductile metals, and it is often induced by the nucleation, growth and coalescence of voids. Of the three stages, void growth is found to be the most important one, since most metals experience plastic deformation during processing or service at the stage. Because the growth process of voids, which are often in sub-micron scale or nano scales, is unable to be captured by means of experiments, researchers often investigate it by means of establishing analytical models or numerical simulations. Over the last decades, numerous analytical models and numerical simulations have been carried out to investigate the mechanism of void growth during plastic deformation. In the case of analytical models, the results obtained by Lubarda et al. [1] and Ahn et al. [2] indicated that dislocation loop emitted from the void surface is the primary mechanism for the void expansion. Fischer and Antretter [3] proposed that the diffusion of vacancies and the mechanical driving force contribute to void growth. In recent years, several other analytical models have been developed and extended to understand void growth in metals [4–9]. However, because the results obtained through analytical models are invisible, the process of void growth is unable to be understood clearly. Therefore, several numerical methods such as finite element method, discrete dislocation dynamics and molecular dynamics have been used.

By means of classical crystal plasticity finite element method (CPFEM), Thakare et al. [10] investigated the void growth near a notch tip in ductile face-centered cubic (FCC) single crystal and paid a special attention to the effects of several factors, including the crystal hardening exponent, the ratio of void diameter to width of ligament connecting the notch and the void, and the crystal orientation, on the plastic flow localization and the void growth. Following them, Yerra et al. [11] investigated void growth and coalescence in single crystals under constant macroscopic triaxial stress, where the influences of crystal orientation on void shape evolution and void growth were analyzed. Biswas and Narasimhan [12,13] studied the void growth and the interaction between notch and micro-void(s) in single crystal, where crystal orientation and through-thickness variation in both hydrostatic stress and equivalent plastic slip during the process of void growth and void-notch interaction were analyzed carefully. Patra and McDowell [14] developed constitutive equations for vacancy generation induced by inelastic deformation, void nucleation caused

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http://dx.doi.org/10.1016/j.jpcs.2016.07.018
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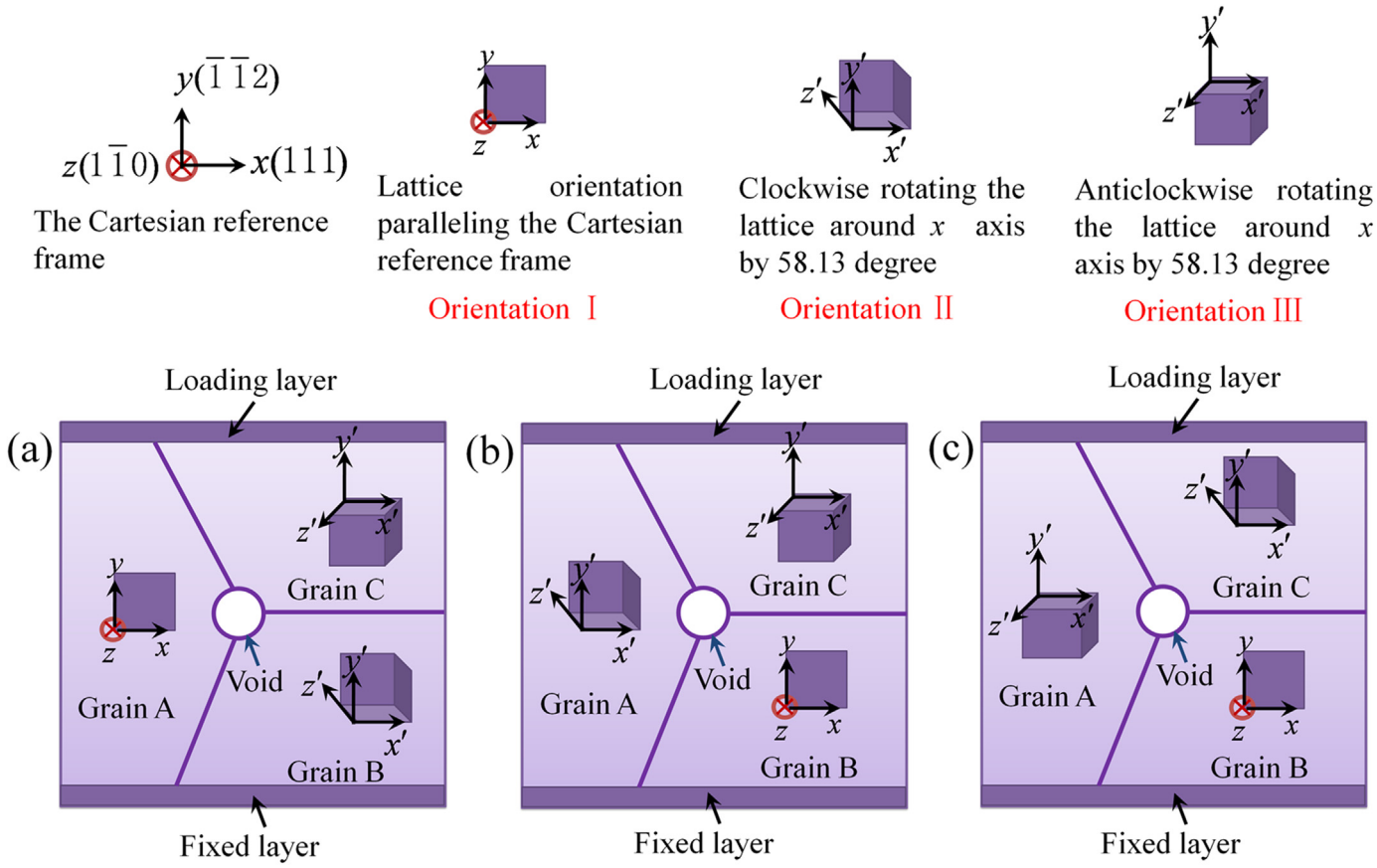

Fig. 1. Simulation models of tricrystal nickel films with different grain orientation distributions: (a) Model I; (b) Model II; (c) Model III.

by vacancy condensation, and diffusion-assisted void growth. However, the diameter of micro-voids and the radius of notch root considered in the above studies are much larger than the actual sizes which usually are several submicrons or nanometers in real materials.

By means of discrete dislocation dynamics (DDD), Segurado and Llorca [15,16] investigated void growth in an isolated FCC single crystal subjected to in-plane strain deformation in the $(\bar{1}10)$ plane, where the size effects on the mechanical behavior and void growth rate in single crystals subjected to hydrostatic tension were analyzed, and micromechanisms of plastic deformation and void growth were revealed. Following them, Liang et al. [17] simulated the interaction between a type-I blunt crack and a near-tip void, where a special emphasis was laid on the void growth, the crack-tip deformation and their size effect. Chang et al. [18] studied plastic void growth in FCC single crystals subjected to hydrostatic tension, where size effect on the void growth rate was developed. However, DDD usually suffers from the approximate nature of prescribed short-range interaction rules between mobile dislocations and voids, and it is lack of the ability to model the dissociation of dislocations. In addition, approximations between dislocation cross slip and other important local mechanisms are required in using DDD. As a result, there is still a large gap in understanding the reason why dislocation slip is able to lead to the fracture of materials. Furthermore, the damage mechanism that is caused by growth and coalescence of voids, which are often in sub-micron scale or nano scales, is unable to be captured by means of DDD.

Molecular dynamics (MD) simulations have been proved to be a powerful candidate for observing the atomic details of fracture behaviors, so more and more researches have devoted themselves to investigating the void growth by means of MD simulations. Potirniche et al. [19] studied the evolution of damage induced by the growth and coalescence of void, where the evolution of void volume fraction and the corresponding stress–strain responses were monitored as the voids grew under the increasing applied tractions. Traiviratana et al. [20] revealed mechanisms of void growth in monocrystalline and bicrystalline copper subjected to tensile uniaxial strains, and they confirmed that the emission of (shear) loops is the primary mechanism of void growth, which agrees with the analytical results obtained by Lubarda et al. [1] and Ahn et al. [2]. Zhao et al. [21] studied cylindrical nano-void growth in FCC single crystal copper subjected to uniaxial tension, where the effects of cell size, crystalline orientation and initial void volume fraction on the macroscopic stress–strain curve, the incipient yield strength and the macroscopic effective Young's modulus were quantified, and the defect evolution in terms of dislocation emission immediately after incipient yielding was investigated as well. Tang et al. [22] investigated the growth and coalescence of voids in magnesium single crystals at the nanoscale, where one void and two void specimens with identical initial void volume fractions were utilized to study the mechanism of growth and coalescence of void. Mi et al. [23] investigated dislocation-based mechanisms of growth and coalescence of void, where a void growth algorithm based on simple-cubic discretization of the rectangular simulation domains is proposed and implemented to characterize the void expansion. Tang et al. [24] investigated ductile tensile failure in metals based on initiation and growth of nanosized voids, and they found that this process is dominated by the emission of a special type of dislocation shear loop, which expands as a partial or perfect dislocation, and then evolves into a prismatic loop through reaction or develops into twins. Tang et al. [25] investigated the growth of spherical nano-voids and the fracture properties of γ-TiAl single crystal, and they