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Relaxation of a disclinated tricrystalline nanowire

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Abstract

Adjoining grains meeting at triple junctions generally suffer from misorientation mismatch, giving rise to disclinations in polycrystalline materials. This paper presents molecular dynamics simulations of the relaxation of a wedge disclination at the triple junction of a tricrystalline cobalt nanowire between 0 and 1200 K. The results show that complex relaxed structures can occur, including cracks and cavities, distorted grain boundaries, dislocations, twin bands, diffuse dislocation walls and amorphized zones, many of which have been observed in nanocrystalline metals. The realized structures depend on the nanowire size, temperature, disclination strength and grain boundary structures. Furthermore, there exists a critical disclination strength below which the disclination is stable and above which it relaxes via competing mechanisms. The critical disclination strength demonstrates a strong size effect at all temperatures.

Keywords: Disclination; Triple junction; Nanowire; Relaxation mechanism

1. Introduction

Triple junctions (TJs) and grain boundaries (GBs) are characteristic constituents of polycrystalline materials [1,2]. As the grain size d decreases to the nanoscale, the volume fractions of both TJs and GBs increase dramatically, from less than 0.01% and ~3% at $d = 100$ nm to ~25% and ~45% at $d = 3$ nm [1]. On the other hand, rotational defects, i.e., disclinations, frequently form at TJs as a consequence of various mechanisms depending on the method of synthesizing the nanocrystalline material [3–8]. In the severe plastic deformation method, dislocation accumulation at GBs causes plastic strain incompatibilities, resulting in TJ disclinations [3]. Tunneling electron microscopy has revealed disclinations with strengths between 1° and 3° at the TJs of fragmented structures in heavily deformed ultrafine-grained nickel, copper and titanium [4–6]. In the inert gas condensation technique followed by compaction, disclinations form in nanoparticles during their growth and in the GBs and TJs during the subsequent consolidation [7]. In preparing nanocrystalline iron via mechanical milling, disclinations have been directly observed via high-resolution transmission electron microscopy (HRTEM) [8].

Disclinations are known to be sources of high stress concentrations [9,10]. They may therefore be unstable and undergo relaxation, and the various types of relaxed structures directly affect the physical properties such as strength, toughness, diffusion and electrical conductivity. In fact, there are a number of experimental studies on the nature of interfaces in nanocrystalline metals [11–16]. For instance, HRTEM investigations of nanocrystalline palladium show bright contrast regions at TJs, which have been interpreted as nanovoids [11,12] or disordered pockets [16]. Similar conclusions were reached regarding the presence of nanovoids at TJs in nanocrystalline iron, palladium and silver based on the positron lifetime spectroscopy technique [13,14]. Detailed HRTEM investigations of nanocrystalline palladium and titanium also suggest that GBs and TJs show a varying degree of disorder [15,16].

A disclination is wedge (or twist) in character if its Frank vector is parallel (or perpendicular) to the axis of

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the defect. The norm of the Frank vector characterizes the rotational misfit and is usually called the disclination power or strength. Wedge disclinations are considered negative (or positive) if the rotational misfit is associated with the insertion (or removal) of material. Disclinations and dislocations in fact form the six "Volterra dislocations" in the continuum theory of defects [17].

Theoretical investigations of disclinated cylinders or nanowires have received much interest [18–23]. Investigations based on continuum elasticity show that a critical disclination can relax via crack nucleation [18,23]. Molecular dynamics studies reveal more complex relaxation mechanisms [19–22]. Refs. [19–21] and Ref. [22] consider a bi-junction and a triple junction wedge disclination, respectively. The results reveal that there exists a critical disclination strength below which the defect is stable and above which it is unstable, and that the unstable defect may relax via crack nucleation, amorphization of the disclination core, or structural reorientation of parts of the crystals. Continuum elasticity also supports the possibility of amorphization from a wedge disclination [24]. The study on bicrystalline nanowires has revealed much insight, but TJs are necessarily excluded from such study. In the recent study of a disclinated TJ [22], the tricrystalline nanowire material is face-centered cubic (fcc) nickel, the temperature considered is 0 K, and crack nucleation is the only relaxation mechanism predicted. The possible complexities arising from a different crystallography, higher temperatures and multiple relaxation mechanisms are not known, and this paper attempts to address these issues. Also, a number of previous works have dealt with crack nucleation at dislocated, rather than disclinated, TJs due to accumulation of dislocations [25–27].

In this paper, we investigate disclinated TJs in a tricrystalline cylindrical nanowire of hexagonal close-packed (hcp) cobalt at five different temperatures via molecular dynamics. A tricrystalline nanowire, which neglects multiple TJs, is the simplest model of a bulk nanocrystalline material. The surface boundary conditions on the nanowire and the polycrystal may also be different. However, the screening distances for the stress field of a disclination in a finite cylinder and in a polycrystal are, respectively, the cylinder radius R and the grain size d, and one may consider results for the cylinder to be appropriate for those of a polycrystal with $d = R$. In practice, it is infeasible to duplicate a bulk polycrystal via an atomistic model due to computational power constraint. The tricrystalline model investigated here already has a complex morphology due to the GB and TJ structures and the hcp crystallography, and has not been previously investigated to our knowledge.

The paper is organized as follows. Following this introduction, the construction of the atomistic model of the disclinated nanowire is outlined in Section 2. The simulation results are presented in Section 3, a further discussion is given in Section 4, and the conclusions of the present work are summarized in Section 5.

2. Atomistic construction of TJ disclination in hcp tricrystal

We consider a wedge disclination whose axis coincides with the central longitudinal axis of a cylindrical nanowire consisting of three 120° grains. The disclination is constructed by merging three bicrystalline wedges with the misorientations of θ_1, θ_2 and θ_3, respectively, such that the wedges are forced to fit into 120° sectors. The misfit of the misorientations gives rise to a disclination. All three bicrystals are assumed to have a common crystallographic direction $[1\bar{1}00]$ aligned with the cylinder axis/triple line, thus the GBs are symmetric $[1\bar{1}00]$ tilt GBs. The GBs are constructed on the basis of the structural unit model, which has first been developed for tilt GBs in fcc metals [28,29] and found valid also for $[1\bar{1}00]$ tilt GBs in hcp metals [30]. In the following, a short outline to help understand the disclination construction is presented.

Fig. 1 illustrates a $[1\bar{1}00]$ projection of an hcp lattice on which squares, stars, circles and triangles indicate atoms on four successive planes belonging to one period along the direction $[1\bar{1}00]$. Any lattice vector lying on the plane $(1\bar{1}00)$ can be considered as a period vector $\vec{H}$ of a GB of a bicrystal that is constructed by a mirror reflection of the sites lying on one side of the plane containing this vector and $[1\bar{1}00]$ direction. As seen in Fig. 1, any period vector $\vec{H}$ is divided in half by the projection of an atom displaced out of the projection plane along the $[1\bar{1}00]$ direction. Thus, the period vectors can be viewed as consisting of two half-period vectors $\vec{h} = \vec{H}/2$. Furthermore, the vector $\vec{H}$ can be represented as a combination of primitive lattice vectors $\vec{a} = [11\bar{2}0]/3$ and $\vec{c} = [000\bar{1}]$:

$$\vec{H} = \alpha\vec{a} + \beta\vec{c} \tag{1}$$

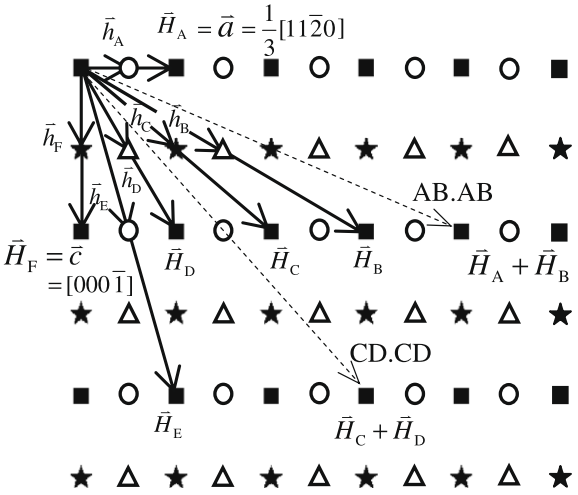

Fig. 1. The $[1\bar{1}00]$ projection of an hcp crystal, showing the period and half-period vectors of GBs constructed by mirror reflection of the sites located on one side of a plane containing a period vector and $[1\bar{1}00]$ axis. Delimiting GBs are designated by letters A through F; intermediate GBs such as AB·AB and CD·CD have misorientations bounded by those of the pair of delimiting boundaries, i.e., A and B, and C and D, respectively.