Materials and Design 52 (2013) 30–35

Contents lists available at SciVerse ScienceDirect

Materials and Design

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

An energy approach to account for crack initiation in nanocrystalline materials

Jianqiu Zhou [a,b,*], Lingling Hu [b], Hongxi Liu [b], Menghan Hu [b]

[a] School of Mechanical & Electrical Engineering, Wuhan Institute of Technology, Wuhan, Hubei 430070, China
[b] School of Mechanical and Power Engineering, Nanjing University of Technology, Nanjing, Jiangsu 210009, China

ARTICLE INFO

Article history:
Received 2 January 2013
Accepted 5 May 2013
Available online 23 May 2013

Keywords:
Nanocrystalline materials
Finest grains
Crack initiation
Energy methods

ABSTRACT

An energy balance method to calculate the initiation of crack at triple junctions in nanocrystalline materials with the finest grains is developed. In the steady state of crack initiation, work done by an applied stress is considered to be dissipated as heat by specific rotational deformation, grain boundary sliding and diffusion. The stress field at crack tips, the energies of rotational deformation, grain boundary sliding and grain boundary diffusion are calculated. The analysis demonstrates that the existence of finest grains will lead to enhanced local fracture toughness.

1. Introduction

Nanocrystalline materials with average grain size in the range from 1 nm to 100 nm show outstanding mechanical properties (ultra-high strength, superior fatigue properties and super hardness) and represent the subject of rapidly growing research efforts motivated by a wide range of applications [1–4]. However, nanocrystalline materials show very low ductility and low toughness as compared to their coarse-grained counterparts, which greatly restricts their applications [5–8]. In these circumstances, it will be of large interest in understanding the fundamental mechanisms governing crack growth processes in nanocrystalline materials.

It has been recognized that, the difference in fracture behavior between nanocrystalline and coarse-grained metals can be attributed to deformation mechanisms dominating in these materials. The lattice dislocation slip serving as the dominant deformation mode in coarse-grained metals is suppressed in nanocrystalline materials [9,10]. At the same time, alternative deformation mechanisms such as intergrain sliding, grain boundary diffusional creep, rotational deformation and nanoscale twin deformation are considered to effectively operate[11–13]. The evidence of enhanced fracture toughness in nanocrystalline materials has been studied and reported. Bobylev et al. [11] showed that intergrain sliding is capable of causing significant blunting of cracks in nanocrystalline materials. Morozov et al. [13] reported on toughness enhancement of nanocrystalline materials, compared to their coarse-grained counterparts, in which case the special rotational deformation intensively occurs. Youssef et al. [8] reported a uniform tensile elongation of 14% and 15.5% elongation-to-failure of nanocrystalline copper synthesized via a unique process of in situ consolidation through mechanical milling. We have found that a considerable amount of finest grains (defined as grains with size between 2 nm and 4 nm, denoted as FGs) exist in nanocrystalline copper specimens. In fact, Gleiter [14] pointed out that these FGs exhibit novel behaviors, i.e., the atomic structure throughout the entire volume of the material as well as the density of the entire material can be tuned. However, the role of FGs is usually neglected in previous studies [10,15]. We believe that FGs may be responsible for some unique mechanical behaviors of nanocrystalline materials.

The main aim of this paper is to theoretically describe the effect of the finest grains on crack growth in nanocrystalline materials. The special rotational deformation conducted by grain boundary processes is considered to occur near crack tips and influence crack growth. An energy balance approach to account for crack initiation at triple junctions in nanocrystalline materials is proposed. In the steady state of crack initiation, work done by an applied stress is considered to be dissipated as heat by the specific rotational deformation, grain boundary sliding and diffusion. The special rotational deformation and grain boundary diffusion are suggested as a toughening micromechanism causing crack blunting in nanocrystalline metals. On the other hand, grain boundary sliding which occurs via grain boundary dislocation movement and leads to the storage of grain boundary dislocations at triple junctions is capable of causing the stress concentration and consequently contributes

* Corresponding author at: School of Mechanical & Electrical Engineering, Wuhan Institute of Technology, Wuhan, Hubei 430070, China. Tel.: +86 27 87992123; fax: +86 27 87992123.
E-mail address: zhouj@njut.edu.cn (J. Zhou).

0261-3069/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.matdes.2013.05.044

to crack growth in the vicinities of triple junctions. The stress field at crack tips and work done by rotational deformation, grain boundary sliding and grain boundary diffusion are calculated.

2. Energy approach and balance

A new composite model containing two types of grains (FGs and normal nanograins (NNGs)) is proposed to interpret the abnormal fracture toughness. The FGs are distributed homogeneously in the NNGs matrix. A schematic representation of the composite model is shown in Fig. 1a. The anisotropic mesh structures, as shown in Fig. 1a, represent the random orientation of adjacent grains. The dimension of FG is close to the size of a normal triple junction (TJ). It has been discovered that the structures and properties of TJs are different from those of grain boundaries they adjoin [16,17]. The diffusivity of TJs is usually two or more orders of magnitude higher than that of grain boundaries due to the rather disordered structures [16]. The fast diffusing TJ cores form a continuous network in nanocrystalline materials instead of being isolated from one another. Hence, the entire volume of the FGs could be treated as a component of TJs. These 'TJs' are larger than normal TJs; we name them super triple junctions (STJs).

The observations of in situ TEM experiments indicated that most of the deformation is associated with the advancement of crack tips [18]. During crack growth, plastic deformation is observed in the neighboring grains. Let us consider a nanocrystalline specimen the structure of which can be illustrated in Fig. 1a with a crack under tensile stress (Fig. 1b. The specimen is assumed to be an elastically isotropic solid. The crack tip is assumed to be located at a super triple junction. It is well known that high local stresses operating near the crack tip can initiate special rotational deformation (Fig. 1c). According to Morozov [13], special rotational deformation occurs in nanograins, by forming immobile disclinations, strengths of which gradually increase during the formation process conducted by grain boundary sliding and diffusion-controlled climb of grain boundary dislocations.

An energy balance method is proposed here. The energy dissipation in the deformation process equals to the external working done on the specimen. That is, in a steady state, the total dissipating energy by the special rotational deformation, grain boundary sliding and grain boundary diffusion is supplied by the external work. Therefore, for the crack in a deformed nanocrystalline spacimen shown in Fig. 1b, the energy balance can be given as:

$$\dot{W} = \dot{W}_{rotational} + \dot{W}_{sliding} + \dot{W}_{diffusion} = \sigma_0 \dot{\varepsilon} \tag{1}$$

where $\dot{W}_{rotational}$, $\dot{W}_{sliding}$ and $\dot{W}_{diffusion}$ represent the energy dissipations by the special rotational deformation, grain boundary sliding and grain boundary diffusion, respectively. σ_0 is the stress loaded on the specimen; $\dot{\varepsilon}$ is the equivalent strain rate.

The Coble-creep equation appropriate for nanocrystalline materials can be deduced as [19]:

$$\dot{\varepsilon} = 4K \frac{\sigma \Omega D_B}{k_B T} \left(\frac{2\delta}{D^3} - \frac{\delta^2}{D^4} \right) \tag{2}$$

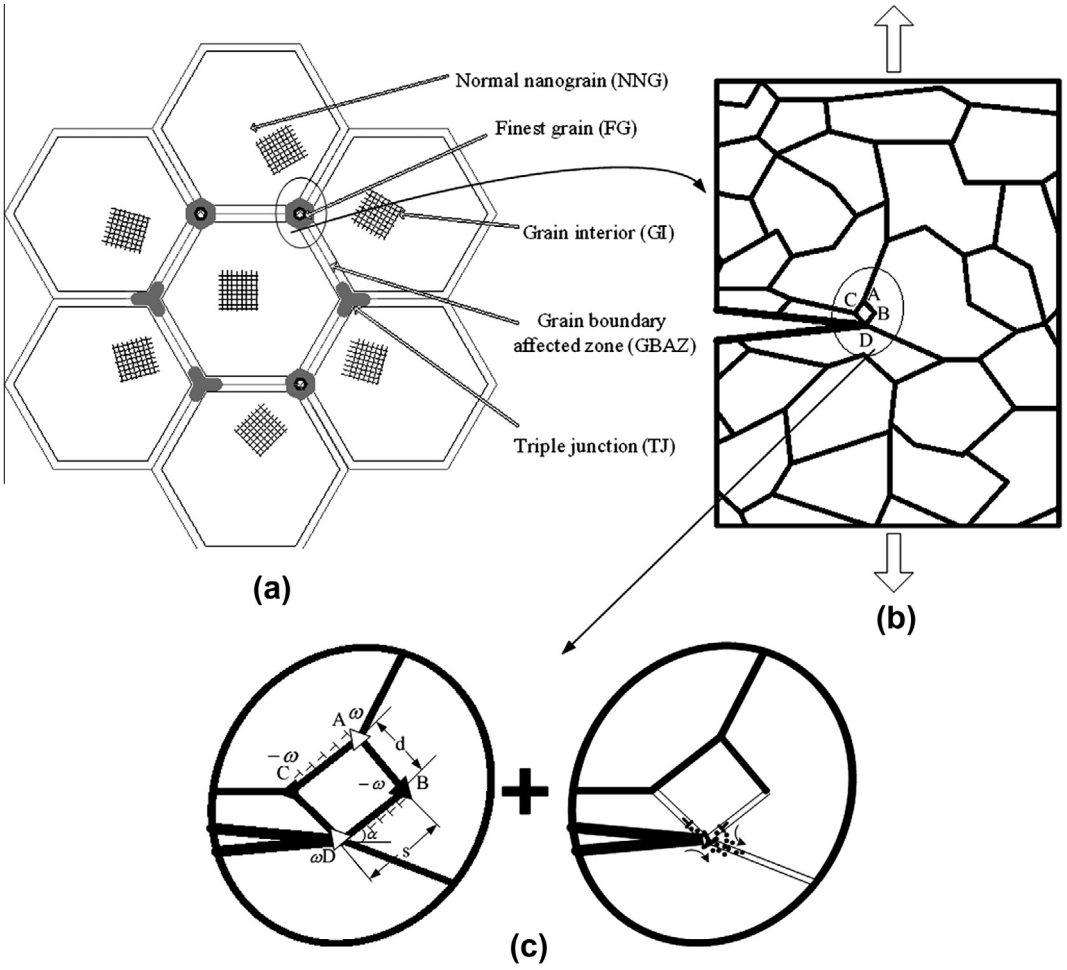

Fig. 1. (a) Schematic representations of the composite model, (b) crack in a deformed nanocrystalline solid with the finest grains. The magnified inset highlights and (c) a disclination quadrupole near the crack tip and the storage of grain boundary dislocations and the enhanced diffusion at a triple junction.