Engineering Fracture Mechanics 201 (2018) 29–35

Contents lists available at ScienceDirect

Engineering Fracture Mechanics

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

The crack nucleation in hierarchically nanotwinned metals

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ARTICLE INFO

Keywords:
Nanocrystalline metals
Hierarchical twin lamellae
Dislocations
Crack nucleation

ABSTRACT

The nanocrystalline (NC) metals with hierarchical twin lamellae exhibit excellent mechanical properties. However, recent efforts are mainly focused on the effects of primary twin boundaries (TB) and grain boundaries (GB) on crack nucleation. Few investigations have been performed on secondary twin boundary (STB) effect on crack nucleation in hierarchically nanotwinned metal. A relevant model is established to describe the crack nucleation criteria quantitatively. Actually, the crack advance mainly depends on the energy of crack nucleation and the energy of pile-up dislocations. Furthermore, predictions about the site of crack nucleation are made for different hierarchically nanotwinned metals. This work will help us better understand the deformation mechanism and the failure behavior in NC materials with hierarchically nanostructures.

1. Introduction

The hierarchically nanotwinned materials exhibit unique mechanic behaviors, such as good ductility, high strength and high hardness [1–9]. Secondary twin lamellae are observed when the primary twin boundary spacing (TBS) reaches to the critical TBS. A self-consistent model was used to understand the global and local mechanical behaviors of the hierarchical materials [10,11]. The hierarchically nanotwinned materials derive high strength from unique deformation mechanism [12]. Also, the hierarchically twinned structures were observed during the martensitic transformation [13,14]. Various researches have confirmed that the hierarchical twin has a significant role in mechanical behaviors. Tao and Qu observed the primary and secondary lamellae in the nanotwinned Cu and Cu-Al alloy by equal-channel angular pressing [15,16]. Besides the experimental achievements, molecular dynamic (MD) simulations provide the possibility of analyzing mechanical behaviors of hierarchical metals quantitatively [17,18].

In the present contribution, a corresponding model was proposed to explore the crack nucleation at GB-TB intersections by Zhang [19]. Moreover, a theoretical model was described to analyze the effects of TBSs and grain size in face-centered cubic (FCC) metals by Zhu [20]. However, Zhang only put the TB-GB intersections into consideration. In the hierarchically nanotwinned materials, dislocations may also pile up at the primary-secondary twin boundary. In this paper, the energy of pile-up dislocations considering the secondary twin boundary effect will be calculated accurately to predict the site of crack nucleation (e.g. TB-GB or TB-STB intersection).

2. The model for boundary intersections

As shown in Fig. 1(a), lots of TB-GB and TB-STB intersections exist in the hierarchically nanotwinned model. During the plastic

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https://doi.org/10.1016/j.engfracmech.2018.08.027
Received 14 May 2018; Received in revised form 24 July 2018; Accepted 28 August 2018
Available online 30 August 2018

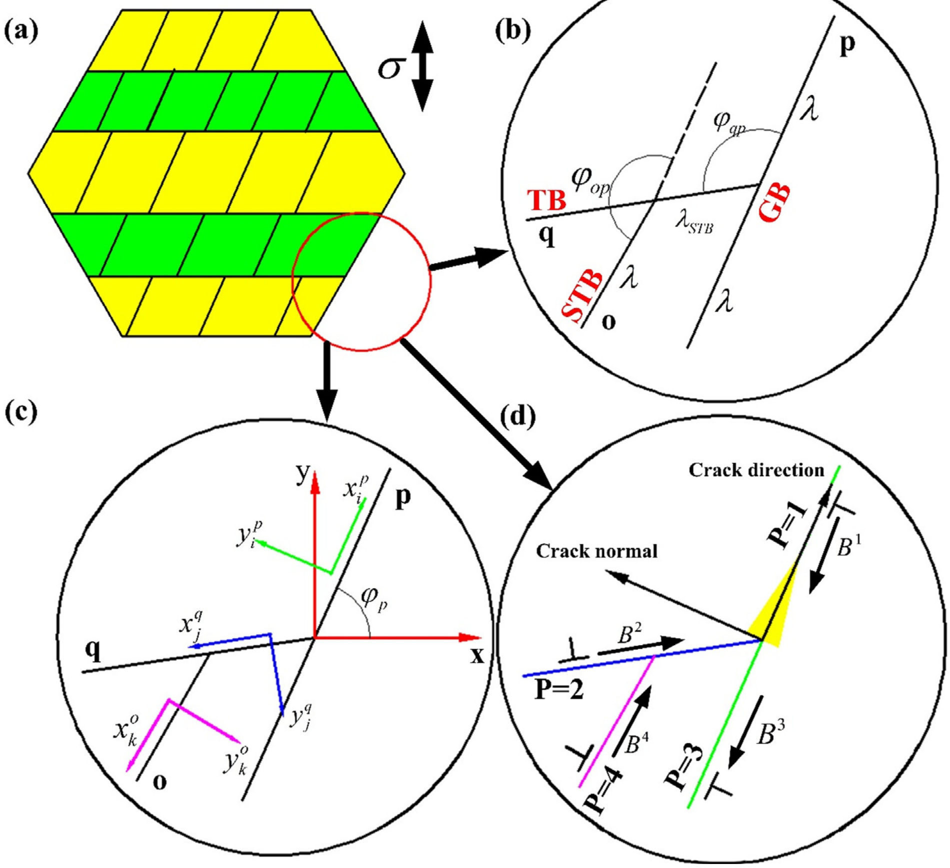

Fig. 1. Schematic drawing of pile-up dislocations at the TB-GB or TB-STB intersection.

deformation process, dislocations pile up on the boundary p, q and o. At the same time, a stress concentration is produced at the TB-GB intersection or TB-STB intersection. When reaching the condition of crack nucleation, the crack will propagate and stress concentration is released.

Fig. 1(b) shows the geometric relationship between each boundary. φ_{qp} is the angle between boundary p and q and φ_{op} is the angle between boundary p and o. As shown in Fig. 1(c), a global rectangular coordinate x-y axes colored by red is defined. The vertical direction is along the direction of loading stress, and the angle between the horizontal direction and boundary p is marked as φ_p. Then we establish three local coordinate systems on each boundary. Fig. 1(d) draws the diagram of pile-up dislocations on each boundary. A wedge crack is at the TB-GB intersection or TB-STB intersection, and the crack advance direction is along the boundary p or q respectively.

In the local frame x_i^p–y_i^p, the in-plane stress components of the dislocation i can be written by [21],

$$\sigma_{xx} = -Ab^p y_i^p \left[\frac{3(x_i^p)^2 + (y_i^p)^2}{((x_i^p)^2 + (y_i^p)^2)^2} \right] \tag{1a}$$

$$\sigma_{yy} = Ab^p y_i^p \left[\frac{(x_i^p)^2 - (y_i^p)^2}{((x_i^p)^2 + (y_i^p)^2)^2} \right] \tag{1b}$$

$$\sigma_{xy} = Ab^p x_i^p \left[\frac{(x_i^p)^2 - (y_i^p)^2}{((x_i^p)^2 + (y_i^p)^2)^2} \right] \tag{1c}$$

In the local frame x_j^q–y_j^q or x_k^o–y_k^o, the in-plane stress components of the dislocation j or k can be written in the similar form,

$$\sigma_{xx} = -Ab^{q,o} y_{j,k}^{q,o} \left[\frac{3(x_{j,k}^{q,o})^2 + (y_{j,k}^{q,o})^2}{((x_{j,k}^{q,o})^2 + (y_{j,k}^{q,o})^2)^2} \right] \tag{2a}$$