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Grain rotation dependent fracture toughness of nanocrystalline materials

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ABSTRACT

A grain size dependent theoretical model is developed to describe the effect of special rotational deformation (SRD) on crack growth in deformed nanocrystalline (nc) materials. The SRD is driven by the stress concentration near the crack tip, and it serves as a toughening mechanism by releases part of the local stresses. The dependence of critical crack intensity factors on grain size was calculated. It was demonstrated that the SRD leads to an increase of critical crack intensity factors by 10–50%.

1. Introduction

Nc materials have been a source of great interest currently due to their unusual mechanical and physical properties [1–8]. In general, nc materials show superior strength but low tensile ductility and low fracture toughness, which limit their applications [1,3,4,6]. However, the evidence of good tensile ductility and/or enhanced toughness in nc materials has been studied and reported [9–14]. Understanding the fundamentals of toughness in the nc materials is of great importance to develop new applications. So far, many models have been developed to explain this phenomenon [15–18]. Most of them attributed the good tensile ductility and/or enhanced toughness to the alternative deformation modes such as lattice dislocation slip, intergrain sliding, Coble creep, triple junction diffusional creep, rotational deformation, and nanoscale twin deformation effectively operating in nc materials.

Many experiments [19–25] have shown that rotational deformation (plastic deformation accompanied by crystal lattice rotations) often occurs in nc materials. Besides, computer simulations [26–28] and theoretical models [29–33] have provided convincing evidence for the important role of rotational deformation in plastic flow processes in various nc materials. Morozov et al. suggested a theoretical model to study the effect of SRD on crack growth in nc materials, however, the relationship between the rotational deformation and grain size has been not well studied, and it needs to be improved. Ovid'ko et al. have pointed that the SRD effectively occurs through the formation of a quadrupole of immobile wedge disclinations whose strengths gradually increase. Their work also gives the energy change associated with the both formation of the quadrupole and the grain size. Romanov et al. indicated that at a certain grain size, there is a critical stress above which the rotation mode of the plastic deformation transfers to another mode. The remaining defects in the grain interior, such as disclination quadrupole and dislocation dipole, possess no field elastic distortions. The above three theories will be introduced briefly in Section 2. It can be seen from the above models that although the above experimental and theoretical results suggest that the rotational deformation contribute to the toughening of nc materials, the relationship between the rotational deformation and grain size has not been well quantitatively studied. In spirit of these previous works, we built a theoretical model to study the hampering effect of the SRD with grain size dependent. This mechanism is different from both standard rotational deformation, which occurs through the movement of wedge disclinations, and diffusion-accommodated grain rotations, which do not contribute to plastic flow [32,33]. The SRD can effectively operate on crack growth in nc materials, but is commonly suppressed in coarse-grained polycrystals [33]. More importantly, the dependence of critical crack intensity fac-

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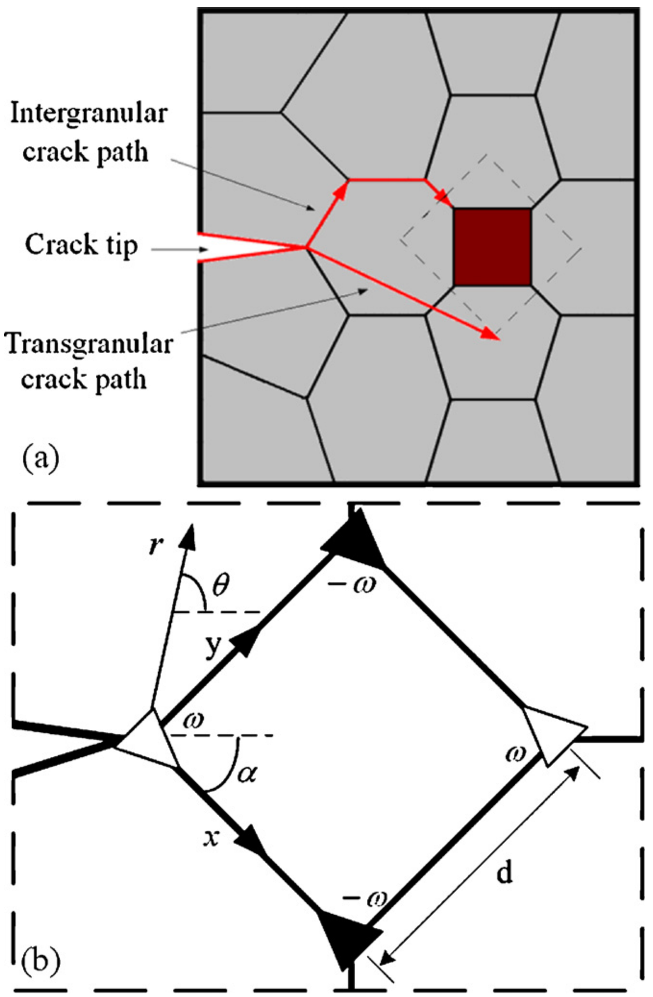

Fig. 1. (a) Special rotational deformation in a deformed nc material containing a mode I crack. (b) Magnified region in (a) highlights a disclination quadrupole near the crack tip.

tors on grain size was calculated, the results appeared to be much meaningful and inspired. So far, there are few literatures doing the similar works.

2. Model and results

In general, there are two ways for the crack propagation in polycrystals: (i) crack crosses the grain (transgranular propagation); (ii) crack travels the interface region between the grains (intergranular propagation), as schematically shown in Fig. 1a. Actually, the present model is applicable for both the transgranular and intergranular fracture mechanisms. In this paper, our aim is to study the effect of SRD. Thus, we only consider a special case that crack tip intersects GBs. and we will not study how the crack propagates. Let us consider the case where a long flat crack evolves under the action of an applied load in the deformed nc specimen under a tensile load (Fig. 1b). For simplicity, we restrict our consideration to a two-dimensional grain structure. High stress concentration near the crack tips can initiate the SRD of grains (Fig. 1b). In the present two-dimensional model, we will consider the SRD of a quadrate grain and the case when the crack tip reaches a junction of boundaries of this grain, as shown in Fig. 1b.

In terms of the theory of defects, the SRD can be described as the formation of a quadrupole of immobile wedge disclinations in such a grain. The strength of the disclinations gradually grows during the formation process [33]. The SRD is conducted by: (i) GB sliding along GBs AB and CD; (ii) diffusion-controlled climb of GB dislocations along GBs AC and BD (Fig. 2a–c). Following the concept on local shear events – shear transformations of local atomic clusters – as carriers of plastic flow in GBs in metals [34,35] and covalent solids [36], we suppose that local shear events carry sliding along GBs AB and CD. The sliding results in the formation of GB dislocations at junctions A, B, C and D [37,38], as schematically shown in Fig. 2a–c. Diffusion-controlled climb of the dislocations

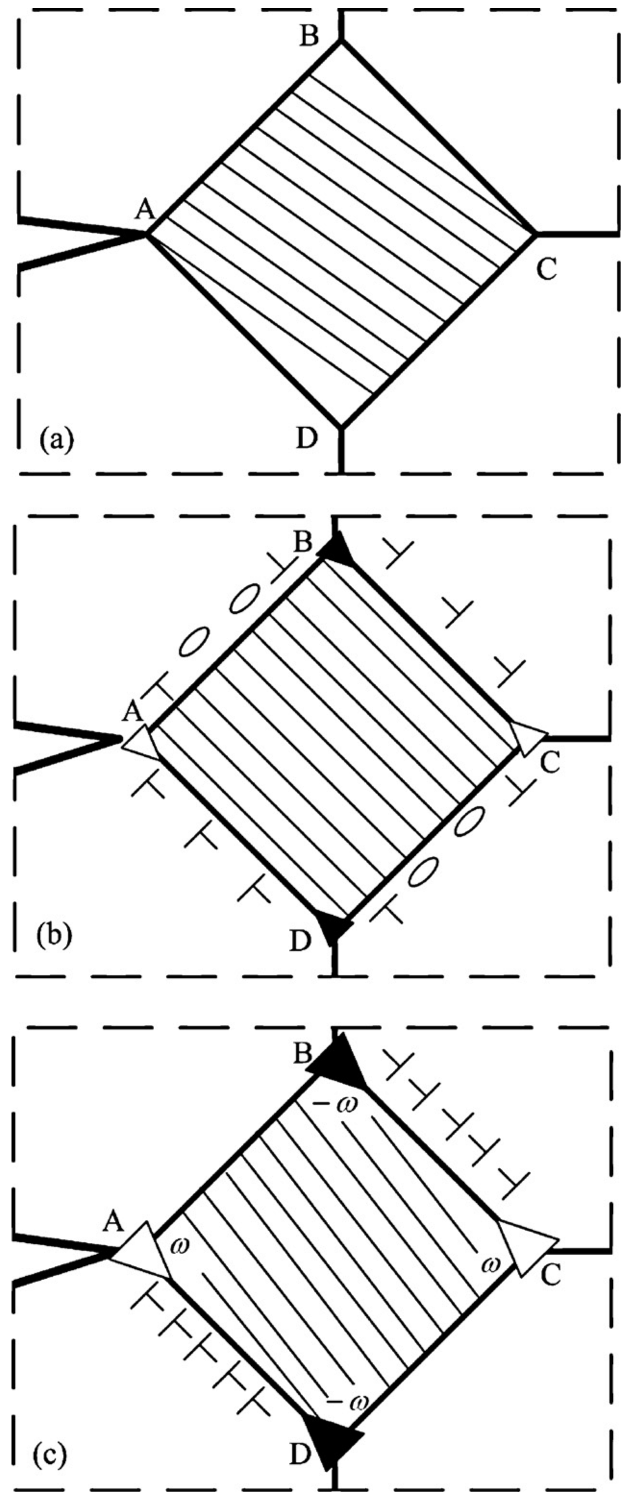

Fig. 2. Special rotational deformation occurs in a nanograin through the formation of immobile disclinations.