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Significantly enhanced crack blunting by nanograin rotation in nanocrystalline materials

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ABSTRACT

Experiments have shown that stress-driven grain growth is closely related to the enhanced crack growth resistance and the exceptional tensile ductility as observed in several nano-metals. However, the quantitative correlation remains unsolved. Here we developed a theoretical model to investigate the effect of nanograin rotation, one of the main modes of stress-driven grain growth, on dislocation emission from the tip of a semi-infinite crack in a nanograined solid. Our findings show that the nanograin rotation can significantly enhance the capability of the crack to emit dislocations, thus leading to strong crack blunting in nanomaterials.

Nanocrystalline (NC) materials are usually strong but lack ductility due to the extremely confined space that suppresses dislocation activities [1,2]. As grain size decreases, grain boundary (GB)-mediated deformation modes begin to dominate, such as GB sliding [3–6], GB migration [7–12], grain rotation [13–15] and stress-driven nano-grain growth [16–21]. Recently, stress-driven grain growth has stimulated an increasing scientific interest because of its intimate correlation with the enhanced ductility, lower friction and resistance to crack growth as observed in several NC metals [7,9,10,16,17,22–35]. A typical example is a gradient nanograined copper during uniaxial tensile deformation, in which most of the nanograins in the gradient region are coarsened from tens of nanometers to submicrometers [17]. Their results show that there are only hollows but no cracks in the nanograined surface layer, whereas micrometer-long cracks initiate at grain boundaries in the coarse-grained interior regions and the number of cracks is increased as tension enhances. This leads to an exceptional strength-ductility combination in the gradient structure. It also indicates that grain coarsening behavior plays an important role in suppressing the crack nucleation and growth in the nano-gradient zone. Another example is an aluminum thin film that shows a discontinuous nanograin growth phenomenon [16]. The reported grain growth renders the thin film with a much higher tensile ductility than that without such a growth behavior.

In the meantime many experiments and molecular dynamics simulations have also shown that nanograin rotation (NGR) serves as an important deformation mode of grain growth in NC materials [15,36–41]. Recently, we developed a theoretical model to describe the NGR process that can be achieved through the climb of grain boundary dislocations [14]. This mechanism has also been identified in experiments and molecular dynamics simulations [37,39,42]. However, due to the difficulty in quantifying the NGR and dislocation behavior near a crack tip in experiments, the quantitative relation between the NGR process and the enhanced ductility and crack growth resistant capability as suggested by experiments [16,17,22] still remains an unsolved issue. Therefore, in this letter we developed a theoretical model to investigate the effect of NGR on the crack blunting behavior of NC materials based on the work of Ovid'ko and Sheinerman [43,44]. The effective fracture toughness is also obtained. Our findings show that NGR can induce a strong crack blunting effect and thus significantly toughen the NC materials.

As revealed in our previous work [14], for a low-angle GB that is equivalent to an edge-type dislocations wall, NGR can be achieved by climbing of GB dislocations, dissociating in the triple junctions to become partial dislocations, gliding along the adjacent GBs and finally annihilating with the other partial dislocations generated by neighboring GBs through similar rotation process. Let us consider a two-dimensional nano-grained elastically isotropic solid, in which a long flat mode I crack is formed during deformation (Fig. 1a). The crack tip locates at the center of the GB ‘AB’ (Fig. 1b). Assuming that n GB dislocations are involved, the NGR process leads to a disclination dipole ‘AB’ with a strength of $\pm\omega = nb/d$ (Fig. 1b), where b is the magnitude of

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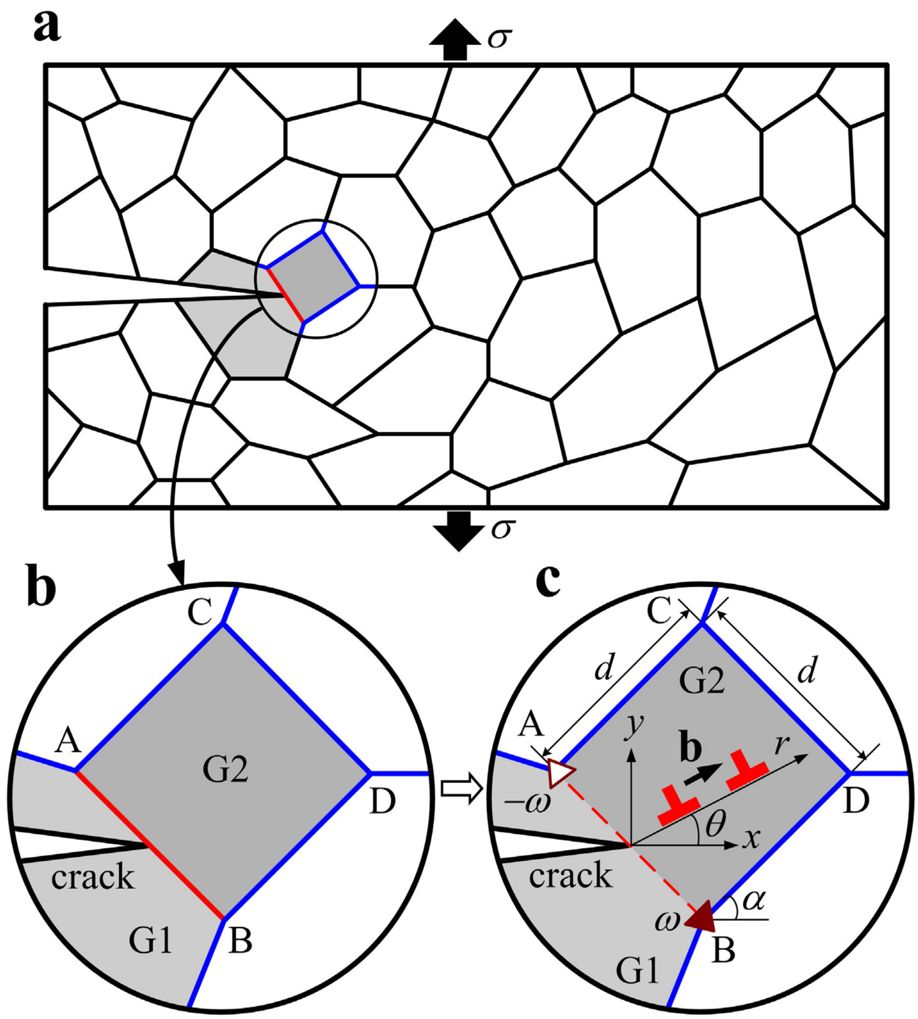

Fig. 1. Schematic of dislocation emission from a mode I crack tip during nano-grain rotation in a nanocrystalline solid. (a) A general view of the nanograined microstructure; (b) a cracked two-grain configuration; and (c) dislocations emitted from the crack tip.

the Burgers vector of the GB dislocation, and d is the length of the GB 'AB' that can be approximated as the grain size (Fig. 1c). As for a high-angle GB that consists of structural units [45], the detailed mechanism of rotation is unclear. However, the rotation of high-angle GB also results in disclinations as observed in experiments [39]. As a result, the rotation of both low and high angle boundaries generates dipoles of disclinations. Here it is convenient to define a parameter that characterizes the level of rotation, i.e., R, for both low and high angle GBs. In this way, the strength of the disclination dipole becomes $\pm\omega = R\theta_0$, $R \in [0,\ 1]$, in which $R = 0$ represents that no rotation occurs, whereas $R = 1$ means the two grains rotate to be merged. Here θ_0 is the initial misorientation of the GB 'AB'. Specifically, for low angle boundaries, $R = n/n_0$. We introduced the effect of NGR process on the dislocation emission from the crack tip by extending the criterion of Ovid'ko and Sheinerman [43,44]. The emission of the first dislocation can occur if the effective stress exerting on it is larger than zero, i.e.,

$$\sigma_{r\theta}^{K_I}\left(r_1^d,\theta\right)+\sigma_{r\theta}^{im}\left(r_1^d,\theta\right)+\sigma_{r\theta}^{\omega}\left(r_1^d,\theta\right)\Big|_{r_1^d=r_c}>0 \qquad (1)$$

where the stresses $\sigma_{r\theta}^{K_I}(r_1^d,\theta)$, $\sigma_{r\theta}^{im}(r_1^d,\theta)$ and $\sigma_{r\theta}^{\omega}(r_1^d,\theta)$ are generated by the applied tensile load σ, the crack free surface (image stress), and the disclination dipole AB resulting from the NGR process, respectively. r_c is the radius of the dislocation core. The superscript 'd' denotes dislocation. The first dislocation after emission moves along its slip plane with an angle of θ, and is finally stopped by the GB 'CD' (Fig. 1c), which requires that $|\theta-\alpha| \le a\tan(0.5) \approx 26.6^{\circ}$, in which α denotes the geometrical arrangement of the grain G2, called as orientation parameter. The α range should be $[-\pi/2, \pi/2]$ for the crack to avoid locating in grain G2. Following the first dislocation, we assume that there are $N+1$ dislocations that can be emitted from the crack tip. The emission of the $(N+1)^{\text{th}}$ ($N = 1, 2, \ldots$) dislocation requires

$$\sigma_{r\theta}^{K_I}\left(r_{N+1}^d,\theta\right)+\sigma_{r\theta}^{im}\left(r_{N+1}^d,\theta\right)+\sigma_{r\theta}^{\omega}\left(r_{N+1}^d,\theta\right)+\sum_{j=1}^{N}\sigma_{r\theta}^{d}\left(r_{N+1}^d,r_j^d,\theta\right)>0 \qquad (2)$$

here $\sigma_{r\theta}^{d}(r_{N+1}^d,r_j^d,\theta)$ is the stress exerted by the j^{th} dislocation at position of (r_j^d,θ) (that is already emitted and stay along the slip direction) on the newly-emitted one at position of (r_{N+1}^d,θ). Using Eqs. (1) and (2) we can obtain the maximum number of the emitted dislocations, i.e., $N_{\max}$, and their equilibrium positions.

The shear stresses $\sigma_{r\theta}^{K_I}(r,\theta)$ and $\sigma_{r\theta}^{im}(r,\theta)$ are given by [46].

$$\sigma_{r\theta}^{K_I}(r,\theta)=\frac{K_{IC}^{\sigma}\ \sin\theta\ \cos(\theta/2)}{2\sqrt{2\pi r}} \qquad (3)$$

$$\sigma_{r\theta}^{im}(r,\theta)=-\frac{Gb_1}{4\pi(1-v)r} \qquad (4)$$