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# A coupling crack blunting mechanism in nanocrystalline materials by nano-grain rotation and shear-coupled migration of grain boundaries

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ABSTRACT

A theoretical model has been developed to investigate the effect of a special cooperative process between two main modes of stress-driven nano-grain growth, i.e., nano-grain rotation and shear-coupled migration of grain boundaries, on the emission of lattice dislocations from a semi-infinite crack in nanocrystalline materials. The results obtained show that the above-mentioned collaborative process is highly conducive to the process of dislocation emission, thus, rendering strong crack blunting in nanocrystalline materials.

## 1. Introduction

Nanocrystalline (NC) materials are usually strong but brittle. However, recent experiments showed that the stress-driven nano-grain growth (NGG) process was a promising deformation mode that could help scientists to circumvent the strength-ductility trade off in NC materials [1–3]. Two general NGG modes have been identified by various researchers, i.e., nano-grain rotation (NGR) and shear-coupled migration (SCM) of grain boundaries [4–11]. Moreover, as demonstrated by many experiments and molecular dynamics as well as mesoscale simulations [4,12,13], NGG and SCM usually appear concomitantly. Most recently, Li et al. [14] predicted a novel coupling behavior of NGR and SCM in their theoretical model, i.e., under an externally applied load, NGR occurred first, which led to a decrease of the initial misorientation parameter $\theta_0$ of a given GB and subsequently SCM appeared, which was called a cooperative NGR–SCM process.

Investigations of the present authors have shown that the SCM mode can considerably enhance the intrinsic ductility [6], toughness [15], crack blunting [16] and dislocation emission [17] in NC materials. The coupled NGR–SCM process proposed by Li et al. [11] has also been identified as an effective toughening mechanism in NC materials [14]. Therefore, it is conceivable that the proposed NGR–SCM coupling behavior could also enhance the dislocation emission from a crack tip, thus, leading to crack blunting and abundant activation of dislocations in grain interior, which eventually renders enhanced strain hardening and ductility, as observed in many NC materials [1–3]. In this letter, the original model of Ovid'ko and Sheinerman [18,19] will be extended to investigate the effect of the above-mentioned coupling behavior on crack blunting in NC materials.

## 2. Model description

Consider a deformed elastic isotropic NC specimen with an embedded long flat mode I crack, which is subjected to an applied tensile stress $\sigma$, as shown in Fig. 1a. For simplicity, a cracked two-dimensional grain with a crack tip located at the center of the GB '*AB*' (Fig. 1b) is analyzed. The GB '*AB*' is modeled as a finite wall of dislocations with identical Burgers vector **b** (see Fig. 1c in Ref. [14]), which is characterized by a tilted misorientation parameter $\theta_0$ and the number of GB dislocations $n_0$. The stresses induced by the crack are assumed to be sufficiently high to initiate a cooperative NGR–SCM process as proposed in [14], where a NGR process between grains G1 and G2 occurs first by the climb and dissociation of $n$ GB dislocations, followed by a SCM process, in which the GB '*AB*' is migrated with a normal distance $m$ and a tangential translation $s$ due to the shear deformation, as shown in

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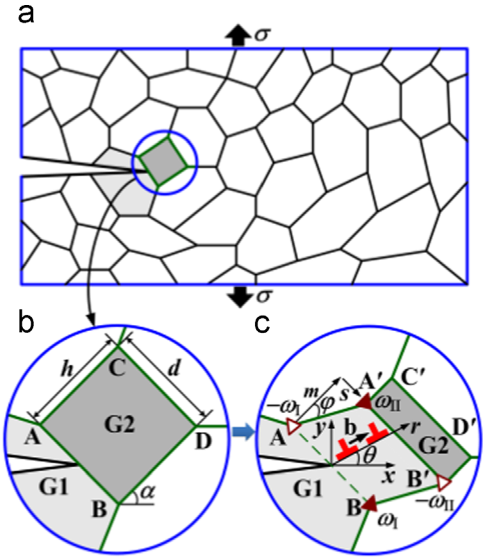

**Fig. 1.** Lattice dislocation emission from a crack tip induced by the cooperative process of nano-grain rotation and shear-coupled migration of grain boundaries in a deformed nanocrystalline solid: (a) general view; (b) initial configuration of grain boundaries; and (c) configuration resulting from dislocation emission (with Burger's vector **b**) after the coupling behavior, where two disclination dipoles (*AB* and *A′B′*) with strengths of $\pm\omega_I$ and $\pm\omega_{II}$, respectively, are formed and the size of grain G1 is increased with diminishing grain G2.

Fig. 1c. A coupling factor $\beta$ is introduced to define the ratio of $s$ to $m$, i.e., $\beta = s/m$ [5]. The magnitude of $n$ represents the level of rotation or coupling between NGR and SCM, i.e., the larger the value of $n$, the higher the level of rotation or coupling is. As a result, two disclination dipoles are formed during the above-mentioned coupling process, i.e., a dipole *AB* with strength $\pm\omega_{\mathrm{I}} = \pm\theta_0$ and another $A'B'$ with $\pm\omega_{\mathrm{II}} = \pm(\theta_0 - nb/d)$, as shown in Fig. 1c. The size of grain G1 is increased with diminishing grain G2 simultaneously. For simplicity, the length $d$ of '*AB*' is taken as the approximate grain size of the NC specimen.

In order to consider the effect of the cooperative NGR–SCM process on crack blunting in a NC specimen, we assume that after the occurrence of the coupling behavior, several edge dislocations with Burger's vector **b** are emitted from the semi-infinite crack tip along the slip plane, which is inclined at an angle $\theta$ with respect to the $x$-axis, as shown in Fig. 1c. According to Ovid'ko and Sheinerman [18,19], the emission criterion for the first dislocation is that the effective stress $\sigma^e_{r\theta}(r_1,\theta)$ at $r_1 = r_c$, where $r_c$ is the radius of the dislocation core, should be larger than zero, i.e.,

$$\sigma^{K_I}_{r\theta}(r_1,\theta) + \sigma^{im}_{r\theta}(r_1,\theta) + \sigma^{\omega}_{r\theta}(r_1,\theta)\Big|_{r_1 = r_c} > 0 \tag{1}$$

where the stress $\sigma^{K_I}_{r\theta}(r_1,\theta)$ is produced by the applied tensile load near the crack tip, $\sigma^{im}_{r\theta}(r_1,\theta)$ depicts the image stress induced by the crack free surface, and $\sigma^{\omega}_{r\theta}(r_1,\theta)$ is the stress induced by the two disclination dipoles resulting from the coupling process.

The first dislocation after emission is assumed to move along the slip plane and finally stops at the new grain boundary $A'B'$, as shown in Fig. 1c. Similarly, the requirement for emission of the $(N+1)$th ($N$=1, 2, …) dislocation is:

$$\sigma^{K_I}_{r\theta}(r_{N+1},\theta) + \sigma^{im}_{r\theta}(r_{N+1},\theta) + \sigma^{\omega}_{r\theta}(r_{N+1},\theta) + \sum_{j=1}^{N} \sigma^{d}_{r\theta}(r_{N+1}, r_j, \theta)\Bigg|_{r_{N+1} = r_c} > 0 \tag{2}$$

where $\sigma^d_{r\theta}(r_{N+1}, r_j, \theta)$ is the stress exerted by the $j$th dislocation on the newly-emitted one. For simplicity, the emitted $(N+1)$ dislocations are assumed to distribute uniformly along the slip direction.

The expressions for the stresses $\sigma^{K_I}_{r\theta}(r,\theta)$ and $\sigma^{im}_{r\theta}(r,\theta)$ that appear in Eqs. (1) and (2) have been presented by Lin and Thomson [20], which are

$$\sigma^{K_I}_{r\theta}(r,\theta) = \frac{K^{\sigma}_{IC}\ \sin\theta\ \cos(\theta/2)}{2\sqrt{2\pi r}} \tag{3}$$

$$\sigma^{im}_{r\theta}(r,\theta) = -\frac{Gb}{4\pi(1-\nu)r} \tag{4}$$

where $K^{\sigma}_{\mathrm{IC}} = \sqrt{4G\gamma/(1-\nu)}$ is the brittle fracture toughness; $\gamma$, $G$, $\nu$ and $b$ are the specific surface energy, the shear modulus, Poisson's ratio and the magnitude of the Burger's vector of the emitted dislocations, respectively.

The shear stress $\sigma_{r\theta}(r,\theta)$, i.e., $\sigma^{\omega}_{r\theta}(r_{N+1},\theta)$ and $\sigma^{d}_{r\theta}(r_{N+1}, r_j, \theta)$, exerts at the point $(r,\theta)$ by a disclination at point $(r_j,\theta_j)$ or a dislocation at point $(r_{dj},\theta)$ can be expressed in terms of the Cartesian stress components $\sigma_{xx}$, $\sigma_{yy}$ and $\sigma_{xy}$ as

$$\sigma_{r\theta} = (\sigma_{yy} - \sigma_{xx})\ \sin\theta\ \cos\theta + \sigma_{xy}\ \cos(2\theta) \tag{5}$$

Generally speaking, $\sigma_{yy} = \mathrm{Re}g$, $\sigma_{xy} = -\mathrm{Im}g$, $\sigma_{xx} = \mathrm{Re}(4\Phi - g)$, $g = \Phi + \overline{\Omega} + (z - \overline{z})\overline{\Phi}'$, where $\Phi$ and $\Omega$ are two complex functions. The complex functions for the disclination quadruple and the emitted dislocations are presented as a Supplementary material appended to this manuscript.

The following procedure is adopted to determine the maximum number of dislocations $N_{\max}$: (i) use Eq. (1) to verify the emission possibility of the first dislocation; (ii) if Eq. (1) is satisfied, then employ Eq. (2) to check the possibility of emission of the second dislocation; (iii) repeat step 2 for the subsequent impending dislocations. The following parametric values of NC Ni are adopted in the present calculation: $G = 73\ \ GPa$, $\nu = 0.34$, $\gamma = 1.725\,J/m^2$, $b$=0.25 nm, $r_c \approx 2b$, $\theta = -\pi/3$, $\alpha = -\pi/2$.

## 3. Results and discussion

Fig. 2 presents the variation of maximum number of dislocations $N_{\max}$ that are emitted from the crack tip with respect to the normalized number of dissociated GB dislocations $n/n_0$ for various nanocrystalline Ni samples, where the effects of the coupling factor $\beta$, initial misorientation parameter $\theta_0$ and grain size $d$ are illustrated in Fig. 2a–c, respectively. Note that the value of $n/n_0$ represents the level of rotation or coupling and $n/n_0 \in (0,1)$; $n/n_0 = 0$ and 1 correspond to pure SCM and NGR processes, respectively. It can be seen that for all the parameters considered the cooperative NGR–SCM process can considerably enhance the number of emitted dislocations from the crack tip, and the larger the rotation level (i.e., coupling level), the higher the value of $N_{\max}$ is. The maximum variation of $N_{\max}$ can reach as high as 7, i.e., from 0 to 7 at $d$=50 nm, $\beta = 1$ and $\theta_0 = 0.3$ as $n/n_0$ is increased from 0 to 1 (circles in Fig. 2c). In this case, the initially brittle NC materials gain strong crack blunting and thus become ductile. Specifically, Fig. 2a shows that the coupled shear (denoted by the coupling factor $\beta$, $\beta > 0$) in the process of SCM is conducive to crack blunting since it enlarges $N_{\max}$. Moreover, grains with higher angle GBs (i.e., larger $\theta_0$) is more favorable for crack blunting than those with lower angle GBs (Fig. 2b), and the variation of $N_{\max}$ with respect to $n/n_0$ is larger in bigger grains (e.g., $d$=50 nm) than that in smaller grains (e.g., $d$=15 nm), as shown in Fig. 2c, which indicates that the coupling NGR–SCM behavior plays a more significant role in coarser grains. The above findings reveal a new effective crack blunting mechanism in NC materials, that is, coupling of NGR and SCM. The results obtained are also helpful to explain the enhanced ductility and strain hardening phenomena observed in many NC metals, in which stress-driven nano-grain growth is thought as the dominating deformation mode [1–3].

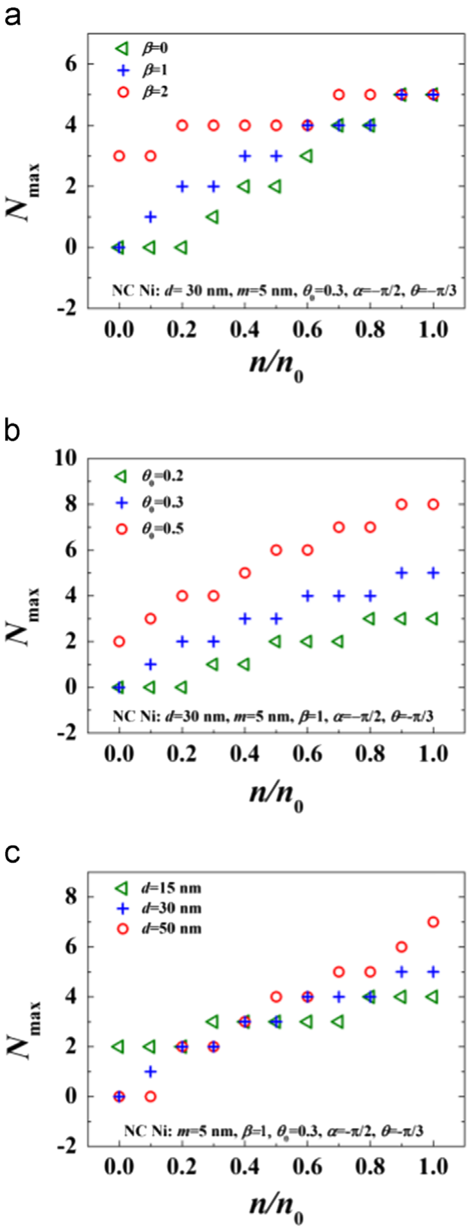

**Fig. 2.** Variation of maximum number of dislocations $N_{max}$ emitted from the crack tip with respect to the normalized number of dissociated grain boundary dislocations $n/n_0$ for various nanocrystalline Ni samples; the effects of coupling factor $\beta$ (a), initial misorientation parameter $\theta_0$ (b) and grain size $d$ (c) are considered.

## 4. Conclusions

In summary, a new crack blunting mechanism is proposed by combining two main modes of stress-driven nano-grain growth, i.e., nano-grain rotation and shear-coupled migration of grain boundaries. The mentioned coupling process could considerably enhance the maximum number of dislocations emitted from a semi-infinite crack tip that leads to strong crack blunting and, thus, could improve the ductility of NC materials.

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## Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.matlet.2014.08.136.

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