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Title Nano-twin and dislocation pileup’s effect on dislocation emission from an elliptical blunt crack tip in nanocrystalline solid

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Abstract

A theoretical model describing the effect of nano-twin and dislocation pileup at twin boundary on the lattice dislocation from an elliptical blunt crack tip in nanocrystalline materials is established. The nano-twin can be represented by a wedge disclination quadrupole and some dislocations accumulate on a twin boundary. The emission criterion of the first edge dislocation emitting from the blunt crack tip are considered, and the analytical solution of stress intensity factor is obtained by applying complex variable function method. Then the influence of the dislocation emission angle, the position and orientation of the twin,the strength of nano-twin,the length and curvature radius of elliptical blunt crack on the critical stress intensity factor for the emission of the first dislocation from blunt crack tip is analyze in detail. The results shows that the effect of nano-twin on dislocations emitting from crack tip depends on the position and azimuth of the nano-twin. There is an optimal position of nano-twin to make the dislocations easiest to emit from the blunt crack tip. The dislocation pileup at the twin boundary will increase the critical stress intensity factors for dislocation emission, making the dislocation emission from crack tip difficult, thus reducing the toughness of the material contributed by dislocation emission.

Keywords dislocation emission; stress intensity factor; blunt crack; nano-twin and dislocation pileup; complex potential method.

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Dear Editors:

On behalf of my co-authors, I am submitting the enclosed material " Nano-twin and dislocation pileup's effect on dislocation emission from an elliptical blunt crack tip in nanocrystalline solid" for possible publication in *Engineering Fracture Mechanics*.

We certify that we have participate sufficiently in work to take public responsibility for the appropriateness of the deduce, calculation, analysis the model.

To the best of our knowledge and belief, this manuscript has not been published in whole or in part nor is it being considered for publication elsewhere.

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Yours Sincerely.

MinYu
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Highlights

(1) The effect of nano-twin on dislocations emitting from crack tip depends on the position and azimuth of the twins. There is an optimal position of nano-twin to make the dislocations most susceptible to emit from crack tip.

(2) The greater the intensity of the twins, the more it can hinder or promote the emission of dislocations at the crack tip. There is a critical inclination of nano-twin oriental corresponding to the maximum critical stress intensity factor making the dislocation of the elliptical crack tip the hardest to launch.

(2) There is the most probable emission angle, and the most probable emission angle increases with the intensity of the nano-twin. The increase of crack length and grain size will make the dislocation emission of crack tip difficult and the dislocation emission will become difficult when the crack tip is passivated.

(3) The dislocation pileup at the twin boundary will increase the critical stress intensity factor for dislocation emission, making the dislocation emission from crack tip difficult, thus reducing the toughness of the material contributed by dislocation emission.

Nano-twin and dislocation pileup's effect on dislocation emission from an elliptical blunt crack tip in nanocrystalline solid

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Abstract. A theoretical model describing the effect of nano-twin and dislocation pileup at twin boundary on the lattice dislocation from an elliptical blunt crack tip in nanocrystalline materials is established. The nano-twin can be represented by a wedge disclination quadrupole and some dislocations accumulate on a twin boundary. The emission criterion of the first edge dislocation emitting from the blunt crack tip are considered, and the analytical solution of stress intensity factor is obtained by applying complex variable function method. Then the influence of the dislocation emission angle, the position and orientation of the twin,the strength of nano-twin,the length and curvature radius of elliptical blunt crack on the critical stress intensity factor for the emission of the first dislocation from blunt crack tip is analyze in detail. The results shows that the effect of nano-twin on dislocations emitting from crack tip depends on the position and azimuth of the nano-twin. There is an optimal position of nano-twin to make the dislocations easiest to emit from the blunt crack tip. The dislocation pileup at the twin boundary will increase the critical stress intensity factors for dislocation emission, making the dislocation emission from crack tip difficult, thus reducing the toughness of the material contributed by dislocation emission.

***Keywords*:** dislocation emission; stress intensity factor; blunt crack; nano-twin and dislocation pileup; nanocrytalline solid; complex potential method.

1 Introduction

Because of the unique physical and mechanical properties, nanocrystalline materials have attracted widespread attention from many scholars, especially its super toughness, hardness and wear resistance. However, in most cases, the shortcomings such as low elongation and poor fracture toughness of nanocrystalline materials have limited its practical application[1-10].However, researchers have found that some face-centered cubic crystalline materials, such as nano-Copper, has both good plasticity and toughness that attracted many scholars to study the mechanism. In recent years, many models have been proposed to explain the unique toughening mechanism, such as grain boundary slip, local migration of grain boundaries, special rotation deformation, deformed nano-twins[11-18].

Most of the research focuses on the contribution of these special deformation mechanisms to the toughening of nanocrystalline materials, and the materials studied are considered as complete crystalline materials. However, in actual materials, defects such as cracks, inclusions, and two-phase particles are unavoidable during the manufacturing or service process. The presence of small defects reduces the strength of the material, leading to low stress failure. The strength and toughness of cracked materials depend on the material's resistance to cracks[15-22]. This resistance is determined by the material's internal properties. In addition, the micro-structure in a small area of the crack tip, such as grain size, two-phase particles, etc., also has a great impact on crack growth. Therefore, studying the interference rules of dislocations with cracks and inclusions of various shapes is helpful to understand the evolution of the microstructure at the crack tip due to the equilibrium stability and movement of dislocations near the crack tip, and its impact on the material. The influence of fracture toughness can also provide scientific basis for the micro-structure design and damage and fracture of nanocrytalline materials[23-32].The ultra-fine grains in the nano-twin materials are divided into nanometer-thick structures by the nano-twin grain boundaries, so there are many twin-grain boundary structures. Its unique mechanical energy originates from the dislocation-twin interactions, and is essentially different from the dislocation-grain boundaries and lattice dislocations in polycrystalline materials.

Ovid'ko and Skiba[33] found the generation of nanoscale deformation twins at locally distorted grain boundaries in nanomaterials. Romanov and Vladimirov[34] proposed that the effect of twinning on cracks can be

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equivalently simulated by a wedge disclination quadrupole. For nanotwined materials, submicron-sized grains are subdivided into nanometer-thick lamellar structure by the twin boundaries, then many twin boundaries -grain boundaries are generated. When dislocations slide parallel to the twin grain boundaries, these dislocations will be blocked by the grain boundaries. As the deformation progressed further, dislocations begin to accumulate on the twin boundaries.These special deformation mechanisms in nanocrystalline materials can not only release the stress concentration at the crack tip height, so as to prevent nano-crack nucleation, but also slow the expansion of existing cracks[28-32].

The interaction between dislocations and other micro-defects will seriously affect the macro-mechanical properties of materials. The emission of dislocations from the crack tip is the key to brittle-tough transformation of the material. For nanocrystalline materials with cracks, under the applied load, as long as the stress intensity factor at the crack tip is sufficiently large, the crack tip will emit dislocations. We have done some research on the interference of nano-twin and dislocations emitting from various crack configurations and in nanocrystalline materials, such as linear crack, surface semi-elliptical crack, and linear interface crack[29-32]. Based on previous research, this article is dedicated to research the effect of nano-twin and dislocation pileup on edge dislocation emitted from an elliptical blunt crack tip.

2 Model building

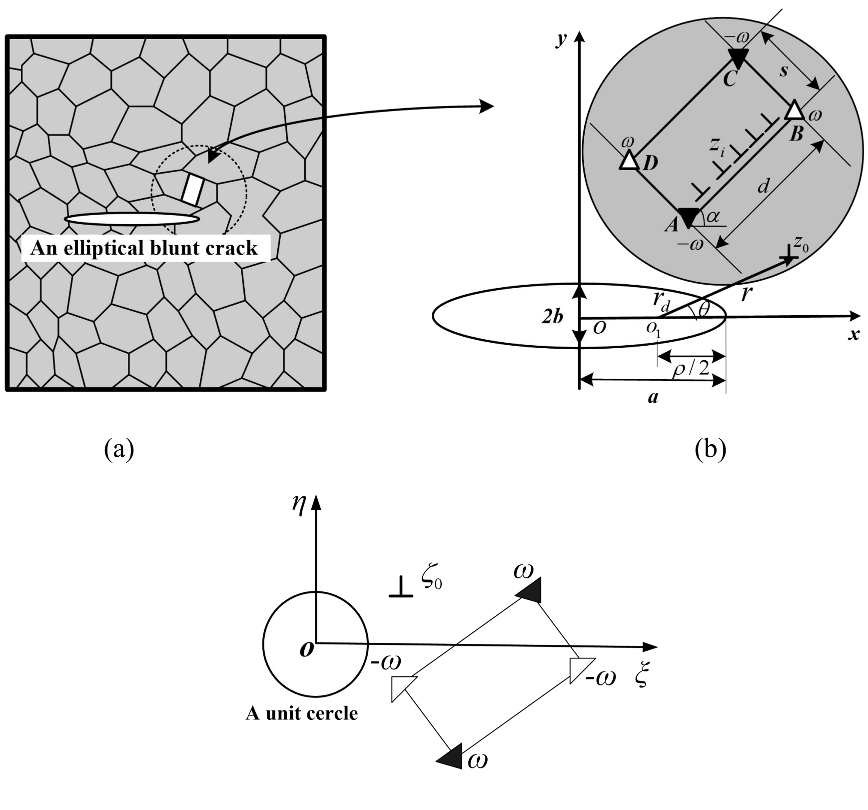


Fig.1 The nano-twin and dislocation pileup near an elliptical blunt crack in a two-dimensional nanocrystalline solid. (a) General view; (b) The magnified inset highlighting the nano-twin represented by two wedge disclination dipoles and a lattice dislocation emission near the elliptical blunt crack tip; (c) ζ -plane after conformal mapping.

As shown in Fig.1(a), a deformed two-dimensional nanocrystallined solid containing an elliptical blunt crack is considered. The deformed nanocrystalline solid under mode I and mode II loadings contains a large number of nanoscale grains divided by grain boundaries. A nano-twin represented by a wedge disclination quadrupole occurs near the elliptical blunt crack and some grain boundary dislocations accumulate in a twin boundary to form dislocation pileup. The computational model that the interaction of elliptical crack and nanoscale twin is detailed diagramed in Fig.1(b). For simplicity, all the defect structures in the solid are assumed to be the same along the z -axis that perpendicular to the xy plane, so just a two-dimensional problem is considered in xy plane. Also, the solid is set to isotropic and elastic, supposing the shear modulus is μ and Poisson’s ratio is ν .

Introducing a Cartesian system (x, y) with the origin point at o, the center of the elliptical crack with a long axis and a short axis a and b, respectively, is at the origin of the Cartesian coordinate. Then, a polar coordinate system (r, θ) with origin at o_1 that $\rho/2$ behind the right end of the elliptical crack is introduced, and the parameter $\rho = b^2/a$ denotes the curvature radius of the elliptically blunt crack tip.

The nano-twin is simulated by a wedge disclination quadrupole $ABCD$ with strength ω, containing two negative disclinations located in A, C and two positive disclinations located in B, D. The wedge disclination quadrupole forms a rectangle, and the length and width of the rectangle are respectively set as d and s, who are also called quadrupole arms, representing the twin size. The angle between the quadrupole arm AB (or CD) and the positive half of the x-axis is set as α. And there are n dislocations accumulated along the twin boundary AB to form the dislocation pileup. Then, the coordinates of the four wedge disclinations A, B, C and D can be expressed as $z_1 = (a-\rho/2) + r_1 e^{i\theta_1}$, $z_2 = z_1 + de^{i\alpha}$, $z_3 = z_2 + se^{i(\alpha+\pi/2)}$ and $z_4 = z_1 + se^{i(\alpha+\pi/2)}$, respectively. And the coordinate of the dislocation $z_i\ (i = 1, ..., n)$ accumulated along at the twin boundary AB is $z_i = z_1 + r_i e^{i\alpha}$ (where r_i is the distance between dislocation z_i and the point A)[30-32].

3 The stress field of nano-twin

According to the hypothesis, the problem can be reduced to a plane strain problem. According to the basic formula of the complex potential method of Elasticity, the stress filed σ_{xx}, σ_{yy} and σ_{xy} can be deduced by two Muskhelishvili's complex potentials $\varphi(z)$ and $\psi(z)$ as[29-30]:

$$\sigma_{xx} = \mathrm{Re}[2\varphi'(z) - \bar{z}\varphi''(z) - \psi'(z)] \tag{1}$$

$$\sigma_{yy} = \mathrm{Re}[2\varphi'(z) + \bar{z}\varphi''(z) + \psi'(z)] \tag{2}$$

$$\sigma_{xy} = \mathrm{Im}[\bar{z}\varphi''(z) + \psi'(z)] \tag{3}$$

where $z = x + iy$ is the complex variable in the complex plane, and the prime represents differentiation of the variable z while the over-bar denotes a complex conjugate.

Assume that the elliptical crack is a free surface, so the boundary condition of the crack can be written as:

$$\sigma_{yy}(t) = 0, \ \sigma_{xy}(t) = 0 \qquad t \in \textit{elliptical crack surface} \tag{4}$$

In order to obtain the analytical solution of the problem, a mapping function is introduced as[29]

$$z = \omega(\zeta) = R(\zeta + m/\zeta) \tag{5}$$

where $\zeta = \eta + i\xi$, $R = (a+b)/2$, $m = (a+b)/(a+b)$. The surface of elliptical crack in the z-plane is mapped into a unit circle in the ζ-plane, and the infinite region outside the Elliptic crack maps to the outer region of the unit circle, as shown in Fig. 1(c).

Substituting the mapping Eq.(5) to Eq.(1)-(3), then the complex potential functions can be rewritten in the ζ-plane as

$$\varphi'(z) = \psi'(\zeta)/\omega'(\zeta) \tag{6}$$

$$\varphi''(z) = \frac{\varphi''(\zeta)\omega'(\zeta) - \varphi'(\zeta)\omega''(\zeta)}{[\omega'(\zeta)]^2} \tag{7}$$

$$\Psi(\zeta) = \psi'(\zeta)/\omega'(\zeta) \tag{8}$$

Referring the work of Fang[31-32], the elastic fields $(\sigma_{xx}^{\omega}, \sigma_{yy}^{\omega}, \sigma_{xy}^{\omega})$ produced by the nano-twin represented by a wedge disclination quadrupole can be deduced by the complex potentials $\varphi_\omega(\zeta)$, $\psi_\omega(\zeta)$:

$$\varphi_\omega(\zeta) = \frac{G}{2}\sum_{k=1}^{4}(-1)^k\left[\omega'(\zeta_k)(\zeta-\zeta_k)\ln(\zeta-\zeta_k) - \bar{a}_k \ln\left(\zeta - \frac{1}{\bar{\zeta}_k}\right) + \bar{a}_k \ln\zeta\right] \tag{9}$$

$$\begin{aligned}\psi_\omega(\zeta) = \frac{G}{2}\sum_{k=1}^{4}(-1)^k&\left[-\omega(\bar{\zeta}_k)\ln(\zeta-\zeta_k) - \bar{a}_k\frac{1+m\zeta^2}{\zeta^2-m} + \bar{a}_k\frac{\bar{\zeta}_k^2+m}{\bar{\zeta}_k\left(1-m\bar{\zeta}_k^2\right)\left(\zeta-\dfrac{1}{\bar{\zeta}_k}\right)}\right] \\ &+\sum_{k=1}^{4}(-1)^{k+1}\omega'(\bar{\zeta}_k)\frac{\bar{\zeta}_k}{\zeta}\left(\zeta-\frac{1}{\bar{\zeta}_k}\right)\ln\left[-\omega'(\bar{\zeta}_k)\frac{\bar{\zeta}_k}{\zeta}\left(\zeta-\frac{1}{\bar{\zeta}_k}\right)\right]\end{aligned} \tag{10}$$

where $G = \mu\omega/2\pi(1-\nu)$, $a_k = R\left(1+\zeta_k^2\right)/\zeta_0 - \omega\left(\bar{\zeta}_k\right)$.

4 The emission force acting on the first dislocation

Dislocation activity is the cause of plastic deformation at the crack tip, which determines the crack propagation behavior. Under the action of the applied load, as long as the stress intensity factor at the blunt crack tip is large enough, the crack tip will emit dislocations[35-36]. Only the edge dislocations are considered here. Supposing that the first edge dislocation emitted by the right end of the elliptical blunt crack is at $z_0=\left(a-\rho/2\right)+r_0\mathrm{e}^{\mathrm{i}\theta_0}$ with the Burgers vector $b_\mathrm{d}=b_y-ib_x$, the total emission force f_emit acting on the first dislocation consists of four parts: the image force f_I, the force f_T produced by the nano-twin , the force f_P produced by the dislocation pile up, and the force f_L caused by the applied load.

Firstly, according to the work of Huang and Li[37], the image force acting on an edge dislocation emitted from an elliptical blunt crack can be obtained as:

$$f_\mathrm{I}=-\frac{\mu b_d^2}{4\pi(1-\nu)(r_0-r_d)} \tag{11}$$

where r_d represents the distance between the origin o_1 and the surface of the elliptical blunt crack and can be calculated as $r_\mathrm{d}=\left[\frac{\sqrt{a^2-0.25a\rho\sin^2\theta_0}-\left(a-\rho/2\right)\cos\theta_0}{\rho\cos^2\theta_0+a\sin^2\theta_0}\right]\rho$. And the item r_0-r_d represents the distance between the dislocation and the blunt crack surface.

Secondly, the force produced by the nano-twin can be calculated by considering the Eqs. (9)-(10) as:

$$\begin{aligned} f_\mathrm{T}=f_{\mathrm{T}x}-\mathrm{i}f_{\mathrm{T}y}&=\left[\sigma_{xy}^{\omega}(\zeta_0)b_x+\sigma_{yy}^{\omega}(\zeta_0)b_y\right]+\mathrm{i}\left[\sigma_{xx}^{\omega}(\zeta_0)b_x+\sigma_{xy}^{\omega}(\zeta_0)b_y\right]\\ &=\frac{\mu b^2}{4\pi(1-\nu)}\left[\frac{\Phi_\omega(\zeta_0)+\overline{\Phi_\omega(\zeta_0)}}{w}+\frac{\overline{\omega(\zeta_0)}\Phi_\omega'(\zeta_0)+\Psi_\omega(\zeta_0)}{\overline{w}}\right]\end{aligned} \tag{12}$$

where σ_{xx}^{ω}, σ_{yy}^{ω} and σ_{xy}^{ω} are the components of the stress field produced by the wedge disclination quadrupole, and, $\Phi_\omega(\zeta_0)=\frac{\varphi_\omega'(\zeta_0)}{\omega'(\zeta_0)}$, $\Psi_\omega(\zeta_0)=\frac{\psi_\omega'(\zeta_0)}{\omega'(\zeta_0)}$, $\Phi_\omega'(\zeta_0)=\frac{\varphi_\omega''(\zeta_0)\omega'(\zeta_0)-\varphi_\omega'(\zeta_0)\omega''(\zeta_0)}{\left[\omega'(\zeta_0)\right]^3}$, $w=\frac{\mu}{4\pi(1-\nu)}\left(b_y-\mathrm{i}b_x\right)$.

Thirdly, the force produced by the dislocation pileup of twin boundary *AB* is considered. We assume that all the stacking dislocations on the twin boundary are edge dislocations, and the number of stacking dislocations on the twin boundaries is n, then the force f_P can be calculated as:

$$f_\mathrm{P}=-\sum_{i=1}^{n}\frac{\mu b_\mathrm{d}^2}{4\pi(1-\nu)(r_{ii}-r_\mathrm{d})} \tag{13}$$

where r_{ii} is the distance between the *i*-th dislocation and the point o_1, and $r_{ii}=\sqrt{r_1^2+r_i^2-2r_1r_r\cos\left(\pi-\alpha+\theta_1\right)}$.

Finally, according to the work of Creager and Paris[38], the force f_L caused by the applied load can be calculated as

$$\begin{aligned} f_\mathrm{L}=b\sigma_{r\theta}^\mathrm{L}&=b\left[\left(\sigma_y-\sigma_x\right)\sin\theta\cos\theta+\sigma_{xy}\left(\cos^2\theta-\sin^2\theta\right)\right]\\ &=\frac{b}{\sqrt{2\pi r}}\left(l_1K_\mathrm{I}^\mathrm{app}+l_2K_\mathrm{II}^\mathrm{app}\right)\end{aligned} \tag{14}$$

where $\sigma_{r\theta}^{T}$ is the stress filed of blunt crack tip produced by remote in-plane load; $K_\mathrm{I}^\mathrm{app}$ and $K_\mathrm{II}^\mathrm{app}$ are the generalized mode I and mode II stress intensity factors (SIFs) produced by remote loadings; and $l_1=\frac{1}{2}\sin\frac{\theta}{2}\left(1+\cos\theta+\frac{\rho}{r}\right)$, $l_2=\cos\frac{3\theta}{2}+\frac{1}{2}\sin\theta\sin\frac{\theta}{2}-\frac{\rho}{2r}\cos\frac{\theta}{2}$.

Therefore, the total emission force f_emit acting on the first dislocation can be written as:

$$f_\mathrm{emit}=\mathrm{Re}\left[f_\mathrm{T}\right]\cos\theta-\mathrm{Im}\left[f_\mathrm{T}\right]\sin\theta+f_\mathrm{I}+f_\mathrm{P}+f_\mathrm{L} \tag{15}$$

The formula of emission force can be obtained by substituting Eqs.(11) –(14) into it.

5 The critical stress intensity factor for dislocation emission

Rice and Tomson[36] have mentioned a commonly accepted criterion for dislocation emission from crack tip. The criterion shows that a dislocation will emit from crack tip if the force acting on it is zero and the distance between the dislocation and the crack surface is not less than the radius of dislocation core. Making $f_\mathrm{emit}=0$ and combing the Eqs.(11)-(14), the critical applied stress intensity factors for the first dislocation emitting from the blunt crack tip can be derived as:

$$K_{\mathrm{IC}}^{\mathrm{app}} = \frac{\sqrt{2\pi r_0}}{b_{\mathrm{d}} l_1}\left(\mathrm{Im}[f_{\mathrm{T}}]\sin\theta - \mathrm{Re}[f_{\mathrm{T}}]\cos\theta - f_{\mathrm{I}} - f_{\mathrm{P}}\right), \quad \text{let } K_{\mathrm{II}}^{\mathrm{app}} = 0 \tag{16}$$

$$K_{\mathrm{IIC}}^{app} = \frac{\sqrt{2\pi r_0}}{b_d l_2}\left(\mathrm{Im}[f_{\mathrm{T}}]\sin\theta - \mathrm{Re}[f_{\mathrm{T}}]\cos\theta - f_{\mathrm{I}} - f_{\mathrm{P}}\right), \quad \text{let } K_{\mathrm{I}}^{\mathrm{app}} = 0 \tag{17}$$

where $r_0 = r_{\mathrm{d}} + b_r$

Using the expression for the critical stress intensity factors $K_{\mathrm{I}}^{\mathrm{app}}$ and $K_{\mathrm{II}}^{\mathrm{app}}$ for dislocation emitting from the tip of an elliptical blunt crack, the effect of nano-twin and dislocation pileup along twin boundary on dislocation emission can be analyzed. For ease of calculation and analysis, the stress intensity factors are normalized as $K_{\mathrm{IC}}^{0} = K_{\mathrm{I}}^{\mathrm{app}} / \mu\sqrt{b_r}$ and $K_{\mathrm{IIC}}^{0} = K_{\mathrm{II}}^{\mathrm{app}} / \mu\sqrt{b_r}$. The nanocrystalline material is assumed to be nano-Ni, so μ=73GPa and ν=0.34 . In addition, the Burgers vector of the first dislocation emitted form blunt crack tip is supposed to be b_{d}=0.25nm .The shape of the elliptical blunt crack can be described by the dimensionless radius of curvature ρ / a and the semi-major axis a .

The effect of disclination strength and the dislocation pileup on the critical normalized SIFs is depicted in Fig.2 when $a = 50\,\mathrm{nm}$, $\rho = 0.5\,\mathrm{nm}$, $\alpha = 0^{\circ}$, $l_0 = 0.25\mathrm{nm}$, $l_1 = 25\mathrm{nm}$, $d = 5\mathrm{nm}$, $s = 1\mathrm{nm}$, $\theta_0 = 15^{\circ}$, $\theta_1 = 0^{\circ}$. $K_{\mathrm{IC}}^{0\mathrm{T}}$, $K_{\mathrm{IIC}}^{0\mathrm{T}}$ indicate only considering the effect of nano-twin while no dislocation piles up at the twin boundary on SIFs for dislocation emission. It can be found that increasing disclination strength increases the critical SIFs and the mode I SIF is larger than the mode II SIF under the same circumstances. The value of the critical SIFs when dislocation pile up at the twin boundary is greater than the value of critical SIFs when no dislocation piles. The phenomenon shows that mode II loadings make the dislocation more likely to emit from the crack tip than the mode I loadings, and the dislocation pileup at the twin boundary will increase the critical SIFs for dislocation emission, making the dislocation emission from crack tip difficult, thus reducing the toughness of the material contributed by dislocation emission.

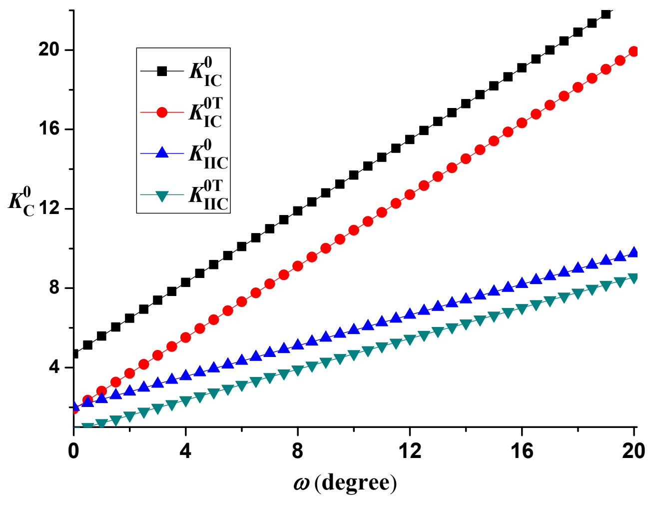


Fig.2 Dependences of the critical normalized SIFs on the disclination strength ω

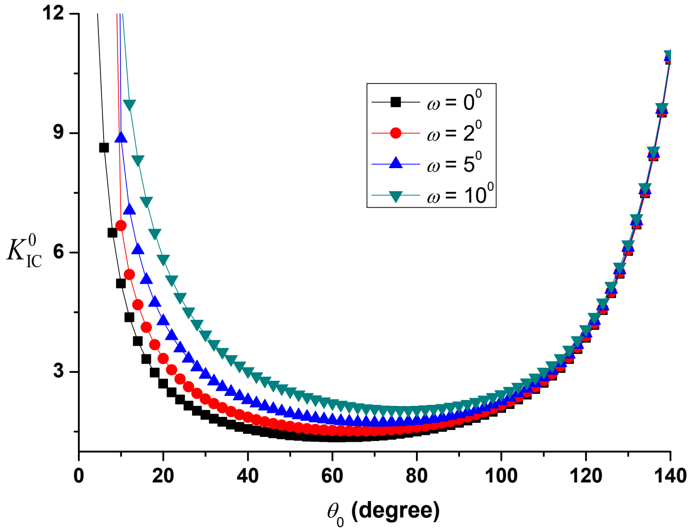
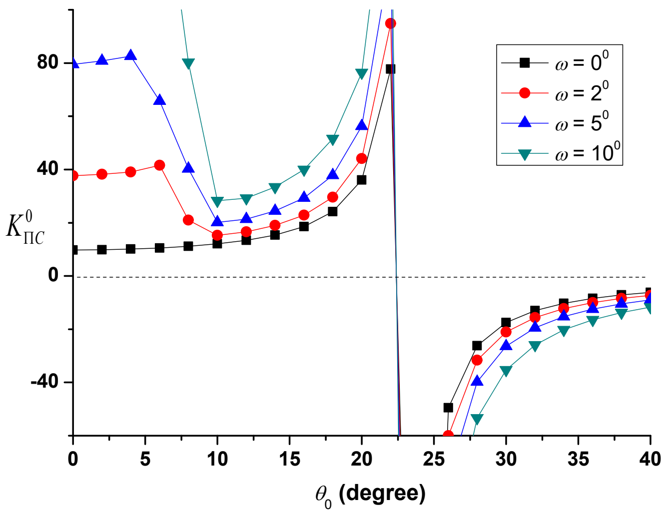
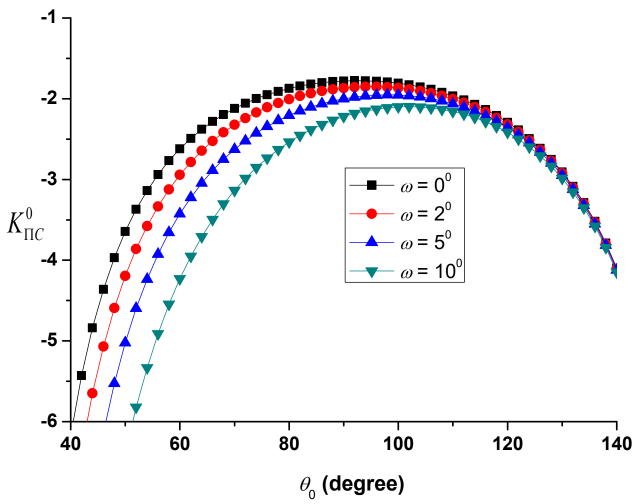


Fig.3 Dependences of the critical normalized K_{IC}^0 on emission angle with different ω



(a)



(b)

Fig.4 Dependences of the critical normalized K_{IIC}^0 on emission angle with different ω

Fig.3 and Fig.4 shows the variation of normalized SIFs on emission angle of the first dislocation when the strength of nano-twin is different for $a = 50\,\text{nm}$, $\rho = 0.5\,\text{nm}$, $\alpha = 0^\circ$, $l_0 = 0.25\text{nm}$, $l_1 = 25\text{nm}$, $d = 5\,\text{nm}$, $s = 1\,\text{nm}$, $\theta_1 = 0^\circ$. It can be seen from Fig.3 that the K_{IC}^0 decreases first and then increases with the increase of the emission angle. Therefore, there is a minimum value of K_{IC}^0 and the angle corresponding to this minimum value is the most probable emission angle of dislocation θ_{e}. When the dislocation emission angle is constant, K_{IC}^0 increases with the increase of the disclination strength, indicating that the greater the intensity of the twins, the more it can hinder the emission of dislocations at the crack tip, which is consistent with the results in Fig. 2. And when $\omega = 0^\circ,\ 2^\circ, 5^\circ,\ 10^\circ$, the most probable emission angle is θ_{e}=$61.2^\circ, 64.5^\circ, 70.6^\circ, 76.8^\circ$, respectively. It is obvious that the most probable emission angle also increases with the intensity of the disclination strength.

For K_{IIC}^0 in Fig.4, with the increase of the dislocation emission angle, the positive stress intensity factor increases slightly, then decreases, and then increases, changing from a positive value to a negative value at about 40º. The negative stress intensity factor decreases first and then increases with the increase of dislocation emission angle, and there is a minimum value. Similarly this minimum corresponds to the most probable emission angle θ_{e}. For positive mode II SIF, θ_{e}=0° when there are no nano-twins (ω=0°); and for negative mode II SIF, θ_{e}=$92.6^\circ, 95^\circ, 98^\circ, 101.6^\circ$ when $\omega = 0^\circ,\ 2^\circ, 5^\circ,\ 10^\circ$, respectively.

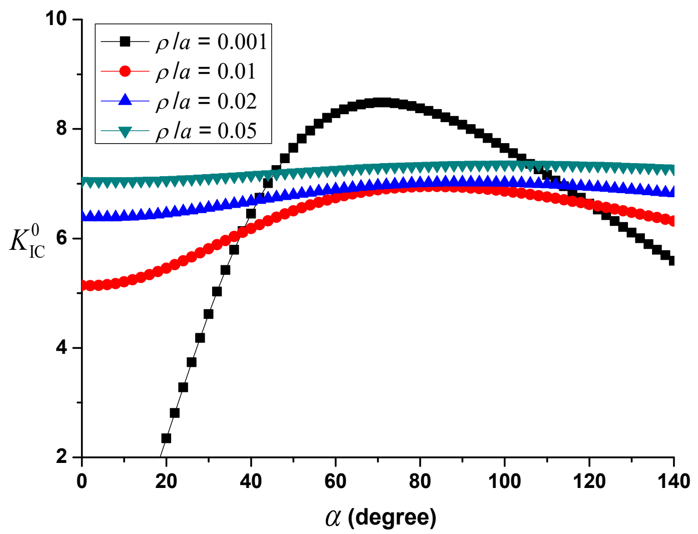


Fig.5 Dependences of the critical normalized K_{IC}^0 on the orientation of nano-twin with different ρ / a

Fig.5 illustrates the variations of the critical normalized mode I SIF with the emission angle for different relative elliptic curvatures when $a = 50\,\text{nm}$, $\omega = 5^\circ$, $\theta_0 = 15^\circ$, $l_0 = 0.25\text{nm}$, $l_1 = 25\text{nm}$, $d = 5\,\text{nm}$, $s = 1\,\text{nm}$, $\theta_1 = 0^\circ$. From the figure, we can see that the stress intensity factor first increases and then decreases with the increase of the emission angle. There is a critical inclination of nano-twin oriental corresponding to the maximum critical stress intensity factor. This inclination angle makes the dislocation of the elliptical crack tip the hardest to launch. The effect of the relative elliptic curvature on the critical normalized mode I SIF is also considered in Fig.6 when $a = 50\,\text{nm}$, $\omega = 5^\circ$, $\alpha = 0^\circ$, $l_0 = 0.25\text{nm}$, $l_1 = 25\text{nm}$, $d = 5\,\text{nm}$, $s = 1\,\text{nm}$, $\theta_1 = 0^\circ$. It can be found that When the dislocation emission angle is determined, the stress intensity factor increases as the curvature of the ellipse increases, which indicates that dislocation emission becomes difficult when the crack tip is passivated.

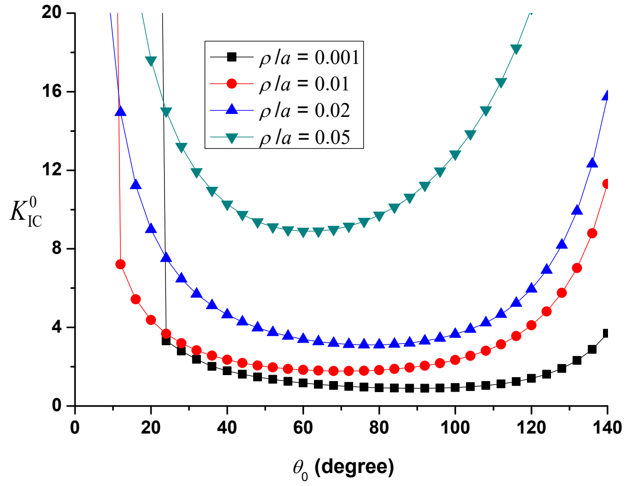


Fig.6 Dependences of the critical normalized K_{IC}^0 on emission angle with different ρ/a

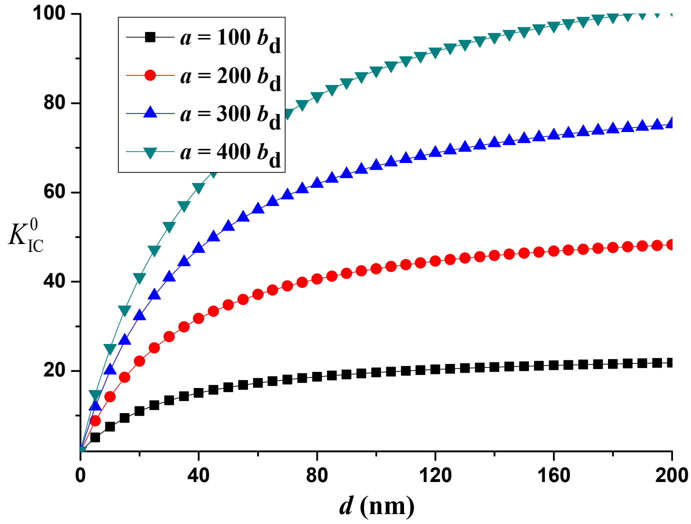


Fig.7 Dependences of the critical normalized K_{IC}^0 on grain size with different crack length

The influence of grain size and crack length on the normalized mode I SIF is shown in Fig.7 when $\omega = 5^\circ$, $\alpha = 0^\circ$, $l_0 = 0.25\text{nm}$, $l_1 = 25\text{nm}$, $\rho = 0.5\text{nm}$, $s = 1\text{nm}$, $\theta_0 = 15^\circ$, $\theta_1 = 0^\circ$. It shows that K_{IC}^0 increases with increasing crack length and grain size, which indicates that in this case, the increase of crack length or grain size will make the dislocation emission of crack tip difficult. The variation of the normalized mode I SIF with the position angle θ_1 of the first wedge disclination is depicted in Fig.8 when its distance from the crack surface l_1 is different for $a = 50\text{nm}$, $\omega = 5^\circ$, $\alpha = 0^\circ$, $l_0 = 0.25\text{nm}$, $d = 5\text{nm}$, $\rho = 0.5\text{nm}$, $s = 1\text{nm}$, $\theta_0 = 15^\circ$. As illustrated, the SIF first increases and then decreases as the angle increases. There is a critical value corresponding to minimize the SIF and make dislocations most likely to be emitted. In addition, when the angle is in a certain range, approximately $14^\circ \le \theta_0 \le 82^\circ$, the closer the nano-twin is, the smaller the SIF is, indicating that the nano-twin can promote the dislocation emission at the crack tip. Conversely, in another range, the SIF increases as the distance from the crack to the nano-twin decreases, which indicates that the nano-twin at this time hinder the dislocation emission at the crack tip. In general, the effect of nano-twin on dislocations emitting from crack tip depends on the position and azimuth of the twins. There is an optimal position of nano-twin to make the dislocations most susceptible to emit from crack tip.

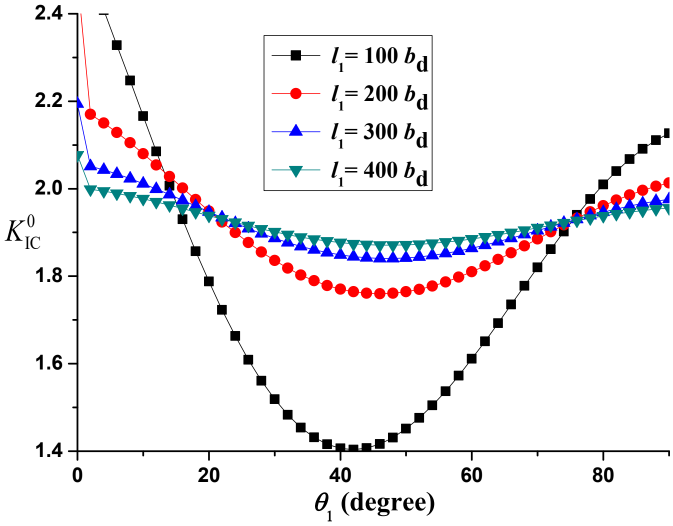


Fig.8 Dependences of the critical normalized K^0_{IC} on position of nano-twin

5 Concluding remarks

In summary, the paper theoretically investigated the effect of the nano-twin and dislocation pileup, which is an important deformation mode in nanocrystalline materials, on the dislocation emission from an elliptical blunt crack tip. The analytical expression of critical stress intensity factors corresponding to the first dislocation emitting from crack tip is deduced. The influence of the dislocation pileup, the position and the strength of nano-twin, the curvature radius of crack tip, the crack length and the grain size on the dislocation emission is discussed in detail. Some useful rules and conclusions are as follows:

(1) The effect of nano-twin on dislocations emitting from crack tip depends on the position and azimuth of the twins. There is an optimal position of nano-twin to make the dislocations most susceptible to emit from crack tip. And the greater the intensity of the twins, the more it can hinder or promote the emission of dislocations at the crack tip. There is a critical inclination of nano-twin oriental corresponding to the maximum critical stress intensity factor making the dislocation of the elliptical crack tip the hardest to launch.

(2) There is the most probable emission angle, and the most probable emission angle increases with the intensity of the nano-twin. The increase of crack length and grain size will make the dislocation emission of crack tip difficult and the dislocation emission will become difficult when the crack tip is passivated.

(3) The dislocation pileup at the twin boundary will increase the critical stress intensity factor for dislocation emission, making the dislocation emission from crack tip difficult, thus reducing the toughness of the material contributed by dislocation emission.

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