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Effect of wedge disclination dipole on dislocation emission from a surface crack tip in nanocrystalline materials

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ABSTRACT

The interaction between a wedge disclination dipole and a linear crack of the surface in nanocrystalline materials is investigated. Utilizing the conformal mapping technique and the Muskhelishvili complex variable method, the explicit closed-form solutions are derived for complex potentials and stress fields. The critical stress intensity factors (SIFs) for the first dislocation emission from the crick tip are also calculated. The effects of the relative parameters on the normalized critical SIFs, such as the disclination strength, the edge dislocation emission angle, the dipole size, the distance between the crack tip and the center of the disclination dipole, the direction angle of the disclination dipole and the crack length, are discussed in detail as well. The results reveal that the shielding effect produced by disclination dipole increases with the increasing disclination strength, which means it can prevent the dislocation emission from the crack tip to decrease material toughness.

1. Introduction

It is well known that dislocation and disclination are two kinds of very important lattice defects in the process of discussing fracture mechanics of the nanocrystalline materials (NCMs). Therefore, the elastic interaction between dislocations/disclinations and cracks has been widely studied by many theoretical and experimental researchers [1–9]. In these researches, they paid more attention to the calculations of the stress field, image force, strain energy of dislocation and the stress intensity factors (SIFs) at the crack tip in their works. As for disclination, a unit disclination is much larger than a dislocation in the aspect of energy. However, when the disclination configurations are in a self-shielded circumstance such as disclination dipoles and disclination loops, the energy may correspondingly become small, and disclinations can exist in crystalline and non-crystalline materials [10]. Disclination elastic fields play an important role in the deformation process of materials, such as determining plenty of the mechanical properties of the physical phenomena. For instance, the deformation mechanism that results from the stress relaxation produced by disclination has been widely investigated by many researchers in NCMs [11–13]. Moreover, numerous works have been conducted concerning the elastic fields and elastic energies caused by shielded disclinations [10,14–17].

Nevertheless, it is extremely common that the surface crack exists in NCMs, and it has a great impact on the mechanical properties of materials as well. The surface crack is a vital damage at the surface of materials, which can produce local stress concentration and eventually lead to deformation or even fracture, thus influence the mechanical properties and quality of materials. Especially, such a phenomenon or damage plays a significant role in single crystal Silicon [18–20]. What is more, indentations and scratches at the surface of materials often generate cracks and eventually result in fracture or damage as well. For the surface crack, many scholars have conducted plenty of researches on the elastic interaction between dislocation/disclination and surface crack [21–24]. At the same time, the influence of surface effects and interface effects on the crack or nanoscale inhomogeneity has also been investigated by researchers [25,26].

In addition, the existence of the disclination configurations can be observed by transmission electron microscopy (TEM) in actual experiments [27,28], and they can be produced by the specific deformation modes, which can explain the specific toughening mechanisms in NCMs [29–33]. In most cases, NCMs have superior strength, strong hardness and good wear resistance but at the expense of low tensile ductility and fracture toughness [34,35]. Nevertheless, certain NCMs with good tensile ductility or enhanced toughness have still been studied and reported [36–38]. The

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fracture behaviors of these materials depend on their dominant deformation modes. Recently, many models have been developed to explain this phenomenon. In most of them, intergrain sliding, triple junction diffusional creep, Coble creep, grain boundary sliding and migration, rotational deformation and nanoscale deformation twinning have been theoretically described as specific deformation modes of NCMs [33,34,39–42].

On the other hand, one of the toughening mechanisms, the dislocation is emitted from the crack tip into the plastic zone, which can reduce the SIFs at the crack tip. In addition to the dislocation/disclination shielding effect, the crack blunting is a significant mechanism which can reduce the stress fields nearby the crack tip as well [24]. Hence, the interactions between dislocations/disclinations and blunt cracks have motivated many investigations [43–49]. When it comes to the dislocation emission from the crack tip, Ohr [50] provided experimental evidence that the dislocation emission from the crack tip can lead to crack blunting. As the crack is blunted to a certain extent, the dislocation emission from the crack tip may be interrupted. The blunted crack will not propagate until the nucleation of a new sharp crack comes into being, and the dislocation may be emitted from the new crack tip again. Later on, many investigations on the interaction between dislocation emission and crack blunting have been also conducted by researchers [51,52].

However, the problem of the wedge disclination dipoles interacting with a surface crack has not been studied as yet because of the complexity of the calculation. In the present paper, the critical SIFs at the tip of the crack are deduced by the conformal mapping technique and the complex variable method. The effects of the stress fields produced by the disclination dipole on the dislocation emission from the crack tip are discussed in detail as well, which can contribute to understanding the deformation mechanisms better in NCMs.

2. Problem statement and solution

The current problem is shown in Fig. 1(a). A free surface $x = 0$ in a semi-infinite plane contains a linear crack whose left-end point is located at the origin O, and OA represents the length L of the linear crack along the positive x-axis, respectively. The wedge disclination dipole consists of a positive disclination with strength ω at B ($z_1 = x_1 + iy_1 = L + de^{i\theta_0} - ae^{i\varphi}$) and a negative disclination with the same strength at C ($z_2 = x_2 + iy_2 = L + de^{i\theta_0} + ae^{i\varphi}$). Here, the dipole arm is $2a$, and disclination lines are perpendicular to the xoy-plane.

For the plane strain problem, stress fields and displacement fields can be expressed by means of two Muskhelishvili's complex potentials $\varphi(z)$ and $\psi(z)$ [53].

$$\sigma_{xx} + \sigma_{yy} = 2[\varphi'(z) + \overline{\varphi'(z)}] \tag{1}$$

$$\sigma_{yy} - \mathrm{i}\sigma_{xy} = \varphi'(z) + \overline{\varphi'(z)} + z\overline{\varphi''(z)} + \overline{\psi'(z)} \tag{2}$$

$$2\mu(u_x + \mathrm{i}u_y) = \kappa\varphi(z) - z\overline{\varphi'(z)} - \overline{\psi(z)} \tag{3}$$

where $z = x + iy$, $\kappa = 3 - 4\nu$, μ is the shear modulus and ν is Poisson's ratio. The superposed bar represents a complex conjugate, and the prime denotes differentiation with respect to the variable z.

Let us introduce the following mapping function [24]:

$$z = \omega(\zeta) = \sqrt{\zeta^2 + L^2} \tag{4}$$

with $\zeta = \eta + i\xi$, which maps the linear crack of the surface in the z-plane into a half space in the ζ-plane ($\eta > 0$), as shown in Fig. 1(b).

With the help of the mapping function Eq. (4), Eqs. (1) and (2) can be rewritten in the ζ-plane as follows:

$$\sigma_{xx} + \sigma_{yy} = 2\left[\Phi(\zeta) + \overline{\Phi(\zeta)}\right] \tag{5}$$

$$\sigma_{yy} - \mathrm{i}\sigma_{xy} = \Phi(\zeta) + \overline{\Phi(\zeta)} + \frac{\overline{\omega(\zeta)}}{\overline{\omega'(\zeta)}}\overline{\Phi'(\zeta)} + \overline{\Psi(\zeta)} \tag{6}$$

where $\Phi(z) = \varphi'(\zeta)/\omega'(\zeta)$, $\Phi'(z) = [\varphi''(\zeta)\omega'(\zeta) - \varphi'(\zeta)\omega''(\zeta)]/[\omega'(\zeta)]^3$ and $\Psi(z) = \psi'(\zeta)/\omega'(\zeta)$.

Let us firstly analyze the singularities of the complex potentials. According to the works of Song et al. [54], the following complex potentials $\varphi_w(z)$ and $\psi_w(z)$ can be chosen:

$$\varphi_w(z) = \frac{D\omega}{2}\sum_{k=1}^{2}(-1)^{k+1}(z - z_k)\ln(z - z_k) + \varphi_{w0}(z) \tag{7}$$

$$\psi_w(z) = \frac{D\omega}{2}\sum_{k=1}^{2}(-1)^{k}\bar{z}_k\ln(z - z_k) + \psi_{w0}(z) \tag{8}$$

where $D = \mu/2\pi(1-\nu)$, $\varphi_{w0}(z)$ and $\psi_{w0}(z)$ refer to the terms resulting from the interaction between the wedge disclination dipole and the linear crack of the surface.

Substituting Eq. (4) into Eqs. (7) and (8), the complex potentials in the ζ-plane are given as

$$\varphi_w(\zeta) = \frac{D\omega}{2}\sum_{k=1}^{2}(-1)^{k+1}H_k(\zeta - \zeta_k)\ln(\zeta - \zeta_k) + \varphi_{w0}(\zeta), \eta > 0 \tag{9}$$

$$\psi_w(\zeta) = \frac{D\omega}{2}\sum_{k=1}^{2}(-1)^{k}\bar{\zeta}_k\ln(\zeta - \zeta_k) + \psi_{w0}(\zeta), \eta > 0 \tag{10}$$

where $H_k = \zeta_k/\sqrt{\zeta_k^2 + L^2}, \quad (k = 1, 2)$.

Applying the Riemann–Schwarz symmetry principle, a new analytic function $\chi_w(\zeta)$ can be introduced:

$$\chi_w(\zeta) = \omega(-\zeta)\frac{\varphi'_w(\zeta)}{\omega'(\zeta)} + \psi_w(\zeta), \eta > 0 \tag{11}$$

Substituting Eqs. (9) and (10) into Eq. (11), the analytic function $\chi_w(\zeta)$ can be regained as below:

$$\chi_w(\zeta) = \frac{D\omega}{2}\sum_{k=1}^{2}(-1)^{k}\left[\omega(\zeta)\ln(\zeta - \zeta_k) + \bar{\zeta}_k\ln(\zeta - \zeta_k)\right] + \chi_{w0}(\zeta) \tag{12}$$

Following Muskhelishvili's treatments, the traction-free boundary condition along the imaginary axis is satisfied by

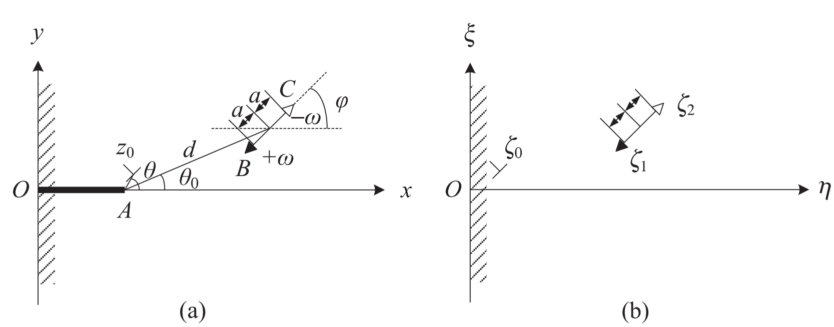

Fig. 1. (a) A wedge disclination dipole near a surface crack tip and dislocation emission from the crack tip. (b) The ζ-plane after conformal mapping.