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Effect of residual surface stress on the fracture of nanoscale materials

Haishun Nan, Baolin Wang*

Graduate School at Shenzhen, Harbin Institute of Technology, Harbin 150001, PR China

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ABSTRACT

The problem of a mode I crack in nanomaterials under a remote mechanical load is investigated. The effect of the residual surface stress on the crack surface is considered and the solutions to the crack opening displacement (COD) and the stress intensity factor (K_I) are obtained. The results show that the surface effect on the crack deformation and crack tip field are prominent at nanoscale. Moreover, COD and K_I are influenced by the residual surface stress not only on the surface near the crack tip region but also on the entire crack surface.

1. Introduction

With increasing applications of micro-/nanoscale materials and structures, such as nanowires (Wu, 2006), nanosprings and nanorings, strength and reliability of these advanced materials and devices become critical. One fundamental and basic issue in understanding the failure behavior of engineering materials and structures is to analyze the deformation and stress field at the crack tip. When the characteristic sizes of materials and structures shrink to microns or nanometers, owing to the large surface–volume ratio, surface effects often play a crucial role in their mechanical behavior (Miri et al., 2011; Wang and Feng, 2009). To explain the effect of surface in solids, Gurtin and Murdoch (1975) and Gurtin et al. (1998) developed a continuum mechanics model of surface elasticity, which recently has been adopted to explore the features of mechanical deformations at nanoscale by incorporating the effects of surface/interface energy (Dingreville et al., 2005; Goldstein et al., 2010; Jin and Carmen, 2008; Liu et al., 2011; Park, 2009; Sharma et al., 2003). For instance, the surface effects on the effective modulus of elastic composites with dilute spherical nanocavities was considered (Yang, 2004) and static and dynamic response of nanoscale beams incorporating surface energy was explored (Liu and Rajapakse, 2010).

The classical fracture mechanics, which neglects the effect of residual surface stress on the fracture of the materials, has been well developed. For nanosized crack problem, the influence of surface stress on the crack surface is not well understood. Since the propagation of cracks in inherent have relation with surface energy, there are some recent work that considered surface influence of surface stress on the stress fields in bodies containing cracks, which may be regarded as asymptotic cases of voids. Using the theory of surface elasticity and analyzing an elliptic void, Wu (1999) studied the effect of constant surface stresses on the configurational equilibrium of voids and cracks. Wang et al. (2008) investigated the influences of surface energy on the stress distributions near a blunt crack tip for Mode I and Mode III cracks by using a local analysis method. Buehler et al. (2003) and Buehler and Gao (2006) investigated the dynamical fracture instabilities due to local hyperelasticity at crack tip by adopting massively parallel atomistic simulations. And after that, as all the above analytical solutions are valid only in a very small region above the crack tip, a numerical study about surface effects on mode-1 crack tip fields is given by Fu et al. (2010). For a mode-III crack, Kim et al. (2010) calculated the full field solution by using the complex variable method. At small length scales, Huang et al. (2009) performed an atomistic study to characterize the formation and extension of nano-sized cracks. Using atomistic reaction pathway calculations, Terdalkar et al. (2010) studied nanoscale fracture in grapheme. The analysis of Terdalkar et al. (2010) identify a kinetically favorable fracture path that features an alternating sequence of bond rotation and bond breaking. Using atomistic and multiscale simulations, Zhang et al. (2005) explored the fracture of defected carbon nanotubes.

However, the studies of surface effect, especially the residual surface stress effect on the fracture, are far from enough. In most previous studies (Wu, 1999; Wang et al., 2008), only the surface stress in the vicinity of the crack tip is considered. Since the crack deformation and stress intensity factor all have strong connection with the surface stress acting on the whole surface of the crack, it is not sufficient to consider only the surface stress near the crack tip region. Thus in the present paper, we considered the residual surface effect on the crack tip fields of a mode-I crack problem by incorporating the surface effect on the whole crack surface. The results show that the classical continuum mechanics

* Corresponding author.
E-mail address: nanhit@yahoo.com.cn (B. Wang).

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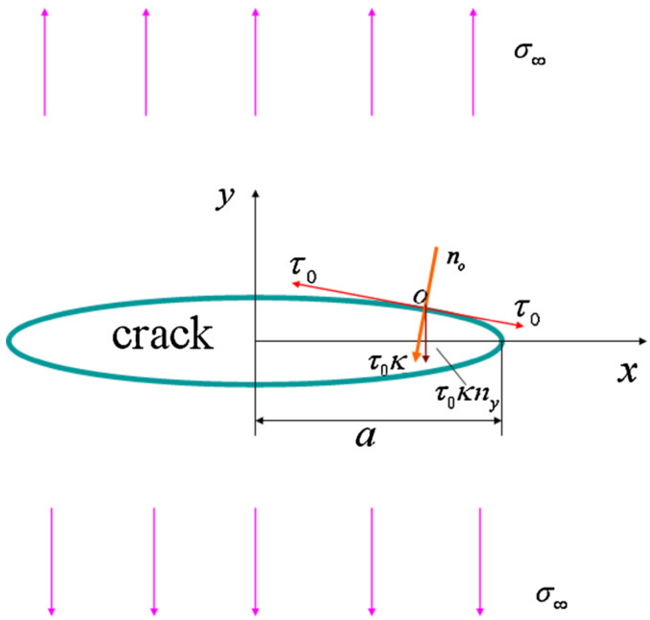

Fig. 1. An infinite medium with a through-thickness crack of length 2*a*.

considerably overestimates the fracture mechanics parameters such as the crack opening displacement and the crack tip stress intensity factor. Further more, COD and K_I are influenced by the residual surface stress not only on the surface near the crack tip region but also on the entire crack surface. Such observation is considerably different from the previous work that only considered the surface effect in the vicinity of crack tip.

2. Basic equations

To begin with, the basic equations of surface elasticity theory were given by Gurtin and Murdoch (1975) and Gurtin et al. (1998). In Gurtin's sense (1998), a surface is regarded as an elastic but negligibly thin membrane and has the properties that is adhered to the underlying bulk material without slipping and has elastic constants different from the bulk. The equilibrium and constitutive equations in the bulk of the material are the same as those in the classical theory of elasticity, but the presence of surface stress gives rise to a nonclassical boundary condition. Without considering the body forces, the equilibrium equations and the isotropic constitutive relations in the bulk read $\sigma_{ij,j}=0$, $\sigma_{ij}=2\mu\varepsilon_{ij}+\lambda\varepsilon_{kk}\delta_{ij}$, i, $j=1, 2$, where μ and λ are material constants of the bulk, σ_{ij} and ε_{ij} are the components of stress and strain tensors, respectively. Assume that the surface is ideally adhered to the bulk. Then the equilibrium conditions on the surface are written as $t_\alpha+\sigma^s_{\beta\alpha,\beta}=0$, $\sigma_{ij}n_in_j=\sigma^s_{\alpha\beta}\kappa_{\alpha\beta}$, where n_i denotes the outward normal unit vector to the surface, t_α is the negative of the tangential component of the tractions $t_i=\sigma_{ij}n_j$ along the α_i direction on the surface, and $\kappa_{\alpha\beta}$ is the surface curvature tensor. According to Gibbs (1906) and Cammarata (1994) the surface stress tensor $\sigma^s_{\alpha\beta}$ is related to the surface energy density γ as $\sigma^s_{\alpha\beta}=\gamma\delta_{\alpha\beta}+\partial\gamma/\partial\varepsilon^s_{\alpha\beta}$, where $\varepsilon^s_{\alpha\beta}$ is the surface strain tensor.

3. Residual surface stress in mode-I crack problem

Now we analyze the plane problem of the infinite medium shown in Fig. 1. It is assumed that all the field variables are functions of x and y only, and the half crack length is denoted by a. Let the medium be loaded by a remote uniform normal stress σ_∞ along the y direction. Here, we investigate a symmetric problem for mode-I crack. In this case, the surface stress along the crack surface would reduced to the one-dimensional and linear form, that is $\sigma^s=\tau_0+E^s\varepsilon$, where τ_0 is the residual surface tension when the bulk is under unstrained, and E^s is the surface Young's modulus. If the change of the atomic spacing in deformation is infinitesimal, compared with the contribution of τ_0, the effect of the component of $E^s\varepsilon$ is negligibly small in most cases (Ou et al., 2008; Wang et al., 2006). Thus the surface stress on the crack surface can be expressed by residual surface stress τ_0 as shown in Fig. 1, and the direction of τ_0 is tangent to the crack surface. The surface stresses are given by residual surface stress τ_0 using the force balance normal to the bulk-surface interface in the deformed configuration from Fig. 1 and can be expressed by $\tau_0\kappa$, where κ is the surface curvature tensor and n_o denote the unit normal vector at any point o on the crack surface. Thus the residual surface stress τ_0 can generate a load perpendicular to the direction of τ_0. Therefore the load along the y-axis is $\tau_0\kappa n_y$, where n_y is the directional cosine of the vector normal to the crack surface.

Note that κ and n_y depend on the crack opening. Thus, the load $\tau_0\kappa n_y$ generated by the residual surface stress τ_0 at the crack is related to the variable x. According to the method of solving the crack problem subjected to dynamic loading (Wang et al., 2000; Erdogan and Gupta, 1972), we introduce a dislocation density function $\phi(x)=2\partial V(x,0)/\partial x$, where V is the crack face displacement along the y-direction. The crack opening displacement (COD) is the maximum opening of the crack, which can be expressed as COD = $2V(0, 0)$. We can also deduct that the radius of crack surface curvature ρ and the directional cosine for the normal to the crack surface n_y can be expressed by ϕ as

$$\rho=1/\kappa=\frac{2(1+\phi^2/4)^{3/2}}{\phi'} \tag{1}$$

and

$$n_y=\frac{1}{\sqrt{1+\phi^2/4}} \tag{2}$$

According to singular integral equation method (Wang et al., 2000; Erdogan and Gupta, 1972), a relation between the applied loadings σ_∞ and the dislocation density function $\phi(r)$ was given on the $y=0$ planes. In the current case, considering the contribution of the load generated by the residual surface stress τ_0, the relation between the applied loadings σ_∞ and the dislocation density function $\phi(r)$ can be rewritten as:

$$\sigma_{yy}(x,0)=\frac{E}{2(1-\nu^2)}\times\frac{1}{2\pi}\int_{-a}^{a}\frac{\phi(r)}{(r-x)}dr+\sigma_\infty+\frac{\tau_0 n_y(x)}{\rho(x)} \tag{3}$$

where E and ν are, respectively, the Young's modulus and Poisson's ratio of the materials. Eq. (3) gives the stress inside the crack as well as outside of the crack. In the case of inside crack, $-a\le x\le a$, the crack face is stress free such that $\sigma_{yy}(x,0)=0$. Then Eq. (4) becomes a singular integral equation which has Cauchy-type integral kernel $1/(r-x)$. Let $\bar r=r/a$ and $\bar x=x/a$, under the theory of the integral equation (Muskhelishvili, 1953), $\phi(r)$ has the form of solution

$$\phi(a\bar r)=\sum_{m=1}^{\infty}\frac{C_mT_m(\bar r)}{\sqrt{1-\bar r^2}},\ -1\le\bar r\le 1 \tag{4}$$

where $T_m(r/a)=\cos(mar\cos(r/a))$ is the Chebyshev polynomials of the first kind, and C_m are unknown constants to be determined. To solve Eq. (3), we can truncated the first M terms of Eq. (4), that is $m=1, \ldots, M$. Substituting the first M terms of Eq. (4) into Eq. (3) and using the well-known integral

$$\frac{1}{\pi}\int_{-1}^{1}\frac{T_m(\bar r)}{(\bar r-\bar x)\sqrt{1-\bar r^2}}d\bar r=U_{m-1}(\bar x) \tag{5}$$