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Misfit dislocation dipoles in wire composite solids

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ABSTRACT

Developed in this note is a theoretical model describing the mobility of a misfit screw dislocation dipole in a wire composite consisting of a stiff cylindrical substrate covered by a soft co-axial cylindrical film. A critical value of the film thickness, which is a function of the parameter measuring the stiffness of the film with respect to the substrate, is identified. It is observed that: (i) there exist two equilibrium positions of the misfit dislocation dipole (one stable and the other one unstable) when the film is thicker than the critical value; (ii) the two equilibrium positions of the misfit dislocation dipole converge to a single saddle point equilibrium position which is neither stable nor unstable when the thickness of the film is at the critical value; (iii) there exists no equilibrium position of the misfit dislocation dipole when the thickness of the film is below the critical value. These features could be useful to the design of wire composites and to the dislocation-related plasticity analysis.

1. Introduction

Studies of dislocations with boundary, interface and even size effect are important in material property characterization (i.e., Hirth and Lothe, 1982; Wang et al., 2007). While Wang and Yang (2005) investigated the possible nucleation of a screw dislocation from a triple junction using the Stroh–Eshelby formalism, Kochmann and Le (2008) studied the dislocation nucleation and pile-ups near the phase boundaries of a model bicrystal by employing the continuum dislocation theory. More recently, various multiscale dislocation models were also proposed to study, i.e., the plastic flow in crystals at submicron-to-nanometer scales (Liu et al., 2009) and the plasticity behavior in an aluminum single crystal (Groh et al., 2009).

The focus of this note is on dislocations in wire composites. The wire composites consisting of a film deposited on a cylindrical substrate allow for novel devices to be developed and thus have been studied intensively, both experimentally and theoretically (Gutkin et al., 2000; Sheinerman and Gutkin, 2001; Lauhon et al., 2002; Song et al., 2005; Lee et al., 2006; Raychaudhuri and Yu, 2006; Trammell et al., 2008). For instance, the behavior of misfit dislocations in film/substrate wire composites was investigated by Gutkin and co-workers (Gutkin et al., 2000; Sheinerman and Gutkin, 2001). However, in the model of Gutkin et al. (2000) the elastic constants were assumed to be the same for the substrate and film comprising the wire composite. This kind of assumption cannot reflect the real scenario of the elastic mismatch between the substrate and the surrounding film. Based on the above considerations, the objective of this note is to investigate the mobility of a misfit screw dislocation dipole in a wire composite consisting of a stiff cylindrical substrate covered by a soft co-axial cylindrical film. Fang et al. (2008) considered a misfit dislocation dipole in an infinite soft matrix reinforced by a stiff circular inhomogeneity. They identified the equilibrium position for the dislocation dipole. Apparently the existence of the additional

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traction-free surface in the film/substrate structure studied here will cause the mobility of the dislocation dipole to be more complicated due to the fact that a traction-free surface will always attract a dislocation. In this note, we first derive the analytical solution and then present some numerical results.

2. Misfit dislocation dipole in wire composite

Here we consider a wire composite of infinite length consisting of a cylindrical substrate of radius R_1 covered by a film of thickness $H = R_2 - R_1 (R_1 < R_2)$ (Fig. 1). Both the substrate and film are assumed to be elastically isotropic with different shear moduli (μ_1 for the substrate and μ_2 for the film). We assume that the substrate is stiffer than the film, i.e., $\mu_1 > \mu_2$, such as the metal/ceramic system in which the substrate is made of ceramic materials. The misfit dislocation dipole is composed of two screw dislocations at x_0 ($R_1 < x_0 < R_2$) and $-x_0$ with Burgers vectors b_z (>0) and $-b_z$ respectively in the softer film and their lines are parallel to the axis of the cylindrical substrate. We ignore the influence of the lattice mismatch on the mobility of the misfit dislocation dipole since we assume that the mismatch induced strain is relaxed by the dipole.

The out-of-plane displacement u_z and the stress components σ_{zy}, σ_{zx} can be expressed in terms of one analytic function $f(z)$, ($z = x + iy$) as (Muskhelishvili, 1953)

$$\begin{aligned} &u_z = \mathrm{Im}\{f(z)\}, \\ &\sigma_{zy} + i\sigma_{zx} = \mu f'(z) \end{aligned} \tag{1}$$

By satisfying the continuity conditions of traction and displacement across the substrate–film interface $|z| = R_1$ and the traction-free condition at $|z| = R_2$, the two analytic functions, $f_1(z)$ defined in the cylindrical substrate and $f_2(z)$ defined in the surrounding film, can be finally obtained as

$$\begin{aligned} f_1(z) &= \frac{\Gamma b_z}{2\pi} \ln \frac{z - x_0}{z + x_0} + \Gamma \sum_{n=1}^{+\infty} A_n z^{2n-1}, \quad (|z| < R_1) \\ f_2(z) &= \frac{b_z}{2\pi} \ln \frac{z - x_0}{z + x_0} + \frac{(1-\Gamma) b_z}{2\pi} \ln \frac{z - R_1^2/x_0}{z + R_1^2/x_0} \\ &\quad + \sum_{n=1}^{+\infty} A_n z^{2n-1} + (1-\Gamma) \sum_{n=1}^{+\infty} R_1^{2(2n-1)} A_n z^{-(2n-1)}, \quad (R_1 < |z| < R_2) \end{aligned} \tag{2}$$

where $\Gamma = \frac{2\mu_2}{\mu_1 + \mu_2} < 1$ is a parameter measuring the stiffness of the soft film with respect to the stiffer substrate, and A_n ($n = 1, 2, \ldots, +\infty$) are real constants given by

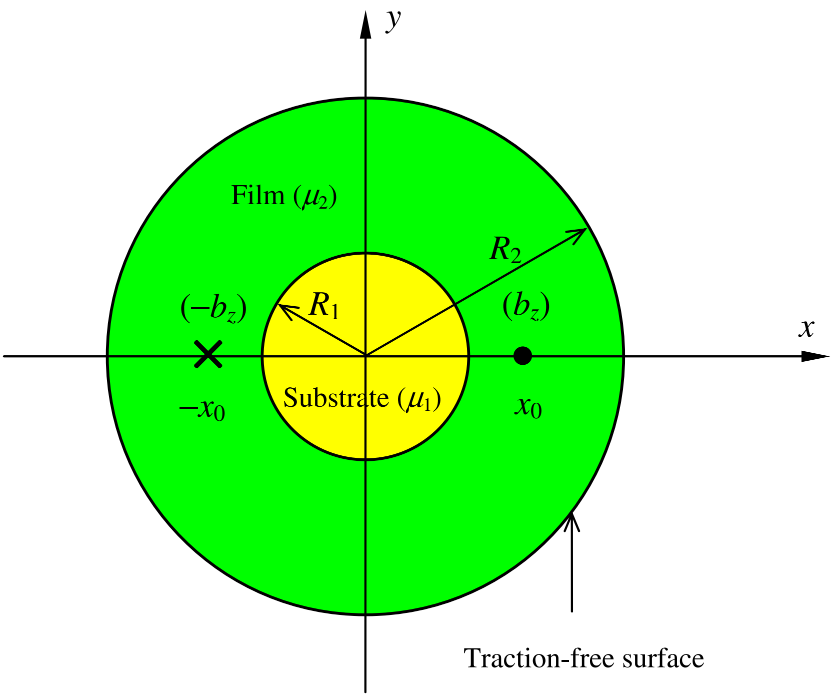

Fig. 1. Misfit dislocation dipole in a wire composite solid.

$$A_n = \frac{b_z}{\pi}\frac{x_0^{2n-1} + (1-\Gamma)R_1^{2(2n-1)}x_0^{-(2n-1)}}{(2n-1)[R_2^{2(2n-1)} + (1-\Gamma)R_1^{2(2n-1)}]} \tag{3}$$

Remark. It can be easily checked that Eq. (2) automatically satisfies the boundary conditions at the substrate–film interface $|z| = R_1$. In addition A_n (n = 1, 2, ..., $+\infty$) is uniquely determined by enforcing the traction-free condition at $|z| = R_2$.

Consequently the stress field within the substrate induced by the dislocation dipole is

$$\sigma_{zy} + i\sigma_{zx} = \mu_1\Gamma\left[\frac{b_z x_0}{\pi(z^2 - x_0^2)} + \sum_{n=1}^{+\infty}(2n-1)A_n z^{2(n-1)}\right], \quad (|z| < R_1) \tag{4}$$

and the stress field within the film induced by the dislocation dipole is

$$\sigma_{zy} + i\sigma_{zx} = \mu_2\left[\frac{b_z x_0}{\pi(z^2 - x_0^2)} + \frac{(1-\Gamma)b_z R_1^2 x_0}{\pi(x_0^2 z^2 - R_1^4)} + \sum_{n=1}^{+\infty}(2n-1)A_n[z^{2(n-1)} - (1-\Gamma)R_1^{2(2n-1)}z^{-2n}]\right](R_1 < |z| < R_2) \tag{5}$$

With these stress components, we can find easily the configurational force on the dislocation (or the Peach–Koehler force). For example, the Peach–Koehler force acting on the positive screw dislocation is found as

$$\tilde{F} = \frac{(1-\Gamma)\tilde{x}}{\tilde{x}^4 - 1} - \frac{1}{4\tilde{x}} + \sum_{n=1}^{+\infty}\frac{\tilde{x}^{2(2n-1)} - (1-\Gamma)^2\tilde{x}^{-2(2n-1)}}{\tilde{x}(1 - \Gamma + R^{2(2n-1)})}, \tag{6}$$

where $\tilde{F} = \frac{\pi R_1}{\mu_2 b_z^2}F_x$, with $F_x = b_z\sigma_{zy}$ being the x-component of the Peach–Koehler force ($F_y = 0$), is a dimensionless value, and $\tilde{x} = x_0/R_1$, and $R = R_2/R_1 > 1$. In the following numerical calculation, the series was truncated at $n = 30$ for a relative error below 1%.

The equilibrium position of the dislocation dipole satisfies the condition that $\tilde{F} = 0$. Our numerical results indicate that when the thickness of the film is above the critical value H_c there exists a stable equilibrium position for the dislocation dipole close to the substrate–film interface due to the interaction among the two dislocations and the interface (the stiff substrate repels the two dislocations while the two dislocations with opposite Burgers vectors attract each other); meanwhile, there exists only one unstable equilibrium position for the dislocation dipole close to the traction-free surface due to the interaction among the two dislocations and the surface (the traction-free surface attracts the two dislocations while the two dislocations with opposite Burgers vectors attract each other); otherwise the dislocation dipole is attracted to the stable

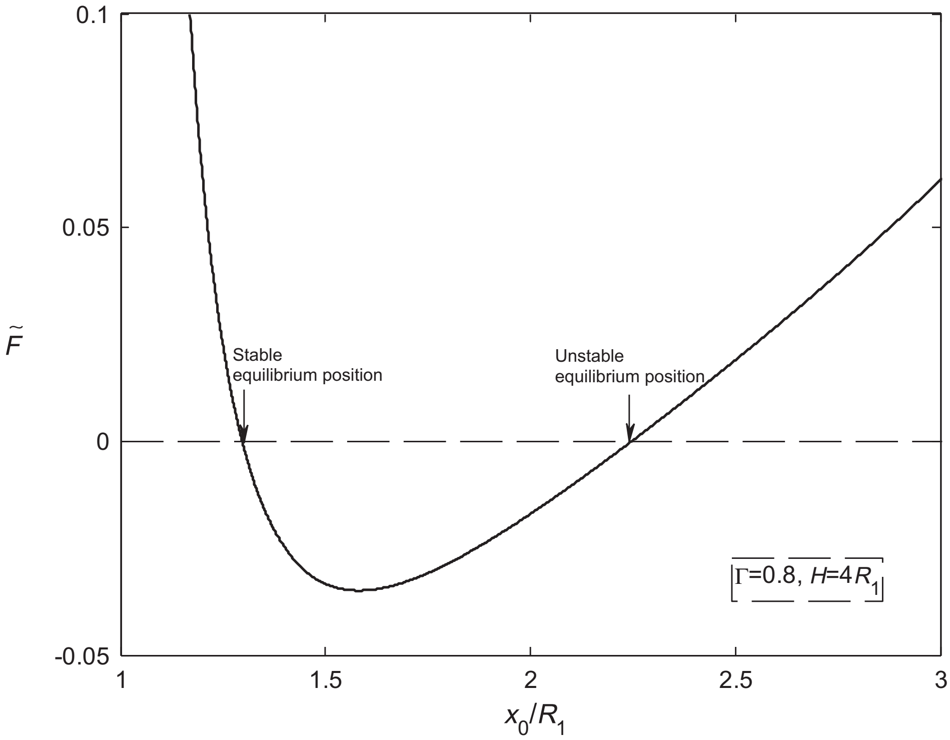

Fig. 2. The Peach–Koehler force acting on the positive screw dislocation component when $\Gamma = 0.8$ and $H = 4R_1$. Two equilibrium positions are observed.

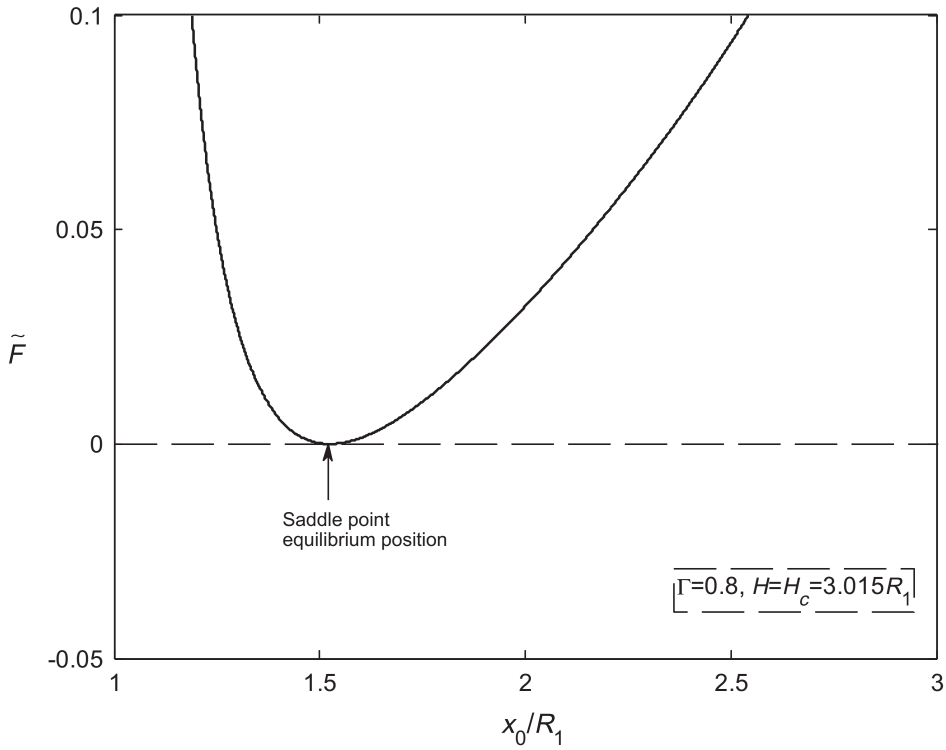

Fig. 3. The Peach–Koehler force acting on the positive screw dislocation component when $\Gamma = 0.8$ and $H = 3.015R_1$. A single saddle point equilibrium position is observed.

equilibrium position. When the thickness of the film is just at the critical value H_c the two equilibrium positions of the misfit dislocation dipole converge to a single saddle point equilibrium position which is neither stable nor unstable. When the thickness of the film is below the critical value H_c, the interaction between the interface and the traction-free surface cannot be ignored. Consequently there exists no equilibrium position for the dislocation dipole when the film is thin enough. Figs. 2–4 demonstrate the above three typical cases for the dislocation dipole. It is observed from Fig. 2 that only if the positive

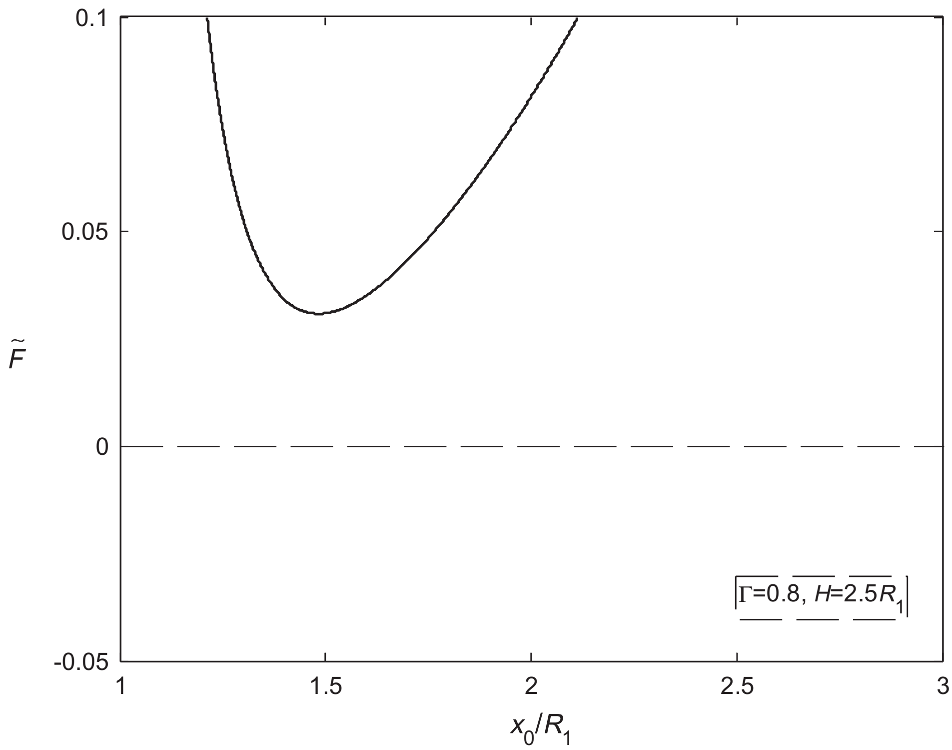

Fig. 4. The Peach–Koehler force acting on the positive screw dislocation component when $\Gamma = 0.8$ and $H = 2.5R_1$. No equilibrium position is observed.

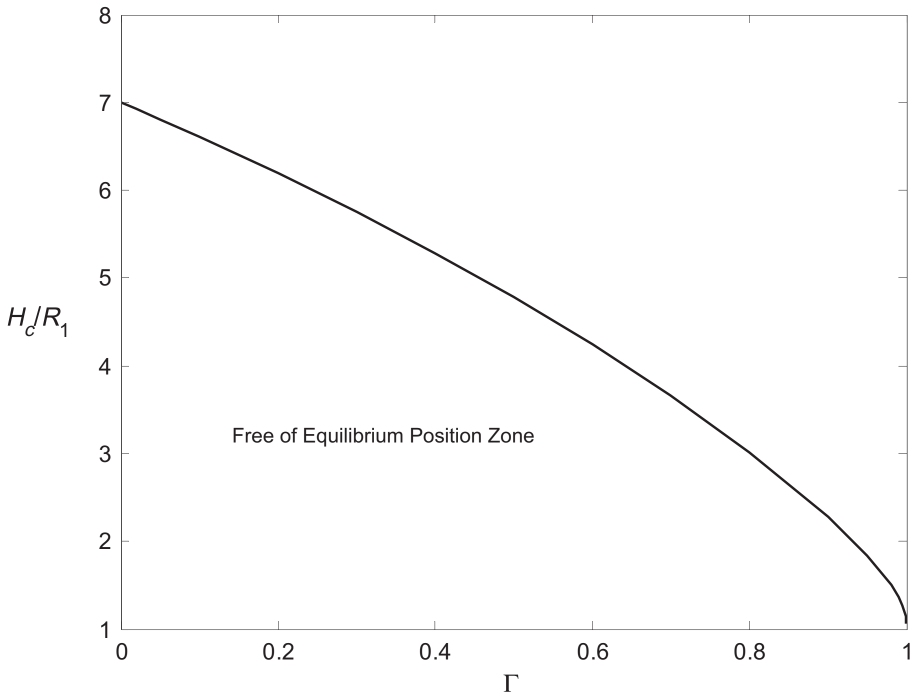

Fig. 5. Variation of the critical thickness of the film H_c as a function of Γ ($0 < \Gamma < 1$).

screw dislocation component is located to the right of the unstable equilibrium position will the dislocation dipole be pulled out of the wire composite; otherwise the dislocation dipole will be attracted to the stable equilibrium position. Fig. 4 demonstrates that the dislocation dipole will always be pulled out of the wire composite no matter where the positive dislocation component is located since the Peach–Koehler force is always positive. In addition Fig. 5 illustrates the variation of the critical thickness of the film H_c as a function of Γ ($0 < \Gamma < 1$). It is observed that H_c is a monotonically decreasing function of Γ. We therefore observe from Fig. 5 that: (i) when $H_c < R_1$ there is always no equilibrium position for the dislocation dipole no matter what the value of Γ is chosen; (ii) when $H_c > 7R_1$ there always exist two equilibrium positions for the dislocation dipole no matter what the value of Γ is chosen.

3. Conclusions

We considered a misfit screw dislocation dipole in a wire composite composed of a stiff cylindrical substrate covered by a soft cylindrical film. Our investigation demonstrated that: (i) there exist a stable equilibrium position and another unstable equilibrium position for the dislocation dipole when the soft film is thick enough, and in this case only if the positive screw dislocation component is located to the right of the unstable equilibrium position will the dislocation dipole be pulled out of the wire composite; (ii) there exists a single saddle point equilibrium position for the dislocation dipole when thickness of the soft film is just at the critical value H_c; (iii) there exists no equilibrium position for the dislocation dipole when the soft film is thin enough, and in this case the dislocation dipole will always be pulled out of the wire composite. The results obtained here can be used to guide the design of wire composites. Finally it should be noticed that the screw dislocation dipole will not induce any Eshelby twist due to a single screw dislocation (Eshelby, 1953), which was experimentally verified recently (Bierman et al., 2008; Zhu et al., 2008; Deppert and Wallenberg, 2008).

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