EFFECTS OF A THIN FILM ON SCREW DISLOCATION AND DISLOCATION DIPOLE EMISSION

Tong-Yi Zhang and Cai-Fu Qian
Department of Mechanical Engineering & Center for Advanced Engineering Materials
Hong Kong University of Science and Technology, Kowloon, Hong Kong

ABSTRACT

The present work analyzes the effects of a passive film, formed at a mode III crack tip during stress corrosion cracking, on screw dislocation emission from the film-covered crack tip and on the screw dislocation dipole emission from the interface between the film and the substrate. The results show that the crack stress field due to the applied load is enhanced by a harder film or abated by a softer film. The critical stress intensity factor for dislocation emission from the film-covered crack tip and the critical stress intensity factor for dislocation dipole emission from the interface are greatly influenced by the film stiffness and the film thickness. When the film is softer than the substrate, both the critical applied stress intensity factors are larger than that for dislocation emission from a crack tip not covered by a film.

KEYWORDS

SCC, Screw dislocation, Screw dislocation dipole, Emission, Stress intensity factor

INTRODUCTION

Stress corrosion cracking (SCC) can cause catastrophic failures of engineering structures and components due to the combined action of applied loads and environment. All SCC failures have in common a macroscopic appearance of brittleness, which means in the engineering sense that the ductility of the material is impaired. However, how the macroscopic ductility is faded at microscopic levels still remains unclear. Many different mechanisms have been proposed to explain the synergistic stress-corrosion interactions that occur at a crack tip, and there are several processes that can contribute to SCC, including anodic dissolution, film growth and cracking, and hydrogen-induced cracking (Parkins, 1992; Jones and Ricker, 1992).

Sieradzki (1982) studied, using angularly resolved X-ray Photoelectron Spectroscopy, embrittlement of High Strength Low Alloy (HSLA) steel in gaseous chlorine. His results indicated that a thin film of $FeCl_2$, forming above a threshold pressure of chlorine gas, is responsible for this SCC. There is evidence from Transmission Electron Microscopy that an oxidized thin film or a de-alloyed "sponge" is formed in susceptible alloys (Sieradzki and Newman, 1985). According to the experimental results, Sieradzki (1982), and Sieradzki and Newman (1985, 1987) proposed a mechanism of film-induced cleavage for SCC based on dislocation-crack interaction. Obviously, fracture will be brittle if no dislocations can be emitted from the crack tip or other dislocation sources nearby. In addition to the crack tip, the interface between the film and the substrate, like grain boundaries (Li, 1963), could be another dislocation source.

Zhang and Qian (1996a and b) have modeled SCC by considering the interaction of a thin-film-covered mode III crack with screw dislocations under an external applied load and, accordingly, derived the exact solutions. The previous results (Zhang and Qian, 1996a and b) show that the crack stress field due to the applied load is enhanced by a harder film or abated by a softer film. Dislocation emission from the crack tip occurs under a lower critical stress intensity factor than that for a dislocation dipole emission from the interface between the film and the substrate. Compared with the dislocation emission from a mode III crack tip without any film around it, dislocation emission from the covered crack tip or dislocation dipole emission from the interface becomes more difficult when the formed film has a shear modulus smaller than the substrate, which implies a brittle behavior of SCC. This note reports highlights of the modeling and results of the previous work (Zhang and Qian, 1996a and b). Furthermore, interaction of a thin-film-covered mode I or mixed mode I + mode II + mode III crack with dislocations having arbitrary Burgers vectors is under preparation.

ANALYSIS

In order to model a crack covered by a thin film, we assume that the film has an elliptical shape of $x_1^2/a^2 + x_2^2/h^2 = 1$. Inside the film there is a crack extending from -c to c along the x_1 axis with $c^2 = a^2 - h^2$. The crack and the film are embedded in an infinite medium under remote loading, as shown in Fig. 1.

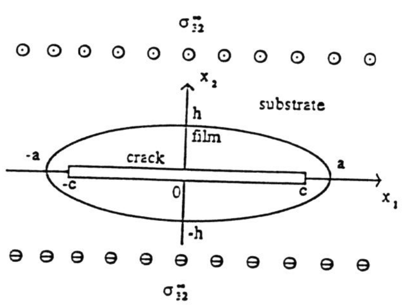

Fig. 1. Schematic illustration of a thin-film-covered Mode III crack under external applied loadins in the z plane.

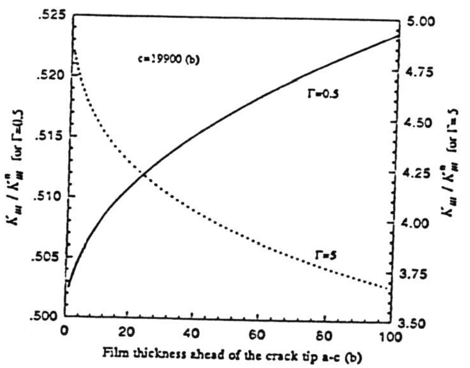

Fig. 2. The normalized stress intensity factors of K_{III}/K_{III}^0 as a function of the film thickness for Γ=0.5 and Γ=5.

Stress Fields Due to an Applied Load

The stress fields inside the film and the substrate due to an applied remote load of σ_{32}^{∞} are formulated and given by

$$\sigma^* = \frac{\Gamma\sigma_{32}^{\infty}}{1+\Gamma+m(1-\Gamma)}\left(z+\sqrt{z^2-c^2}+\frac{c^2}{z+\sqrt{z^2-c^2}}\right)\frac{1}{\sqrt{z^2-c^2}}, \tag{1}$$

$$\sigma = \frac{\sigma_{32}^{\infty}}{2\sqrt{z^2-c^2}}\left(z+\sqrt{z^2-c^2}+\frac{4R^2(1-\Gamma)+c^2(1+\Gamma)}{1+\Gamma+m(1-\Gamma)}\frac{1}{z+\sqrt{z^2-c^2}}\right), \tag{2}$$

where complex stress $\sigma = \sigma_{32} + i\sigma_{31}$, $\Gamma = \mu^*/\mu$ is a ratio of the shear modulus of the film to that of the substrate, μ is the shear modulus of the material, $z = x_1 + ix_2$, $R = (a+h)/2$, $m = (a-h)/(a+h)$, and the asterisk denotes the film. From the stress field, the stress intensity factor at the right crack tip is calculated as

$$K_{III} = \frac{2\Gamma\sigma_{32}^{\infty}\sqrt{\pi c}}{1+\Gamma+m(1-\Gamma)} = \frac{2\Gamma}{\Gamma(1-m)+1+m}K_{III}^0, \tag{3}$$

where K_{III}^0 is the nominal stress intensity factor without any film. Since m<1, the stress intensity factor is enhanced if the shear modulus of the thin film is larger than that of the substrate. Being a function of m, the stress intensity factor depends on the film thickness. Figure 2 indicates the normalized stress intensity factor as a function of the film thickness of a-c in units of the Burgers vector b, respectively, for $\Gamma = 0.5$ and $\Gamma = 5$. The normalized stress intensity factor decreases with increasing film thickness if the film is harder than the substrate, as shown in Fig. 2 for $\Gamma = 5$. In this case, the normalized stress intensity factor decreases from 5 to 1 as the film thickness changes from zero to infinity. When the film is softer than the substrate, the normalized stress intensity factor increases with increasing film thickness, as shown also in Fig. 2. For $\Gamma = 0.5$, the normalized stress intensity factor ranges from 0.5 to 1 as the film thickness increases from zero to infinity. When the crack length is much larger than the film thickness, Eq. (3) can be reduced to

$$K_{III} = \Gamma K_{III}^0, \quad \text{for } h \ll c. \tag{4}$$

In this case, the stress intensity factor is enlarged by Γ times.

Stress Fields of a Dislocation Located Inside the Film or the Substrate

For a screw dislocation inside the film, stress fields within the film and substrate are evaluated and given below:

$$\sigma^* = \left[\frac{\mu^* b}{2\pi}\left(\frac{1}{\zeta-\zeta_d}-\frac{1}{\zeta-m/\bar{\zeta}_d}\right)+\mu^*\sum_{n=1}^{\infty}n(\overline{A_n^*}m^n\zeta^{-n}+A_n^*\zeta^n)\right]\frac{z+\sqrt{z^2-c^2}}{2R\sqrt{z^2-c^2}}, \tag{5}$$

$$\sigma = -\mu\frac{z+\sqrt{z^2-c^2}}{2R\sqrt{z^2-c^2}}\sum_{n=1}^{\infty}nA_{-n}\zeta^{-n-1}, \tag{6}$$

where the overbar means the complex conjugate, b is the Burgers vector, and both A_{-n} and A_n^* are constants (Zhang and Qian, 1996a). For a screw dislocation inside the substrate, stress fields within the film and substrate are given by

$$\sigma^* = \frac{z+\sqrt{z^2-c^2}}{2R\sqrt{z^2-c^2}}\mu^*\sum_{n=1}^{\infty} n(\overline{B_n^* m^n \zeta^{-n}} + B_n^*\zeta^n), \tag{7}$$

$$\sigma = \mu\left[\frac{b}{2\pi(\zeta-\zeta_d)} - \sum_{n=1}^{\infty} nB_{-n}\zeta^{-n-1}\right]\frac{z+\sqrt{z^2-c^2}}{2R\sqrt{z^2-c^2}}, \tag{8}$$

where both B_{-n} and B_n^* are constants (Zhang and Qian, 1996b). From the stress fields induced by the applied load and the dislocation(s), we can calculate the critical stress intensity factors for screw dislocation emission from the crack tip and screw dislocation dipole emission from the interface.

DISLOCATION EMISSION FROM THE CRACK

Recently, Rice (1992) re-solved the emission problem using the Peierls-Nabarro model. The critical stress intensity factor for dislocation emission from a crack tip is determined by the unstable stacking fault energy. However, the unstable stacking fault energy is not available in the literature for most materials, especially for passive films. In the present work, we emphasize how a hard or soft passive film can influence dislocation emission from the crack tip. Therefore, we determine the critical stress intensity factor for dislocation emission from the Rice-Thomson model (1974), wherein we assume that the size of the dislocation core in the film is the same as that in the substrate. Thus, the effect of the shear modulus ratio and the film thickness can be clearly demonstrated. The critical applied stress intensity factor in a two-dimensional calculation of the Rice-Thomson model is given by (Lin and Thomson, 1986)

$$K_{cri}^{crack} = -\frac{\sqrt{2\pi r_0}}{b} f(r_0), \tag{9}$$

where r_0 is the radius of the dislocation core. The nominal critical stress intensity factor is then given by

$$K_{cri}^{crack} = \frac{\mu b}{2\sqrt{2\pi r_0}} - \frac{\mu(\Gamma-1)b\sqrt{c}}{4R\sqrt{\pi}}\sum_{n=1}^{\infty}\left[\left(\frac{c+\sqrt{2cr_0}}{2R}\right)^{2n} - \left(\frac{2Rm}{c+\sqrt{2cr_0}}\right)^{2n}\right]\frac{1}{\Gamma(1-m^n)+1+m^n}. \tag{10}$$

The radius of the dislocation core is chosen as one Burgers vector in plotting the critical applied stress intensity factor for dislocation emission.

Figure 3 shows that the critical applied stress intensity factor decreases as the shear modulus ratio increases. This phenomenon becomes more significant when the film thickness is small, as shown in Fig. 3 for the film thickness of 2 b, 5 b and 10 b, where $K_{cri}^{\Gamma=1}$ is the critical applied stress intensity factor for dislocation emission from a crack tip without being covered by a film. The film thickness effect is illustrated in Fig. 4 for $\Gamma = 0.5$ and $\Gamma = 5$. As can be seen in Fig. 4, for both cases of $\Gamma = 0.5$ and $\Gamma = 5$, the influence of the film on the critical applied stress

intensity factor becomes smaller and smaller as the film thickness gets larger and larger. There are two reasons for this phenomenon. Firstly, the normalized applied stress intensity factor increases (or decreases) for $\Gamma = 5$ (or $\Gamma = 0.5$) as the film thickness decreases, as shown in Fig. 2. This means the driving force for dislocation emission becomes stronger (or weaker) for $\Gamma = 5$ (or $\Gamma = 0.5$) as the film is thinner. Secondly, if the film is harder (or softer) than the substrate the image force induced by the interface attracts (or pushes) the dislocation towards to the interface (or crack) and consequently, the total image force acting on the dislocation is smaller (or larger). As a result, the critical applied stress intensity factor for dislocation emission is smaller for a harder film or larger for a softer film, and the changes are substantial for thin films with thickness less than 20 b, as shown in Fig. 4.

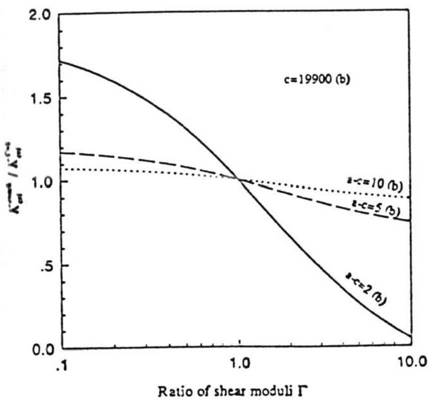

Fig. 3. The normalized critical applied stress intensity factor $K_{cri}^{crack} / K_{cri}^{\Gamma=1}$ for dislocation emission from the crack tip as a function of the shear modulus ratio for the film thickness a-c=2 b, 5 b and 10 b.

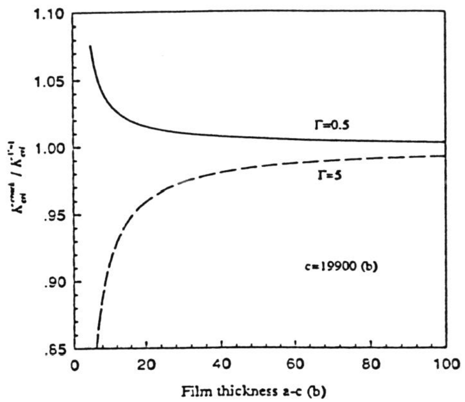

Fig. 4. The normalized critical applied stress intensity factor $K_{cri}^{crack} / K_{cri}^{\Gamma=1}$ for dislocation emission from the crack tip as a function of the film thickness for Γ=0.5 and Γ=5.

DISLOCATION DIPOLE EMISSION FROM THE INTERFACE

For a screw dislocation dipole, one dislocation is located in the film and has a Burgers vector -b, and the other is located in the substrate and has a Burgers vector b. Under external applied loadings, the force exerted on each dislocation per unit dislocation length (the unit of length is b in the present work) can be expressed in three terms

$$f = f_{app} + f_{imag} + f_{int} \tag{11}$$

where f_{app} is the force due to external applied loading, f_{imag} is the image force due to its own image dislocations and f_{int} is the force exerted by its counterpart dislocation and associate image dislocations.

By analogy to the dislocation emission from the crack tip, we use the following criterion for the emission of a dislocation dipole from the interface. Dipole emission will occur from the interface when the zero in the total force acting on one of the two dislocations occurs at a distance between the two dislocations, being equal to or smaller than the effective core size of the dislocation dipole. In the present work, the effective core size of the dislocation dipole is taken as 2 b for simplicity. Once one of the two dislocations is moved away from the interface, the distance between the two dislocations will increase and the interaction force will decrease and, consequently, its counterpart dislocation will also move away from the interface. As a result, the two dislocations are emitted from the interface simultaneously. The critical stress intensity factor for dislocation dipole emission from the interface is defined as the smaller of the two critical values calculated from the criterion for the two dislocations.

The two critical applied stress intensity factors K^*_{app} and K_{app} needed to emit the dislocations respectively in the film and substrate at 1 b away from the interface are shown in Fig. 5 as a function of the ratio of shear moduli. It is seen that K^*_{app} is always slightly smaller than K_{app}, and both increase almost linearly with the ratio of the shear moduli. Therefore, the critical applied stress intensity factor to emit the dislocation dipole from the interface is chosen as $K^{dipo}_{cri} = K^*_{app}$. Fig. 6 plots the critical applied stress intensity factor K^{dipo}_{cri} vs. the film thickness ahead of the crack tip. It is clear that increasing the film thickness will increase the critical stress intensity factor because the stress field decreases very fast with increasing distance from the crack tip. As a result, it is more difficult to emit a dislocation dipole from the interface when the film is harder and the film thickness is larger, and it is easier to emit the dipole if the film is softer and the film thickness is smaller.

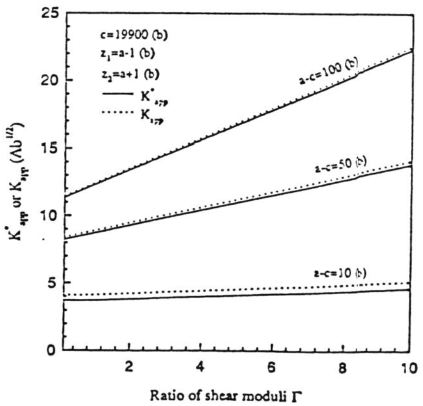

Fig. 5. The critical applied stress intensity factors needed to emit dislocations in the film and substrate at 1 b away from the interface are proportional to the ratio of shear moduli.

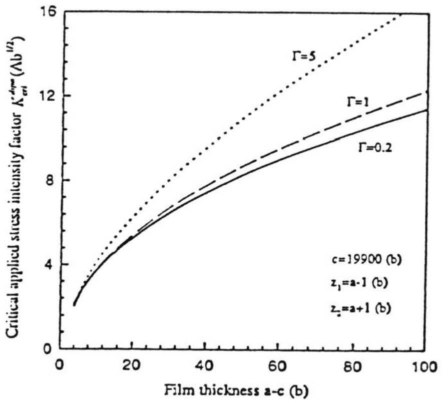

Fig. 6. The critical applied stress intensity factor needed to emit a dislocation dipole with the core size of 2 b from the interface increases with increasing the film thickness.

Fig. 7 combines the critical applied stress intensity factors K^{crack}_{cri} and K^{dipo}_{cri} respectively for dislocation emission from the crack tip with a dislocation core radius of 1 b and dislocation dipole emission from the interface with a dislocation dipole core size of 2 b. It is seen that compared with the critical applied stress intensity factor K^{crack}_{cri} for dislocation emission from the crack tip, the critical applied stress intensity factor K^{dipo}_{cri} for dislocation dipole emission from the interface is strongly affected by the film thickness. For a given film thickness, K^{crack}_{cri} is much smaller than K^{dipo}_{cri}, which means that dislocation emission from the crack tip occurs before a dislocation dipole is emitted from the interface. It is also seen from Fig. 7 that, if the film around the crack is softer than the substrate ($\Gamma<1$), both the critical applied stress intensity factors for dislocation emission from the crack tip and for dislocation dipole emission from the interface are larger than that for dislocation emission from the crack tip if there is no film covering it (i.e. $\Gamma=1$). During SCC, the film which is usually a spongy layer formed by de-alloying (Sieradzki and Newman, 1985b) may have a smaller shear modulus than the substrate, thus, the dislocation emission would be more difficult after forming the film and, consequently, the fracture would be more brittle.

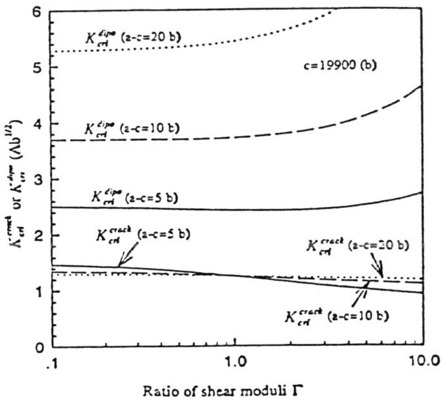

Fig. 7. Comparison of the critical applied stress intensity factors K^{crack}_{cri} and K^{dipo}_{cri} needed respectively to emit a dislocation from the crack tip and to emit a dislocation dipole from the interface.

CONCLUSIONS

For simplicity, a stress corrosion crack is modeled in the present work as a thin film-covered mode III crack. The exact solutions are obtained for both the applied stress field and the dislocation stress field. Dislocation emission from the crack tip and dislocation dipole emission from the interface between the film and the substrate have been studied. The results indicate that the crack stress field due to the applied load is enhanced by a harder film or abated by a softer film. If the film thickness is much smaller than the crack length, then, the stress intensity factor can be simply expressed as the product of the nominal stress intensity factor times the shear modulus ratio. Both the critical stress intensity factors for dislocation emission from the crack tip and dislocation dipole emission from the interface are greatly influenced by the film stiffness and thickness. Dislocation emission from the crack tip occurs prior to dislocation dipole emission from the interface. When the film is softer than the substrate, both the critical applied stress intensity factor for dislocation emission from the crack tip and the critical applied stress intensity factor for dislocation dipole emission from the interface are larger than that for dislocation emission from a crack tip without being covered by a film.

ACKNOWLEDGMENTS

Financial support from the Hong Kong Research Grants Council through an RGC grant HKUST819/96E is gratefully acknowledged.

REFERENCES

Li, J.C.M. (1963). Petch relation and grain-boundary sources, *Trans*, **AIME 227**, 239-247.

Lin, I.H. and R. Thomson (1986). Cleavage, dislocation emission, and shielding for cracks under general loading, *Acta Metall.* **34**, 187-206.

Jones, R.H. and R.E. Ricker (1992). Mechanisms of stress-corrosion cracking. In: *Stress-Corrosion Cracking* (R.H. Jones, ed.). pp. 1-40. ASM International.

Parkins, R.N. (1992). Current understanding of stress-corrosion cracking. *JOM, December issue*, 12-19.

Rice, J.R. and R. Thomson (1974). Ductile versus brittle behavior of crystals, *Phil. Mag.* **29**, 73-97.

Rice, J.R. (1992). Dislocation nucleation from a crack tip: an analysis based on the Peierls concept, *J. Mech. Phys. Solids.* **40**, 239-271.

Sieradzki, K. (1982). The Effect of thin film formation at crack tips on fracture. *Acta Metall.* **30**, .973-982.

Sieradzki, K. and R.C. Newman (1985). Brittle behavior of ductile metals during stress-corrosion cracking. *Phil. Mag.* **A51**, 95-132.

Sieradzki, K. and R.C. Newman (1987). Stress-corrosion cracking, *J. Phys. Chem. Solids* **48**, 1101-1113.

Zhang, Tong-Yi and Cai-Fu Qian (1996a). Interaction of a screw dislocation with a thin-film-covered mode III crack, *Acta Metall. Mater.*. in press.

Zhang, Tong-Yi and Cai-Fu Qian (1996b). Interaction of a thin-film-covered mode III crack with screw dislocations: emission of a screw dislocation dipole from the interface, *Mech. Mater.*. in press.