CRACK PROBLEMS IN SINGLE CRYSTALS OF HEXAGONAL STRUCTURE

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Abstract

Crack problems in single crystals of hexagonal structure are reexamined from a new perspective. It is shown that, when the crack is on the basal plane, the asymptotic forms of the elastic crack-tip fields are identical with those in orthotropic media. Equivalent inclusion method in conjunction with Eshelby's S tensor of a strongly oblate spheroid in transversely isotropic materials is used to solve penny-shaped crack problems. The stress intensity factors corresponding to uniform tension and shear are determined respectively. Griffith's energy criterion for brittle cracking and Irwin's energy release rate are discussed in the present context. Finally, the weight function for an axisymmetrically loaded penny-shaped crack is derived. It is found that the axisymmetric weight function is independent of the material constants and is identical with the isotropic case.

1. Introduction

In this article, crack problems in single crystals of hexagonal structure are reexamined from a new perspective. The crack is assumed being contained in the (0001) basal plane. We briefly review the crack-tip displacement fields in an orthotropic solid so that the definition of symbols and notation can be clarified and unified. In section 3, We explicitly show that the mathematical expressions of the elastic crack-tip fields in transversely isotropic materials are completely identical with those associated with orthotropic media. In section 4, by the method of equivalent inclusion in conjunction with Eshelby's [1] S tensor for a thin oblate spheroid in transversely isotropic materials, problems of a penny-shaped crack subjected to remote uniform loading are solved and the associated stress intensity factors are determined. Related elastic energy consideration and its connection to Griffith's [2] theory of rupture, Irwin's [3] energy release rate of the crack tip, as well as the axisymmetric weight function are analyzed and discussed.

2 Crack opening displacements in an orthotropic medium

We choose a rectangular coordinate such that three planes of elastic symmetry are coincident with the coordinate planes. The crack is on the $x_1 x_2$-plane.(i.e. the crack surface is normal to x_3 axis as shown in Fig.1.) It is known that the crack-tip displacement field can be characterized by three stress intensity factors K_I, K_{II} and K_{III} as shown in Sih and Leibowitz[4].. Specifically, the displacements of the crack surface (referring to Fig.1, with $\theta = \pi$) are

Plane symmetric deformation

$$u_1 = K_I \sqrt{\frac{2r}{\pi}} \operatorname{Re}\left\{\frac{i(\mu_1 p_2 - \mu_2 p_1)}{\mu_1 - \mu_2}\right\} \ , \ u_3 = K_I \sqrt{\frac{2r}{\pi}} \operatorname{Re}\left\{\frac{i(\mu_1 q_2 - \mu_2 q_1)}{\mu_1 - \mu_2}\right\} \ , \ u_2 = 0 \quad (1)$$

Plane skew-symmetric deformation

$$u_1 = K_{II}\sqrt{\frac{2r}{\pi}}\,\text{Re}\left\{\frac{i(p_2 - p_1)}{\mu_1 - \mu_2}\right\} \quad , \quad u_3 = K_{II}\sqrt{\frac{2r}{\pi}}\,\text{Re}\left\{\frac{i(q_2 - q_1)}{\mu_1 - \mu_2}\right\} \quad , \quad u_2 = 0 \qquad (2)$$

Anti-plane deformation

$$u_2 = K_{III}\sqrt{\frac{2r}{\pi}}\,\frac{1}{\sqrt{C_{44}C_{66}}} \quad , \quad u_1 = u_3 = 0 \qquad (3)$$

in which $p_1 = \beta_{11}\mu_1^2 + \beta_{13}$, $q_1 = \beta_{13}\mu_1 + \dfrac{\beta_{33}}{\mu_1}$, $p_2 = \beta_{11}\mu_2^2 + \beta_{13}$, $q_2 = \beta_{13}\mu_2 + \dfrac{\beta_{33}}{\mu_2}$ and Lekhnitskii's [5] complex parameters μ_1 and μ_2 are the roots (with positive imaginary part) of the following equation,

$$\beta_{11}\mu^4 + (2\beta_{13} + \beta_{55})\mu^2 + \beta_{33} = 0 \qquad (4)$$

where β_{ij} are the reduced elastic constants of compliance. In fact β_{ij} can be related to the elastic constants of stiffness C_{ij} by the following equations

$$\beta_{11} = \frac{C_{33}}{C_{11}C_{33} - C_{13}^2} \quad , \quad \beta_{13} = \frac{-C_{13}}{C_{11}C_{33} - C_{13}^2} \quad , \quad \beta_{33} = \frac{C_{11}}{C_{11}C_{33} - C_{13}^2} \quad , \beta_{55} = \frac{1}{C_{55}} \qquad (5)$$

The third Lekhnitskii's complex parameter μ_3 is given by $\mu_3 = i\sqrt{\dfrac{C_{66}}{C_{44}}}$. It is noted that complete information concerning the elastic crack tip fields can be found in [4].
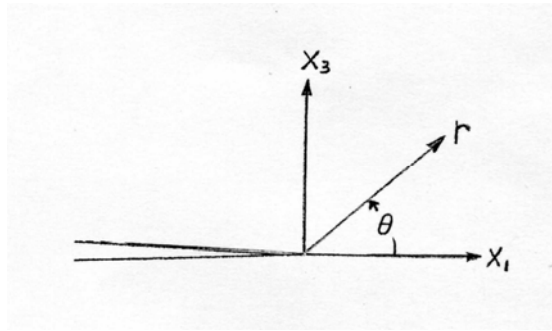

FIGURE 1. The coordinate axes and crack orientation

3. Crack tip fields for cracks on the basal plane of hexagonal crystals

Referring to Fig.1, the basal plane is parallel to the $x_1 x_2$ plane in which the crack is contained. The crack front is along the x_2-axis. Traditionally, in solving elasticity problems in a transversely isotropic material, it is expedient to introduce three material characterizing

numbers: v_1, v_2 and v_3 (Pan and Chou [6]). v_1, v_2 are the (positive) roots of the following equation

$$C_{33}C_{44}v^4 + \left[C_{13}(2C_{44} + C_{13}) - C_{11}C_{33}\right]v^2 + C_{11}C_{44} = 0 \tag{6}$$

and $v_3 = \sqrt{\dfrac{C_{66}}{C_{44}}}$. By comparing (4) and (6) with aid of (5) and noting that $C_{44} = C_{55}$ in transversely isotropic materials, we may conclude that $\mu_1 = iv_1$, $\mu_2 = iv_2$ In addition, $\mu_3 = iv_3$ is self-evident. This fact indicates that the asymptotic forms of the elastic crack-tip (displacement and stress) fields for cracks on the basal plane are identical with those shown in the preceding section. Furthermore, following identities will be useful in our subsequent analysis:

$$v_1 + v_2 = \mathrm{Im}\{\mu_1 + \mu_2\} = \left(\frac{C_{11}C_{33} - C_{13}(2C_{44} + C_{13}) + 2C_{44}\sqrt{C_{11}C_{33}}}{C_{33}C_{44}}\right)^{1/2}$$

$$v_1 v_2 = -\mu_1 \mu_2 = \sqrt{\frac{C_{11}}{C_{33}}} \, , \quad \sqrt{\frac{C_{33}}{C_{11}}}(v_1 + v_2) = \sqrt{\frac{C_{33}}{C_{11}}}\,\mathrm{Im}\{\mu_1 + \mu_2\} = \mathrm{Im}\left\{-\frac{1}{\mu_1} - \frac{1}{\mu_2}\right\}$$

4.Penny-shaped crack problems

The equivalent inclusion method is used in this section to determine the geometrical change of a penny-shaped crack under the influence of remote uniform loading. The crack is treated as the limiting form of a strongly oblate spheroidal cavity. In other words, the crack is described by

$$\frac{x_1^2}{a^2} + \frac{x_2^2}{a^2} + \frac{x_3^2}{c^2} = 1$$

with $c/a \to 0$ (see the coordinates shown in Fig.2). It is sufficient to consider two cases of applied loading σ_{33}^A and τ_{13}^A independently for the present purpose. The success of the equivalent inclusion method hinges on the determination of Eshelby's S tensor. The exact expressions for the S tensor have been derived recently by Chiang [7]. In fact only following components are needed

$$S_{1133} = S_{2233} = -\frac{\pi}{4}\left(\frac{c}{a}\right)\left[\left(\frac{1}{v_1 + v_2}\right)\left(1 - \frac{C_{13}}{C_{33}}\sqrt{\frac{C_{33}}{C_{11}}}\right)\right]$$

$$S_{3333} = 1 - \frac{\pi}{2}\left(\frac{c}{a}\right)\left[\left(\frac{1}{v_1 + v_2}\right)\left(\sqrt{\frac{C_{11}}{C_{33}}} - \frac{C_{13}}{C_{33}}\right)\right]$$

$$S_{1313} = S_{2323} = \frac{1}{2} - \frac{\pi}{8}\left(\frac{c}{a}\right)\left[\left(\frac{1}{v_1 + v_2}\right)\left(\frac{C_{11}}{C_{44}} - \frac{C_{13}^2}{C_{33}C_{44}}\right) + \sqrt{\frac{C_{66}}{C_{44}}}\right]$$
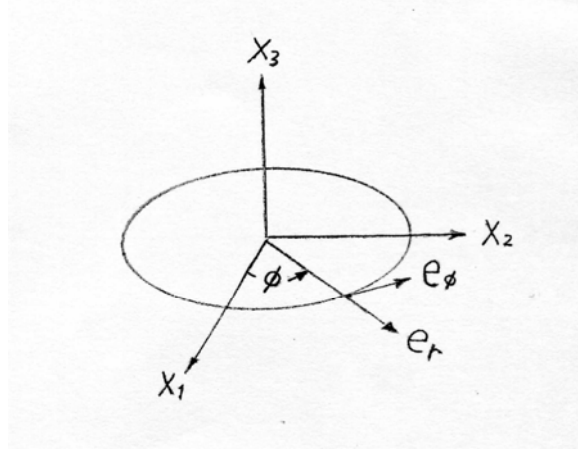
Other components can be found in [7].

FIGURE 2. The rectangular and polar coordinates

4.1 The displacement of crack surface due to σ_{33}^A

The procedure of the equivalent inclusion method has been outlined in [1,7], only relevant results are presented here. The only non-vanishing eigen strain ε_{33}^* corresponding to σ_{33}^A is determined by the following equation

$$[C_{31}S_{1133} + C_{32}S_{2233} + C_{33}(S_{3333} - 1)]\varepsilon_{33}^* = -\sigma_{33}^A \tag{7}$$

or $\varepsilon_{33}^* = \dfrac{1}{Q_I}\left(\dfrac{2a}{\pi c}\right)\sigma_{33}^A$ where $Q_I = \left(\dfrac{1}{v_1 + v_2}\right)\dfrac{C_{11}C_{33} - C_{13}^2}{\sqrt{C_{11}C_{33}}}$. In other words, the induced

displacement of the crack (upper) surface due to σ_{33}^A is

$$u_3 = \dfrac{1}{Q_I}\left(\dfrac{2a}{\pi}\right)\sqrt{1 - \dfrac{x_1^2}{a^2} - \dfrac{x_2^2}{a^2}}\,\sigma_{33}^A \;\;,\; u_1 = u_2 = 0 \tag{8}$$

Here the origin of the coordinate is at the center of the crack. Referring to the local coordinate at the edge of the crack shown in Fig.2, near the edge of the crack , the crack surface displacement is given by

$$u_3 = \dfrac{1}{Q_I}\left(\dfrac{2a}{\pi}\right)\sqrt{\dfrac{2r}{a}}\,\sigma_{33}^A \tag{9}$$

where r is the radial distance from the crack edge. Comparing (9) with the K_I displacement field in (1) and noting that

$$\text{Re}\left\{i\dfrac{\mu_1 q_2 - \mu_2 q_1}{\mu_1 - \mu_2}\right\} = \beta_{33}\,\text{Im}\left\{-\dfrac{1}{\mu_1} - \dfrac{1}{\mu_2}\right\} = \dfrac{C_{11}}{C_{11}C_{33} - C_{13}^2}\sqrt{\dfrac{C_{33}}{C_{11}}}(v_1 + v_2) \tag{10}$$

We find $K_I = \dfrac{2}{\pi}\sigma_{33}^A\sqrt{\pi a}$ which is independent of the material constants. This result has been shown through different procedures by Kassir and Sih [8].

4.2 The displacement of crack surface due to τ_{13}^A

In this case, the only non-vanishing eigen strain due to τ_{13}^A is ε_{13}^* which is determined by

$$2C_{44}\left(2S_{1313}-1\right)\varepsilon_{13}^* = -\tau_{13}^A \tag{11}$$

or $\varepsilon_{13}^* = \dfrac{1}{Q_{II}+Q_{III}}\left(\dfrac{2a}{\pi c}\right)\tau_{13}^A$ where $Q_{II} = \left(\dfrac{1}{\nu_1+\nu_2}\right)\left(\dfrac{C_{11}C_{33}-C_{13}^2}{C_{33}}\right)$ and $Q_{III} = \sqrt{C_{44}C_{66}}$. The displacement u_1 of the crack surface associated with ε_{13}^* is

$$u_1 = \dfrac{2}{Q_{II}+Q_{III}}\left(\dfrac{2a}{\pi}\right)\sqrt{1-\dfrac{x_1^2}{a^2}-\dfrac{x_2^2}{a^2}}\,\tau_{13}^A \tag{12}$$

Here the origin of the coordinate is at the center of the crack. Referring to the local coordinate at the edge of the crack (Fig.2) and resolving the displacement into radial and circumferential components, i.e. $u_1\cos\phi$ and $-u_1\sin\phi$. Then, the near-edge crack surface displacement can be written as

$$u_r = \dfrac{2}{Q_{II}+Q_{III}}\cdot\dfrac{2}{\pi}\sqrt{2ar}\,\tau_{13}^A\cos\phi \quad , \quad u_\phi = \dfrac{-2}{Q_{II}+Q_{III}}\cdot\dfrac{2}{\pi}\sqrt{2ar}\,\tau_{13}^A\sin\phi \tag{13}$$

By writing (2) and (3) in terms of the coordinates e_r and e_ϕ in Fig.2, we find

$$u_r = K_{II}\sqrt{\dfrac{2r}{\pi}}\cdot\dfrac{1}{Q_{II}} \quad , \quad u_\phi = K_{III}\sqrt{\dfrac{2r}{\pi}}\cdot\dfrac{1}{Q_{III}} \tag{14}$$

By comparing (13) and (14) we may conclude that

$$K_{II} = Y_{II}\dfrac{2}{\pi}\tau_{13}^A\sqrt{\pi a}\cdot\cos\phi \quad , \quad K_{III} = -Y_{III}\dfrac{2}{\pi}\tau_{13}^A\sqrt{\pi a}\cdot\sin\phi \tag{15}$$

where $Y_{II} = 2Q_{II}/(Q_{II}+Q_{III})$ and $Y_{III} = 2Q_{III}/(Q_{II}+Q_{III})$. Numerical results for Y_{II} and Y_{III} of several hexagonal crystalline elements are given in Table 1. It is noted that $Y_{II}+Y_{III} = 2$. and for transversely isotropic materials $C_{66} = (C_{11}-C_{12})/2$. When the material is isotropic, we have the known result[8,9]

$$Y_{II} = \dfrac{2}{2-\nu} \quad , \quad Y_{III} = \dfrac{2(1-\nu)}{2-\nu} \tag{16}$$

where ν is the Poisson's ratio of the material.

TABLE 1. Numerical results of Y_{II} and Y_{III} for some hexagonal crystals. Elastic constants are taken from Reid[10]

Material	C_{11}/GPa	C_{12}/GPa	C_{13}/GPa	C_{33}/Gpa	C_{44}/GPa	Y_{II}	Y_{III}
Be	292.3	26.7	14.0	336.4	162.5	1.0244	0.9756
C(Graphite)	1160	290	109	46.6	2.3	1.1779	0.8221
Mg	59.52	25.6	21.4	61.74	16.47	1.1937	0.8063
Ti	162.4	92.0	69.0	180.7	46.7	1.2505	0.7495
Co	306.3	165.1	101.9	357.4	75.3	1.2611	0.7389

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5. Energy change due to the presence of a crack

Again, we assume only σ_{33}^A and τ_{13}^A are present, so the potential energy reduction can be written as

$$\Delta U = \underset{c/a \to 0}{Lim} \frac{1}{2} \iiint_{cavity} \left(\sigma_{33}^A \varepsilon_{33}^* + 2\tau_{13}^A \varepsilon_{13}^*\right) dV = \frac{8}{3} a^3 \left(\frac{\left(\sigma_{33}^A\right)^2}{2Q_I} + \frac{\left(\tau_{13}^A\right)^2}{Q_{II} + Q_{III}} \right) \tag{17}$$

On the other hand, forming a penny-shaped crack of radius a, the material will increase the (surface) energy by $2\pi a^2 \Gamma$ where Γ is the surface energy per unit area. According to Griffith's fracture model, the critical condition is governed by

$$\frac{\partial}{\partial a}\left(-\Delta U + 2\pi a^2 \Gamma\right) = 0 \tag{18}$$

This leads to the critical stress condition

$$\frac{\left(\sigma_{33}^A\right)^2}{2Q_I} + \frac{\left(\tau_{13}^A\right)^2}{Q_{II} + Q_{III}} = \frac{\pi \Gamma}{2a} \tag{19}$$

Obviously the above equation is meaningful only when σ_{33}^A is positive(tension).When σ_{33}^A is compressive, the first term in (19) should be ignored if the crack surface is frictionless. Equation(19) indicates that the failure surface plotted in the stress space $\left(\sigma_{33}, \tau_{13}\right)$ is an ellipse whose size is proportional to the inverse of the crack size. Nevertheless, the validity of (19) is very restricted since the presence of τ_{13}^A tends to cause the crack to grow in an asymmetric manner.

6. Energy release rate

Irwin [10] has proposed an energy criterion for the crack growth which turns out to have more advantages than Griffith's model in terms of engineering applications. The energy release rate (crack extension force) G is defined as the energy change during an increment of crack extension. If the penny-shaped crack is assumed to grow quasi-statically on the basal plane, the crack-tip stress and displacement fields allow us to establish the connection

between the energy release rate G and the stress intensity factors by the crack closure work calculation as follows

$$G = \underset{\Delta a \to 0}{Lim} \frac{2}{\Delta a} \int_0^{\Delta a} \frac{1}{2} \left[\sigma_{33}(r)u_3(r - \Delta a) + \tau_{31}(r)u_1(r - \Delta a) + \tau_{32}(r)u_2(r - \Delta a) \right] dr$$

$$= G_I + G_{II} + G_{III} = \frac{v_1 + v_2}{2} \beta_{33} \sqrt{\frac{C_{33}}{C_{11}}} K_I^2 + \frac{v_1 + v_2}{2} \beta_{11} K_{II}^2 + \frac{1}{2\sqrt{C_{44}C_{66}}} K_{III}^2 \qquad (20)$$

Now, if we assume that the crack would grow when G reaches a critical value (e.g. under the influence of σ_{33}^A and τ_{13}^A , the crack start propagating at $\phi = 0°$ and $180°$ in Fig.2) then substituting the stress intensity factors found in section 4 into (20) we have

$$\frac{\left(\sigma_{33}^A\right)^2}{2Q_I} + \frac{\left(\tau_{13}^A\right)^2}{\left(Q_{II} + Q_{III}\right)^2 / 2Q_{II}} = \frac{\pi G_c}{4a} \qquad (21)$$

It is noted that when $\tau_{13}^A = 0$, (21) is identical with (19) if G_c is identified with 2Γ as expected. Like equation (19), (21) indicates that the failure surface is an ellipse. Since for all hexagonal crystals $Q_{II} > Q_{III}$, critical value of τ_{13}^A predicted by (21) is always lower than that by (19) when keeping other parameters fixed. This implies that the crack has a tendency to grow asymmetrically when τ_{13}^A is present. Furthermore, it should be recognized that in addition to the surface energy, in real materials other physical process such as plastic deformation should be taken into account in the estimate of G_c .

7. The weight function for an axisymmetrically loaded crack

The concept of weight function originated by Bueckner [11] and re-interpreted by Rice [12] has provided a convenient method to calculate the stress intensity factors once a reference solution is available. In this section, the result of axisymmetrically loaded cracks is derived. Let $K_I^{(1)}$ and $K_I^{(2)}$ denote the stress intensity factors of a penny-shaped crack subjected to two different loading conditions respectively. In the absence of body forces, using Betti's reciprocal theorem with a virtual crack extension δa , we have

$$\pi a \left(v_1 + v_2\right) \beta_{33} \sqrt{\frac{C_{33}}{C_{11}}} K_I^{(1)} K_I^{(2)} = \iint T^{(1)} \frac{\partial u^{(2)}}{\partial a} dS \qquad (22)$$

where S is the crack surface. $T^{(1)}$ is the (normal) traction of loading-(1) and $u^{(2)}$ is the displacement (along x_3 axis) of the crack surface due to loading-(2) .

If we identify loading- (2) with the uniform pressure over the crack surface, then we find

$$K_I^{(1)} = \frac{1}{\pi a \sqrt{\pi a}} \iint \frac{T^{(1)}}{\sqrt{1 - \left(\dfrac{r}{a}\right)^2}} dS = \frac{2}{\sqrt{\pi a}} \int_0^a \frac{T^{(1)} r dr}{\sqrt{a^2 - r^2}} \qquad (23)$$

Equation (23) is independent of the material constants and in fact is identical with isotropic case[8]. With (23) the stress intensity factors for any arbitrary axisymmetric loading can be evaluated by a simple integration.

8. Concluding remarks

It has been shown in this article that the asymptotic forms of elastic crack-tip fields of cracks on the basal plane are identical with those for orthotropic media. Furthermore, it should be pointed out that when the crack is oriented with x_1-x_3 being the basal plane (Fig.1) then the elastic crack-tip fields become identical with those in isotropic materials as this situation corresponds to a degenerate case of orthotropic media.

Under small-scale-yieldng conditions, the size of the plastic zone is governed by the local stress intensity factors. For a penny-shaped crack subjected to pure shear stress τ_{13}^A, the plastic zone surrounding the crack border has been determined [13] by assuming the plastic zone is restricted on the basal plane. On the other hand when σ_{33}^A is present, the situation becomes very complicated since pyramidal and/or prismatic slip modes other than basal slip mode may be activated. This complicated problem is currently under investigation. The results will be reported in due time.

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