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Fracture Behavior of a Completely Brittle Crack in Consideration of Restraining Stress between Atomic Planes

原子面間結合力を考慮した完全ぜい性き裂の破壊挙動

Yutaka SASAKI, Yutaka SATO and Katsuhiko WATANABE
佐々木 裕*・佐 藤 裕**・渡 辺 勝 彦**

1. Introduction

The so-called ideal cleavage strength of a solid is usually estimated by considering the restraining stress between atomic planes[1]. Similarly the behavior of a completely brittle crack may, in principle, be subject to the atomic restraining stress in crack plane. We can suggest that a crack grows when the atomic restraining stress at crack-tip becomes irreversible with the increase of an external force. But this idea has been used only conceptually and we have seen few analyses which actually follow the change of the atomic restraining stress to estimate the behavior of a crack in continuum. In this study, using the discontinuous model proposed previously[2], we try the finite element analyses of crack behavior considering the restraining stress between atomic planes. Through the results we show some fundamental issues about completely brittle fracture, and make clear the meanings and roles of fracture mechanics parameters such as stress intensity factor etc..

2. Modeling of a Completely Brittle Crack by Discontinuous Model

2. 1 Discontinuous Model

Consider a two-dimensional problem. Figure 1 shows the situation in which a discontinuous plane is considered ahead of a notch whose radius of curvature is ρ. In the discontinuous model, a plane before deformation (Fig. 1(a)) is stretched after deformation (Fig. 1(b)), and it can be a model for analysis when some constitutive relation compatible with the one for continuum parts is given for the plane[2]. The strain in the discontinuous plane cannot be defined in the same way as for continuum parts. Therefore we introduce a characteristic length $\lfloor h \rfloor = \lfloor h_{22}\ h_{21} \rfloor$, and define *strain-like* quantities as

$$\tilde{\varepsilon}_{11} = \frac{1}{2}\frac{\partial}{\partial X_1}(u_1^+ + u_1^-)$$

$$\tilde{\varepsilon}_{22} = \frac{1}{h_{22}}(u_2^+ - u_2^-) \qquad (1)$$

$$\tilde{\gamma}_{21} = \frac{1}{2h_{21}}(u_1^+ - u_1^-) + \frac{1}{2}\frac{\partial}{\partial X_1}(u_2^+ + u_2^-)$$

Here, u_1^+, u_1^-, u_2^+ and u_2^- are the displacements on the upper and lower planes in X_1 and X_2 derections, respectively. When we employ an appropriate constitutive equation between these *strain-like* quantities and the stresses for the discontinuous plane, and, as to the continuum parts, employ an ordinary constitutive relation, the discontinuous model can be analized actually[2].

2. 2 Introduction of a Constitutive Relation Representing the Atomic Restraining Stress

In the model in Fig. 1, suppose that the continuum parts are linear elastic and only Mode I load is applied hereafter (symmetric about the discontiniuous plane), and let's try to introduce a constitutive relation representing the atomic restraining stress into the discontinuous plane. That is, suppose that the quantity corresponding to Poisson's ratio is zero for simplicity and, the relation between the restraining stress σ_{22} and the *strain-like* quantity $\tilde{\varepsilon}_{22}$ is given, as shown in Fig. 2, by

$$\sigma_{22} = \begin{cases} \sigma_{max}\sin(2\pi\tilde{\varepsilon}_{22}/\lambda), & \text{if } (0 \leq \tilde{\varepsilon}_{22} \leq \lambda/2) \\ 0, & \text{if } (\lambda/2 < \tilde{\varepsilon}_{22}) \end{cases} \qquad (2)$$

Here, λ is the wave length of sinusoidal function, and σ_{max} is the ideal cleavage strength. Since the values of

*NTT DATA Communication Systems Corporation
**Dept. of Applied Physics and Applied Mechanics, Institute of Industrial Science, University of Tokyo

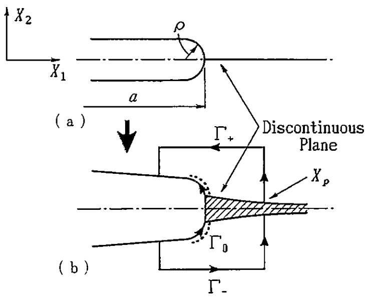

Fig. 1 Discontinuous Crack Model

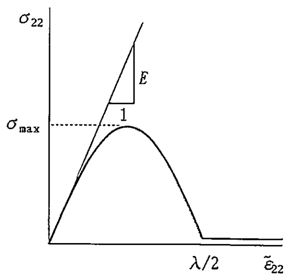

Fig. 2 Relation between *Strain-like* Quantity $\tilde{\varepsilon}_{22}$ and Restraining Stress

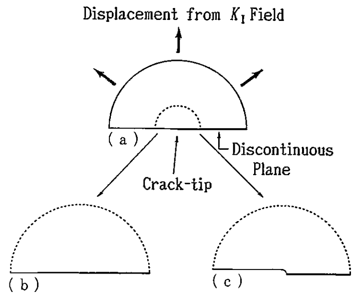

Fig. 3 Crack Model for Analyses

σ_{11} and σ_{12} are comparatively small (σ_{12} will be zero for symmetry), the relation between σ_{11} and $\tilde{\varepsilon}_{11}$, and that between σ_{12} and $\tilde{\gamma}_{21}$ can be assumed to be linear.

As to the characteristic length h_{22} through which the *strain-like* quantity $\tilde{\varepsilon}_{22}$ is defined, it should be noted that physically it corresponds to the distance between atomic planes in the unstressed state as $\delta_{22}=u_2^+-u_2^-$ is equal to the relative displacement between atomic plancs in the stressed state. The same may be said of h_{21}.

2. 3 Crack Parameters

The conventional crack parameters are defined for the continuum with a completely sharp crack ($\rho=0$) under a particular consititutive relation. In order to remove these restrictions, the *CED* (*Crack Energy Density*) was proposed as a crack parameter which always has a clear physical meaning[3]. So, we will discuss the matter centering the *CED*. The *CED* is defined as "the work done per unit area in the plane containing crack front line during deformation, that is, the strain energy area density". The *CED* $\mathscr{E}$ at the crack-tip of the model in Fig. 1 is given by

$$\mathscr{E}=\mathscr{E}^*+\mathscr{E}^N \tag{3}$$

$\mathscr{E}^*$ is the contribution from the stretched discontinuous plane, and $\mathscr{E}^N$ is the contribution from the notch-tip path Γ_0 in Fig. 1. When $\phi(t)$ is the crack-tip opening displacement at the time *t*, and σ^* (δ_{22}) is the restraining stress as the function of the relative displacement δ_{22}, $\mathscr{E}^*$ is given by

$$\begin{aligned}\mathscr{E}^* &= \int_0^{\phi(t)} \sigma^*(\delta_{22})\, d\delta_{22} \\ &= \left(\frac{\lambda}{2\pi}\right)^2 E h_{22}\left(1-\cos\frac{2\pi\phi(t)}{\lambda h_{22}}\right)\end{aligned} \tag{4}$$

considering that E is Young's modulus and $\sigma^*(\delta_{22})$ is given by Eq. (2). On the other hand, $\mathscr{E}^N$ is given by

$$\mathscr{E}^N=\int_{\Gamma_0} W dX_2 \tag{5}$$

when W is the strain energy density. It is noteworthy that the value of $\mathscr{E}^*$ becomes equal to the surface energy $2\gamma_S$ when the *strain-like* quantity $\tilde{\varepsilon}_{22}$ reaches $\lambda/2$.

While $\mathscr{E}$, $\mathscr{E}^*$ and $\mathscr{E}^N$ can be evaluated directrly from the equations above, especially $\mathscr{E}$ can be evaluated also by the following path-independent integral[4].

$$\begin{aligned}\mathscr{E}_J &= J \\ &= \int_{\Gamma_-+\Gamma_+} (W dX_2 - T_i u_{i,1} d\Gamma) \\ &\quad + \int_0^{\delta(X_p)} \sigma^*(\delta_{22})\, d\delta_{22}\end{aligned} \tag{6}$$

Here, $\Gamma_-+\Gamma_+$ is an arbitrary path surrounding the crack-tip in Fig. 1. T_i and u_i are the surface traction and the displacement on the path $\Gamma_+ + \Gamma_-$, respectively, and δ_{22} (X_p) is the relative displacement at the point X_p.

When we define $\mathscr{E}_K$ as the *CED* for a completely sharp crack in a linear elastic solid, the relation among $\mathscr{E}_K$, energy release rate $\mathscr{G}$ and stress-intensity factor K

$$\mathscr{E}_K=\mathscr{G}=\frac{(1-\nu^2)K^2}{E} \tag{7}$$

holds for plane strain state[5]. Here, ν is Poisson's ratio.

3. Finite Element Analyses and Evaluation of Crack Parameter

3. 1 Object and Method for Analyses

In order to analize crack behaviors in the atomic size order, we pay attention to the limited small region around crack-tip, and plane strain analyses of the region are carried out by applying the displacement field prescribed by Mode I stress-intensity factor K on the boundary. Since the non-linear region is very small, it is thought to be natural to assume the K field in the region surrounding the non-linear region. Taking account of the symmetrical character, the semi-circular region shown in Fig. 3(a) is taken as the object for analyses. The discontinuous plane of which the constitutive relation is given by Eq. (2) is inserted ahead of the crack front. Two kinds of analyses are carried out. A completely sharp crack, and a notch with a finite radius of curvature ρ in the unstressed state are supposed in Figs. 3(b) and 3(c), respectively. Since an actual crack in a solid often exsists with some width, the model in Fig. 3(c) may be more actual.

Taking the fact stated in Sec 2.2 into consideration, the characteristic length of the discontinuous plane h_{22} is 0.4×10^{-6}mm (atomic size order). The distance from crack-tip to the boundary R is $250\times h_{22}$, and the radius of curvature ρ in Fig. 3(c) is 0.4×10^{-6}mm. The minimum mesh size around the crack-tip is set about a quarter of the distance between atomic planes in the unstressed state so that we can follow the non-linear behavior near the crack-tip. Four-noded isoparametric elements and four-noded discontniuous plane elements with three Gauss integrating points are employed for the continuum parts and for the discontinuous plane, respectively.

3. 2 Results of Analyses

Figure 5 shows the relation between *CED* and K that plays the role of parameter of external force. In the figure, $\mathscr{E}_J$ and $\mathscr{E}^*$ are the results by the path-independent integral Eq.(6) and Eq.(4) through the crack-tip opening displacement, respectively, and $\mathscr{E}_K$ is the result by Eq.(7) and means the *CED* which is expected to be obtained when $\rho=0$ and the discontinuous plane is not considered. Essentially $\mathscr{E}^*$ and $\mathscr{E}_J$ should take the same value, and it is considered that $\mathscr{E}^*$ is estimated smaller than $\mathscr{E}_J$ here because the quantities near the crak tip are apt to be estimated smaller than the true values in the finite element analysis. So, it is resonable to regard $\mathscr{E}_J$ as more exact solution. The difference between $\mathscr{E}_J$ and $\mathscr{E}_K$ is caused by the non-linearity near the crack-tip.

Figure 5 shows the variation of each *CED* with the increase of the external force parameter K for the case of Fig. 3(c). Here, $\mathscr{E}^*+\mathscr{E}^N$ should take the same value as that of $\mathscr{E}_J$ by the path-independent integral, and it is thought that $\mathscr{E}^*+\mathscr{E}^N$ is evaluated to be smaller because the values near the crack-tip are used directly. So, $\mathscr{E}_J$ is regarded as more exact solution of *CED*. $\mathscr{E}_K$ is evaluated by Eq.(7) in the same way as in Fig. 4.

4. Fracture Criterion of a Completely Brittle Crack and Meaning of Fracture Mechanics Parameter

4. 1 Fracture of a Completely Sharp Crack

It is seen from Fig. 4 that the following relation holds taking also Eq. (8) into acount.

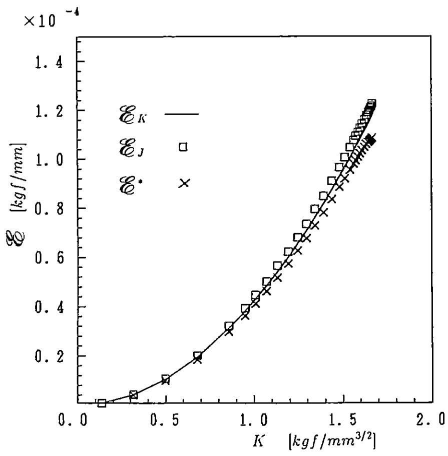

Fig. 4 *CED* Value with load (ρ=0mm)

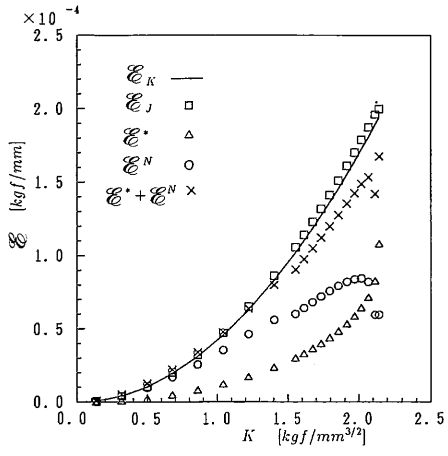

Fig. 5 *CED* Value with load ($\rho=0.4\times10^{-6}$mm)

$$\mathscr{E}^*(=\mathscr{E}=\mathscr{E}_J)\approx\mathscr{E}_K=\frac{(1-\nu^2)K^2}{E}=\mathscr{G} \tag{8}$$

It is expected that this relation holds generally taking account of the path independency of J-integral and the fact that the difference of the situation near the crack-tip has little influence on the region far from the crack-tip. So, it can be said that our expectation was confirmed through numerical analyses. In the crack model here, it is supposed that the deformation at the crack-tip becomes irreversible when the *strain-like* quantity $\tilde{\epsilon}_{22}$ reaches $\lambda/2$, that is, $\mathscr{E}^*$ creaches the surface energy $2\gamma_S$. Therefore, the relation that $\mathscr{E}^*=2\gamma_S$ $(=\mathscr{E}_c^*)$ is clearly the necessary and sufficient condition of fracture. When K_c^* and $\mathscr{G}_c^*$ are the values of K and $\mathscr{G}$, respectively, at the time when $\mathscr{E}^*$ reaches $2\gamma_S$, we have the relation

$$\mathscr{E}_c^*=2\gamma_S\approx\frac{(1-\nu^2)K_c^{*2}}{E}=\mathscr{G}_c^* \tag{9}$$

by considering Eq. (8), and this implies that K_c^* and $\mathscr{G}_c^*$ can be regarded almost constant since $2\gamma_S$ takes a value peculiar to a material (exactly speaking, K_c^* and $\mathscr{G}_c^*$ are dependent on the shape of specimen and boundary condition) and that the condition almost equivalent to the necessary and sufficient condition of fracture $\mathscr{E}^*=2\gamma_S$ is given by

$$\mathscr{G}=2\gamma_S \text{ or } K=\sqrt{\frac{2E\gamma_S}{1-\nu^2}} \tag{10}$$

The exsistence of the K stress field around the crack-tip is usually emphasized as the meaning of K. However, the reason why K is available as a crack parameter although the situation at the crack-tip is completely defferent from that of K field (actualy σ_{22} at the crack-tip in the discontinuous plane begins to decrease in the neighborhood of $K=1.0\text{kgf/mm}^{3/2}$ in Fig. 4) is that the relation of Eq. (8) holds, that is, there exists the one-to-one correspondence between K and $\mathscr{E}^*$ that has the clear phisical meaning and reflects the actual situation of the crack-tip, and this fact is most essential to explain the meaning of K (the same is said of $\mathscr{G}$).

The relation of Eq. (10) is so-called Griffith's brittle fracture criterion, and this condition has been thought of generally as the necessary condition of fracture. However, through the above argument we can find that this condition is also the condition corresponding to the sufficient condition.

4.2 Fracture of a Notch Type Crack

Figure 5 shows that the following relation holds.

$$\mathscr{E}(=\mathscr{E}^*+\mathscr{E}^N=\mathscr{E}_J)\approx\mathscr{E}_K=\frac{(1-\nu^2)K^2}{E}=\mathscr{G} \tag{11}$$

It can be expected in the same way as for Eq. (8) that this relation holds generally. Also in this case, $\mathscr{E}^*=2\gamma_S$ $(=\mathscr{E}_c^*)$ is the necessary and sufficient condition of fracture, and when we represent the value $\mathscr{E}^N$ at the time when $\mathscr{E}^*=2\gamma_S$ by $2\gamma_N$, this condition can be expressed also by

$$\mathscr{E}=2(\gamma_S+\gamma_N)\,(=\mathscr{E}_c) \tag{12}$$

When K_C and $\mathscr{G}_C$ are the values of K and $\mathscr{G}$ at the time when Eq. (12) holds, we have the relation

$$\mathscr{E}_C=2(\gamma_S+\gamma_N)\approx\frac{(1-\nu^2)K_c^2}{E}=\mathscr{G}_C \tag{13}$$

from Eq. (11), and this implies that the condition almost equivalent to the necessary and sufficient condition of fracture Eq. (12) is given by

$$\mathscr{G}=2(\gamma_S+\gamma_N) \text{ or } K=\sqrt{\frac{2E(\gamma_S+\gamma_N)}{1-\nu^2}} \tag{14}$$

It should be noted here that γ_S is dependent on the value of ρ, therefore, when ρ is not constant, K_C and $\mathscr{G}_C$ are not constant either, and this may cause the scatter of the value of K_C or $\mathscr{G}_C$ in the evaluation of fracture toughness of brittle crack.

5. Conclusion

By using the discontinuous model, we showed that it is possible to analize the crack behavior of a completely brittle crack in consideration of the restraining stress between atomic planes and obtained some fundamental knowledges about the brittle fracture and the roles of fracture mechanics through the results of the finite element analyses.

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