Numerical Simulation of Ductile Crack Initiation in Metallic Material Using Interface Element Based on Lennard-Jones Type Potential Function †

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Abstract

The fracture behavior of a cracked body is characterized by the property of the plastic zone in small scale yielding conditions and process zone in large scale yielding conditions. Based on the Lennard-Jones type potential function, an interface crack model (ICM) was proposed for the analysis of fracture behavior of ductile materials in this report. The local J-integral along the interface elements was defined as a critical parameter for crack initiation. The new crack surface will form when the applied J-integral far from the crack tip equals the critical local J-integral. A center-cracked specimen with a/W=0.5 is numerically analyzed making use of the ICM. The effects of the parameters in the ICM on the relationship of the local J-integral and the far J-integral were numerically investigated.

KEY WORDS: (Fracture Mechanics) (Interface Element) (J-integral)

1. Introduction

It is well known from the Linear Elastic Fracture Mechanics (LEFM) that the stresses at the crack tip are infinite. The LEFM was originally developed to deal with the fracture phenomena of metallic materials with high strength and brittle materials like ceramics, glasses and rocks for which the plastic deformation is negligible. However, plastic deformation is generally observed in metallic materials even when the failure is a typical brittle fracture. The plastic deformation occurs in the region where the stresses exceed the yielding strength of the material. In order to deal with plastic deformation near the crack tip, the concept of LEFM is slightly modified for small scale yielding problems. When the materials are ductile, as most of the structural steels, the size of the plastic zone exceeds the limits of LEFM. For this kind of problem, the Elastic-Plastic Fracture Mechanics (EPFM) with J-integral and CTOD concept were developed[1-3].

In the LEFM, the energy dissipation due to the crack propagation occurs in an infinitesimal zone at the crack tip, where the stress field is assumed to be infinite. On the other hand, in real materials, the energy is dissipated in a process zone ahead of the crack tip during the process of crack growth. The size of the process zone is finite and the stress field in this zone is limited by the plastic deformation. The nonlinear fracture mechanics uses a semi-empirical approach in large scale yielding. Asymptotic analyses of steady state crack growth based on continuum mechanics have shown that crack growth changes the stress and deformation in the near-tip field[4,5].

Recently, considerable attention is drawn to the microscopic fracture process. For the elastic-plastic materials, experimental investigations have shown that the fracture process is restricted very near to the crack tip. Based on the Dugdale model for crack tip plasticity, the cohesive zone model was popularly used to model the ductile fracture, postulating that the traction acting on the separating surface in the so-called fracture process zone represents the effect of atomic or molecular attractions[6].

Based on the fact that surface energy must be supplied for the formation of a new surface, a new model to describe the fracture phenomena was recently proposed[7]. In this model, the mechanism of energy dissipation is embedded in the interface element using a surface energy function. A Lennard-Jones type potential function is employed as the surface energy function. Such interface elements are arranged along the crack propagation path within the specimen modeled using conventional finite elements. This method has been applied to peeling tests of bonded plates, push-out tests of fibers in a matrix, dynamic crack propagation and

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ductile tearing of steel plate. Though it is simple, it is a very versatile method to simulate the initiation and the propagation of various types of cracks.

In this report, the mechanical behavior of the plastic zone in small scale yielding and that of process zone in larger scale yielding are closely examined. Based on the computed results of J-integral and CTOD, an interface crack model (ICM) is proposed to predict the initial fracture toughness of metallic materials under the conditions ranging from small scale yielding to large scale yielding.

2. Crack Tip Plasticity and Process Zone

It is very fundamental but difficult to give a proper description of plastic zone size and shape in small scale yielding. Although the finite element method and experimental method can be used to verify the plastic zone size more effectively, the classic models of plastic zone can give a very good profile about the plastic zone. Based on the fact that the most typical brittle fracture of metallic materials are accompanied by some plastic deformation, the size of the plastic zone and the stress distribution near crack tip can be determined. There are two theories to estimate the plastic region size in the vicinity of crack tip, namely, Irwin's plastic zone and Dugdale's plastic zone as shown in **Fig.1**.

Irwin's analysis of plastic zone size attempts to account for the fact that the stress above the yield stress σ_0 cannot be cut off in a simple manner. For the analysis to be straightforward there are several restrictions: the plastic zone shape is considered to be circular, only the section along the x-axis is analyzed, and the material is considered to be elastic-perfectly plastic. The plastic size is determined by Eq.(1).

$$r_y = \frac{1}{\pi}\frac{EJ}{\sigma_0^{\,2}} \qquad (1)$$

where, r_y is the plastic zone size in x-direction, E the Young's module and J the J-integral.

Dugdale analysis assumes that all plastic deformation concentrates in a strip ahead of the crack, i.e. the strip yield model. Dugdale continued with the argument that a stress singularity does not exist at the notional crack tip, since the stress does not go higher than the yield stress if the material is elastic-perfectly plastic. According to the Dugdale's analysis, the plastic zone size is,

$$r_y = \frac{\pi}{8}\frac{EJ}{\sigma_0^{\,2}} \qquad (2)$$

The Dugdale's plastic zone is somewhat larger than the diameter of the plastic zone proposed by Irwin.

The size of the plastic zone discussed above is derived for the plane stress state with a selected plastic zone shape. According to the classical yielding criteria, the plastic zone shapes under the small yielding condition are given by the following equations.

$$r(\theta) = (\frac{1}{2} + \frac{3}{2}\sin^2\theta + \frac{1}{2}\cos\theta)r_y \qquad \text{plane stress} \qquad (3)$$

$$r(\theta) = [\frac{3}{4}\sin^2\theta + \frac{1}{2}(1-2\nu)^2(1+\cos\theta)]r_y \qquad \text{plane strain} \qquad (4)$$

It can be seen from Fig.1 that the shape of the plastic zone changes significantly with the stress state. In the x axial (θ=0), the size of plastic zone along the x-axis is $1.0r_y$ in the plane stress state and $0.11r_y$ in the plane strain state. In general, the stress state in real structures is located between the plane stress and the plane strain, and the plastic zone shape and size change between plane stress and plane strain state, i.e. $1.0\text{-}0.11r_y$

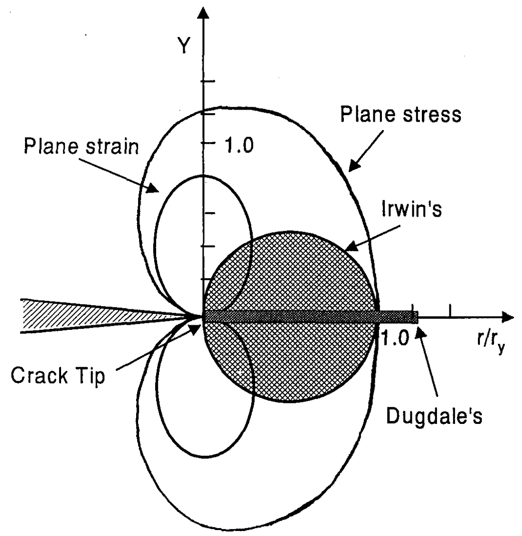

Fig.1 The profile of plastic zone size in different models of small scale yielding

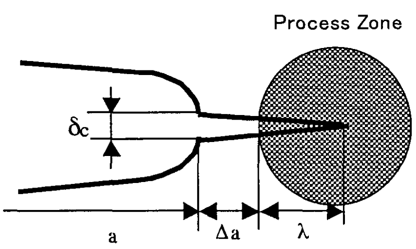

Fig.2 The process zone with large damage in large scale yielding condition

along the crack plane.

In large scale yielding condition, the plastic zone is as larger as the macro crack size and considerable damage occurs near the crack tip. Experimental investigations have shown that the fracture process is restricted very near to the crack tip. The so-called process zone shown in **Fig.2** was proposed to describe the feature in this damage region. In elastic-plastic fracture mechanics, it is generally assumed that a process zone will be formed and grow around the crack tip with the increase of the external loads acting on a cracked body. The classical fracture theory based on conventional continuum mechanics does not consider the behavior of the microscopic fracture nor its effect on the crack extension. Simply it is assumed that stress fields out of the process zone can control the fracture process. Recently, much attention is drawn to modeling the so-called process zone both in metallic materials and in nonmetallic materials.

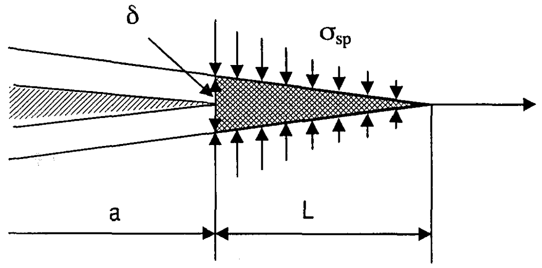

Fig.3 The interface crack model (ICM) with interface element in distance L

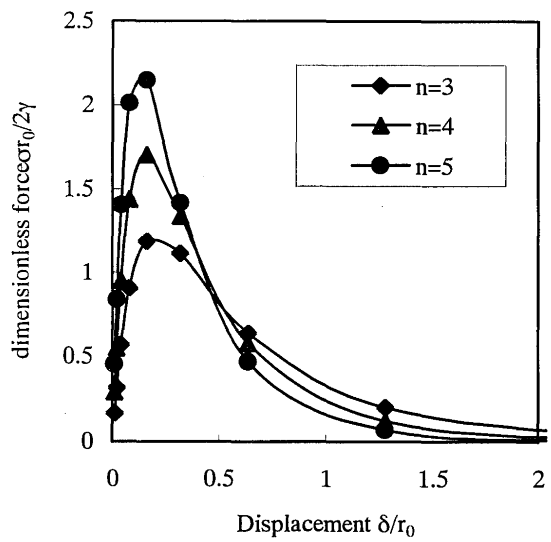

Fig.4 The separation force between crack surfaces in Interface Crack Model

3. Interface Crack Model (ICM)

In order to simulate the crack initiation of the metallic materials, an interface crack model is introduced and illustrated in **Fig.3**. A zip-fastener strip joining the two elastic-plastic solids represents the crack formation. In general, the traction across the strip is taken to be a function of the accumulation of micro-cracking and void growth. The interface elements introduced in the model consist of two surfaces and have no thickness when the load is not acting. When the load is applied, the two surfaces separate from each other.

The distance between the surfaces is denoted by δ. The mechanical characteristics of the interface element are defined through a potential function $\phi(\delta)$. The Lennard-Jones type potential energy function is employed in this report, i.e.

$$\phi(\delta) = 2\gamma\left\{\left(\frac{r_0}{r_0+\delta}\right)^{2m} - 2\left(\frac{r_0}{r_0+\delta}\right)^{m}\right\} \tag{5}$$

where, the parameters γ, m and r_0 are the material constants. In particular, 2γ is the surface energy per unit area.

By taking the derivative of $\phi(\delta)$, the relation between the traction σ and the separation δ at the interface which is gradually opening is derived as shown by Eq.(6).

$$\sigma(\delta) = \frac{4\gamma m}{r_0}\left\{\left(\frac{r_0}{r_0+\delta}\right)^{m+1} - 2\left(\frac{r_0}{r_0+\delta}\right)^{2m+1}\right\} \tag{6}$$

The traction reaches its maximum when the separation becomes δ_m given by Eq.(7).

$$\frac{\delta_m}{r_0} = \left[\left(\frac{2m+1}{m+1}\right)^{\frac{1}{m}} - 1\right] \tag{7}$$

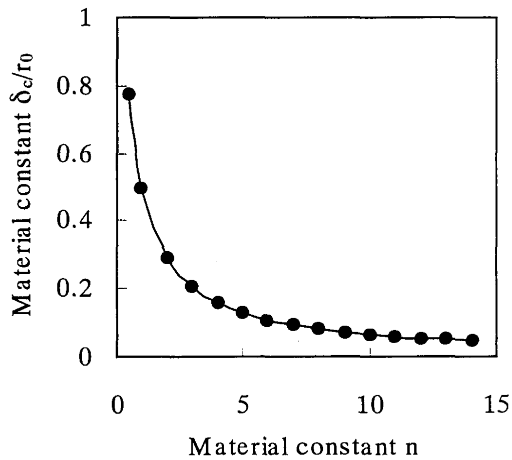

Fig.5 The critical value of displacement at maximum traction in Interface Crack Model

Figure 4 shows the bonding force per unit area of the surface. The parameter m controls the shape of the bonding stress-separation curve. After the maximum value is reached, the bonding stress decreases rapidly with the increase of δ. **Figure 5** shows the effect of parameter m on the δ_m/r_0. It is shown that the δ_m/r_0 decreases with the increase of parameter m.

4. The definition of the local J-integral

In the interface crack model, the interface elements are located near the crack tip. Considering the interface crack model as shown in Fig.3, a local J-integral along the border between the interface elements and the ordinary elements can be obtained from the definition of J-integral as shown by Eq.(8).

$$J = \int_\Gamma (W dy - T_i \frac{\partial u_i}{\partial x} ds) \tag{8}$$

where, W is the strain energy density, T_i is the traction along the line integral contour Γ, and u_i is the displacement. Since the J-integral is path independent the closed contour along the lower and upper sides of the interface elements can be taken. Considering that the displacement δ is very small compared with interface crack model size, only stress normal to the x-axis acts on the contour. Thus,

$$J_{LO} = -\int_\Gamma \sigma_{sp} \frac{\partial v}{\partial x} dx \tag{9}$$

Where, σ_{sp} is the stress along the interface element border. Taking J_{LO} counterclockwise along Γ means proceeding along the lower side of the interface elements from a to a+L in the x+ direction and back along the upper side from a+L to a in the x- direction. Thus,

$$J_{LO} = (\int_a^{a+L} \sigma_{sp} \frac{\partial v}{\partial x} dx^+ - \int_{a+L}^{a} \sigma_{sp} \frac{\partial v}{\partial x} dx^-)$$

(10)

Noticing that $v=\delta$, $\phi(\delta_T) = \int \sigma_{SP} d\delta |_{\delta_T}$ and $\phi(0)=2\gamma$, the following equation can be derived.

$$J_{LO} = 2\gamma \left\{ 1 - \left[(\frac{r_0}{r_0+\delta_T})^{2m} - 2(\frac{r_0}{r_0+\delta_T})^m \right] \right\} \tag{11}$$

Specially, J_{LO} would equal 2γ when the crack tip opening displacement δ_T becomes large enough compared to the parameter r_0 as shown in **Fig.6.** It is shown that the larger the constant m is the faster the J_{LO} gets to 2γ. It is the critical situation for crack initiation when J_{LO} equals 2γ. From Eq.(7) and (11), the relationship between the J_{LOC} or 2γ and σ_m, r_0, m can be described as shown by Eq.(12).

$$J_{LOC} = 2\gamma = \frac{\sigma_m r_0}{f(m)} \tag{12}$$

where:

$$f(m) = 2m \left[\left(\frac{m+1}{2m+1} \right)^{\frac{m+1}{m}} - \left(\frac{m+1}{2m+1} \right)^{\frac{2m+1}{m}} \right] \tag{13}$$

It can be seen from the equation that the critical J_{LOC} is proportional to the σ_m, r_0 and $f(m)$. **Figure 7** shows the effect of the parameter m on function $f(m)$. The function $f(m)$ can be approximated by a linear function with sufficient precision, i.e.

$$f(m)=0.4901m-0.2202 \tag{14}$$

According to Eq.(14), $f(m)$ becomes 1.0 when m equals 2.01. Consequently, $J_{LOC}=2\gamma=\sigma_m r_0$. The

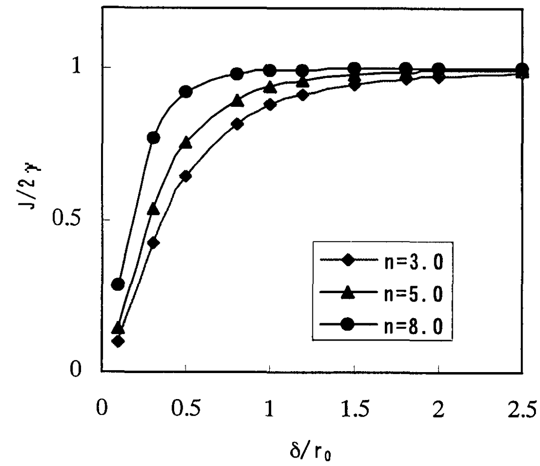

Fig.6 The theoretical J-integral along the interface elements border in interface crack model (ICM) with the effect of constant *m*

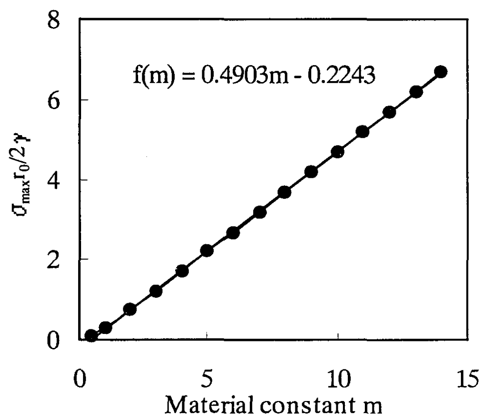

Fig.7 The function *f(m)* with constant *m* for determining the critical local J-integral

parameters σ_m, r_0 and m can be considered as the material constants which are related to the critical situation through Eq.(12).

5. Results and Discussion

The center-cracked specimen shown in **Fig.8** is analyzed numerically. In the computation, the ratio of crack length a to specimen width W is assumed to be 0.5. Due to the symmetry, only the upper-right of the specimen is meshed as shown in **Fig.9** using 1100 element and 2450 nodes. The mesh is refined in the region near the crack tip. The interface elements are arranged along the crack extension path with length L from the crack tip. The minimum size of the elements including interface elements near the crack tip is about 1/1000 of the ligament length. The J-integral far from the crack tip is estimated as the average value of J-integrals for five different paths.

5.1 Small scale yielding condition

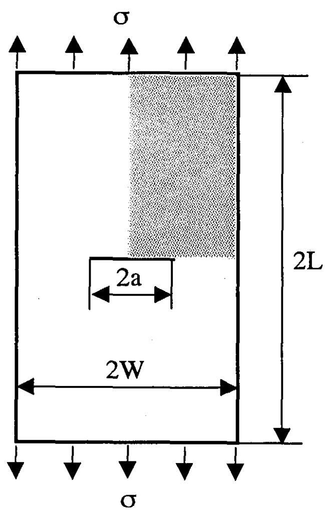

Fig.8 The center-cracked specimen with a/W=0.5, W=50mm, L=120mm

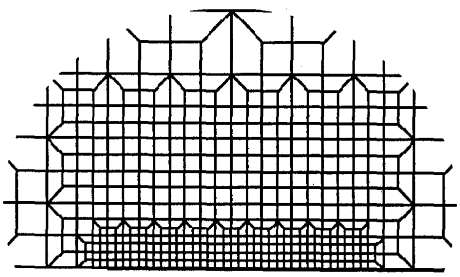

Fig.9 The finite element mesh near crack tip with the minimum size 1/1000 of ligament.

In the linear elastic fracture mechanics, the fracture is controlled by a so-called stress intensity factor K. According to the Griffith energy balance approach, the relationship between K and energy release rate, G, or J-integral can be determined. When the applied stress intensity factor K or the J-integral J reaches the critical value K_C or Jc, fracture occurs. In case of ICM, the resistance or the toughness of the material is embedded in the interface element as the surface energy 2γ. As shown in Fig.6, the local J-integral increases when the crack is opening but never exceeds 2γ. Thus, the crack starts to grow when the applied or the far J-integral becomes equal to 2γ. **Figure 10** shows the relationship between dimensionless δ/δ_m and r_0/L when the J-integral far from the crack tip equals 2γ or the local J-integral along the border of interface elements. As mentioned before, the parameter L means the length in which the interface elements are arranged. The maximum stress in the interface element is assumed to be 588MPa, which is taken as the same value as the yielding stress of the material considered. It can be seen also from Fig.10 that the value δ/δ_m increase with the decrease of r_0/L and the effect of L on the J-integral is not so large when the L is relatively small. It can be seen from Fig.10 that the value δ/δ_m changes with the parameter r_0/L. In this computation, the cracked body is in the elastic condition. Then the maximum stress in the interface element is limited to the yield stress of the material. Thus, the interface elements are expected to behave as the yield zone. The parameter L, which is the length of the interface element can be regarded as the plastic zone in small scale yielding condition. Though the value of the parameter L can be determined from the

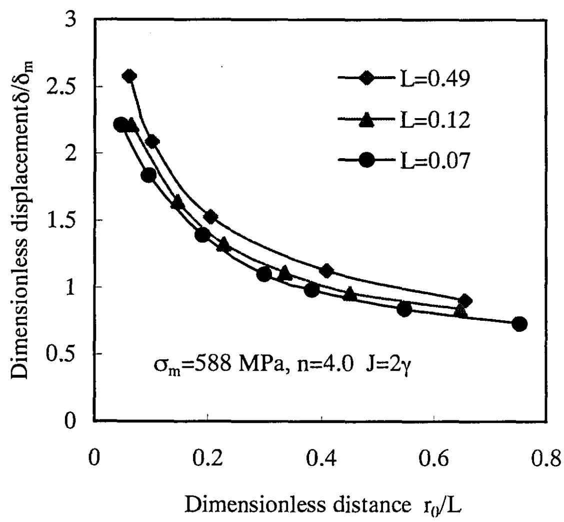

Fig.10 The dimensionless crack tip displacement with distance parameter r_0/L in deferent L..

size of the yield zone, the value of r_0 can be chosen arbitrarily dependent on the critical condition. To select the unique value of r_0, the condition that, $\delta = \delta_m$ is introduced. Under this condition, the unique combination of L and r_0 can be determined from the point corresponding to $\delta/\delta_m=1$ in Fig.10.

The effect of yield stress on the δ/δ_m is illustrated in **Fig.11**. It can be seen that the δ/δ_m increases with the decrease of yield stress. It means that the larger the maximum stress of interface element, the smaller the δ when the far J-integral equals to the value 2γ for given r_0/L. **Figure 12** shows the effect of constant *m* on the δ/δ_m. The critical opening displacement δ for the given value of r_0/L decreases with the increase of the exponent *m*.

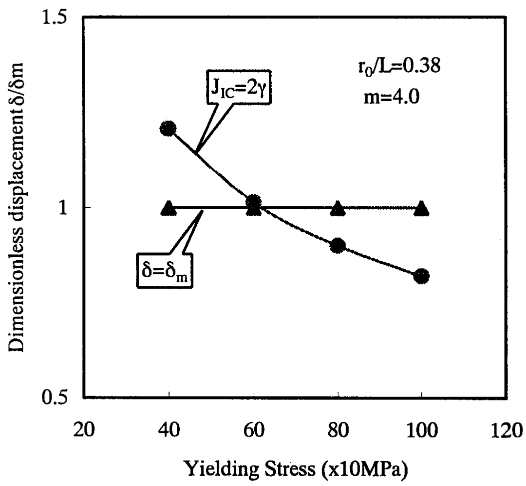

Fig.11 The influences of yielding stress on the dimensionless crack tip displacement.

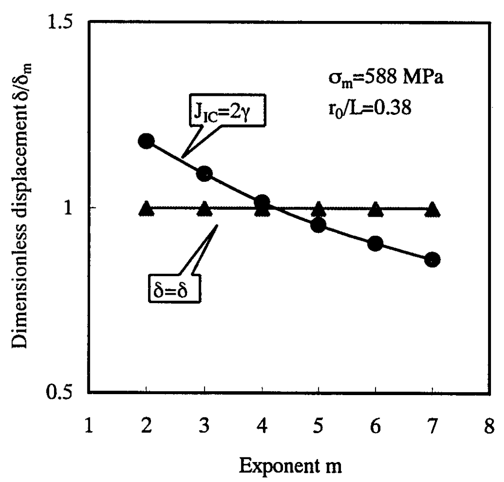

Fig.12 The influences of the constant m on the dimensionless crack tip displacement.

5.2 Large scale yielding condition

In the elastic-plastic condition, it is also assumed that the maximum stress in the interface element does not exceed the yield stress of the material. **Figure 13** shows the relation between the far J-integral and the applied load for different combination of r_0 and L. It is seen from Fig.13 that the interface element itself has almost no influence on the far J-load curve in elastic-plastic conditions. When the length of the interface element L is very large, the influence of the interface element can not be ignored. **Figures 14** and **15** show the relation between the far J-integral and crack tip displacement for different values L and m. Also, the J-integral estimated by the interface crack model and the

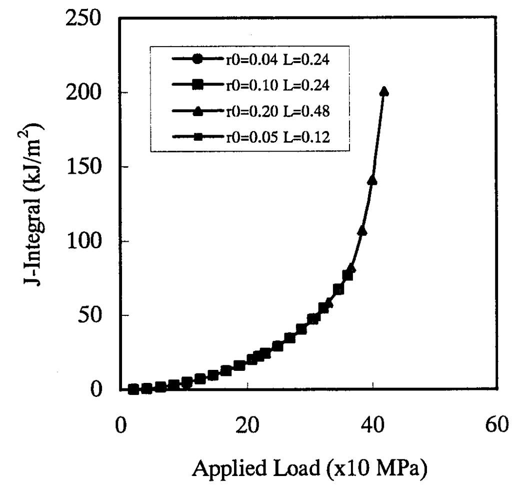

Fig.13 The effect of parameter L on the J-load line in elastic-plastic condition with m=4.0 and σ_0=488Mpa.

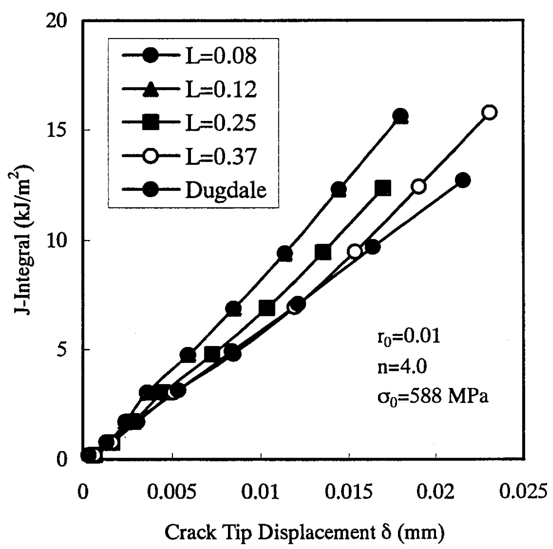

Fig.14 The J-integral far from crack tip with crack tip displacement at deferent distance parameter L.

classical Dugdale Model are compared in Figs.14 and 15. In general, the relationship between the J-integral and the crack tip displacement can be approximated as a linear function, i.e.

$$J = M\delta\,\sigma_0. \tag{15}$$

The value M varies between 1.15 and 2.95. In case of the Dugdale Model, the M equals 1.0. The parameter L influences the relationship between the J-Integral and the crack tip displacement when L is larger than 0.12. The slope of the curve decreases with the increase of L. The parameter m expresses the separation property of the crack. The larger the value m, the easier the crack separates. It can be seen from Fig.15 that the larger the value m is, the smaller the J-integral. **Figure 16** shows two cases of elastic and elastic-plastic situation with interface element. It can be seen from Fig.16 that the two lines become close to each other when the far J-integral is less than a certain value. In elastic case or small scale yielding case, the local J is almost the same with far J-integral. But in case of large scale yielding, the local J-integral is different from the far J-integral because of the large damage near the crack tip. Therefore, making use of this model we can build the relation between the local J-integral and far J-integral.

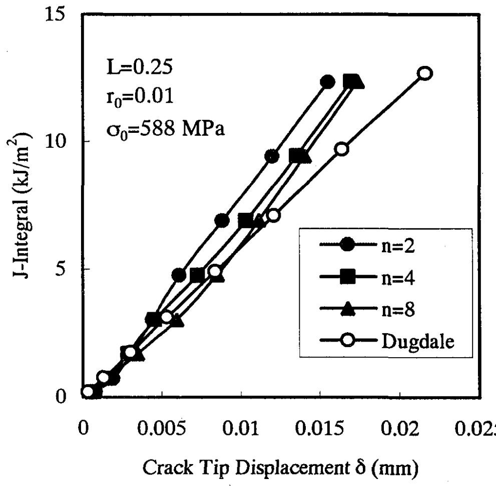

Fig.15 The influence of constant m on the J-integral far from crack tip with crack tip displacement.

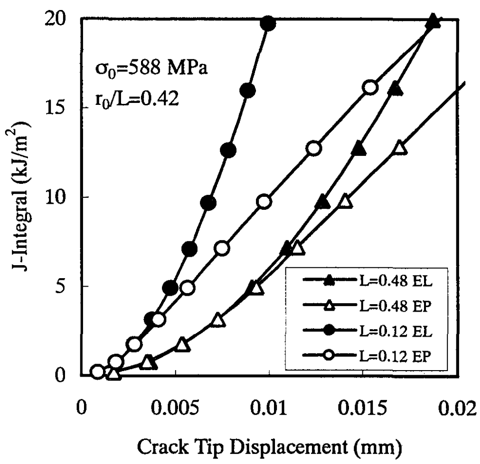

Fig.16 Comparison of J-integral far from crack tip in small scale yielding and large scale yielding condition.

5.3 The profile and future work on the Interface crack model

The ductile fracture of metallic materials can be described as a progressive process, which involves the nucleation, growth and coalescence of voids or micro-cracks. At the vicinity of a pre-existing macro-crack, a large damage evolution occurs due to the high stress and strain concentrations. It has been shown from experiments that the damaged zone is confined very near to the macro-crack tip. The fracture toughness, the crack resistance and the tearing modulus of the ductile materials may be strongly affected by the presence of such localized damages near the crack tip. In small scale yielding conditions, the plastic zone size around the crack tip is proportional to the stress intensity factor, K. In large scale yielding conditions, the process zone size around the crack tip would be proportional to the J-integral. Therefore, the initiation and the growth of the ductile crack is controlled by the state of the plastic zone in the case of small scale yielding and the process zone in case of large scale yielding conditions.

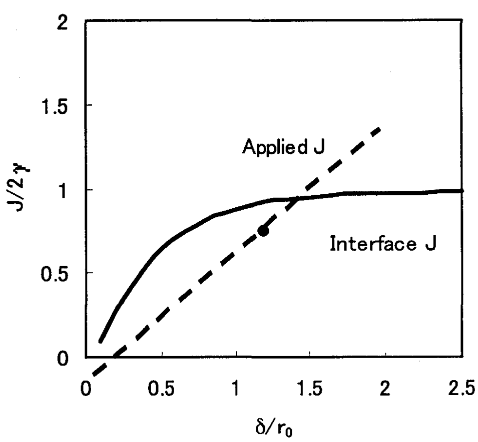

Fig.17 The relationship between J-integral far from crack tip and local J-integral defined by ICM.

The Interface Crack Model proposed in this report can be used to simulate the crack opening property and to estimate the fracture parameter in critical conditions. **Figure 17** shows the relationship between the applied J-integral far from the crack tip and local J-integral defined by ICM. It can be seen that the local J-integral and applied J-integral does not increase in the same manner. After the intersection point where the applied J-integral becomes equal to the local J-integral, the local J-integral will keep the same value and the crack start to grow. Therefore, the crack initiation and propagation can be modeled by the ICM. The behavior of the crack depends on the local J-integral which is characterized by the constants involved in the ICM, namely σ_m, m, r_0 and L. The important work about the ICM in the future is to demonstrate its capability to analyze the crack propagation problem and to clarify the relation between the parameters σ_m, m, r_0, L involved in the ICM and the measurable material properties.

6. Conclusion

Based on the Lennard-Jones type potential function, an interface crack model (ICM) is proposed in this report. In the ICM, one kind of interface element is introduced near the crack tip to simulate the ductile fracture for Mode I crack in plane strain condition. The main conclusions drawn from the present study are as follows.

1) The ductile fracture of metallic materials can be simulated making use of the interface crack model. The local J-integral is defined along the interface crack model contour as a initiating J-integral. The new crack surface will be formed when the applied J-integral far from the crack tip equals to the critical local J-integral.
2) There are several parameters included in the IC model, namely 2γ, m, r_0 and L. The parameter 2γ refers to the energy release rate for the new surface formation. The parameter m mainly controls the shape of the potential function. The parameter r_0 and L are the size parameters, with which the process zone can be characterized. Possibly, they may be related to the inclusion size and its distribution in the metallic materials.
3) In small scale yielding conditions, the size parameter L can be related to the length of the plastic zone near crack tip. In large scale yielding conditions, it can be related to the length of the process zone.

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