Anisotropic Damage Constitutive Law for Cleavage Failure in Crystalline Grain by Cohesive Zone Model*

by Yuichi Shintaku**, Kenjiro Terada*** and Seiichiro Tsutsumi***

The objective of this study is to propose new anisotropic damage constitutive law that represents the separation process on cleavage plane in a polycrystalline aggregate. The proposed law is formulated by embedding of an exponential type of the cohesive zone model (CZM) in a standard crystal plasticity constitutive law. The separation of the cleavage plane can be realized by exponential type of the CZM based on an atomic potential. On the other hands, the crystal plasticity constitutive law is used to simulate the deformation due to the crystalline slip on each crystallographic system. Thus, the proposed damage constitutive law is capable of representing the microscopic mechanism characterized by both the fracture behavior of the cleavage plane and the plastic deformation of the crystallographic slip. Several numerical simulations are conducted to demonstrate the capability of the proposed damage constitutive law. In particular, it is confirmed that the proposed model enables us to simulate the crack propagation in arbitrary directions, and the resultant anisotropic strength in a single crystal grain.

Key Words: Brittle fracture, Cleavage failure, Anisotropic damage model, Crystal plasticity, Cohesive zone model

1. Introduction

One of the critical issues in fracture mechanics is the dispersion of fracture toughness when a polycrystalline metal is broken by brittle fracture1). The difference of the fracture toughness is caused by the microscopic stress concentration and plastic deformation in the scale of crystalline and sub grain, although the macroscopic behavior appears to be elastic. The deformation behavior of each grain varies according to the crystal orientations defined by the crystal lattice and crystallographic slip planes. Also, a crystal grain shows anisotropic strength because of the separation of the cleavage plane, which is often observed in experiments for polycrystalline aggregate of a body-centered cubic metal2). The anisotropic strength is also confirmed from the uniaxial tensile test of a single crystal grain with different crystal orientations3).

Although the cohesive zone model (CZM) is often utilized for the assessment of a fracture toughness of brittle materials, it is difficult to simulate crack nucleation at arbitrary locations and propagation in arbitrary directions because a latent fracture surface must be pre-defined between finite elements4). To overcome this limitation, we have recently proposed a cohesive-force embedded damage model for isotropic elastic materials. In this study, we extend the model to deal with the anisotropic behavior of single crystalline grains. The proposed anisotropic damage constitutive law is formulated based on the assumption that the cohesive crack is located on each cleavage plane. More specifically, the new deformation gradient due to the crack opening is introduced into the conventional crystal plastic model5) and determined by the exponential type of the CZM6) to realize brittle fracture. Several numerical simulations are conducted to demonstrate the capability of the proposed damage constitutive law.

2. Anisotropic damage constitutive law for cleavage failure in crystalline grain by cohesive zone model

2.1 Multiplicative decomposition of deformation gradient: Elasticity, plasticity, and crack opening

The total deformation gradient is decomposed into the three parts, i.e., the elastic deformation due to distortion of crystal lattices, the plastic deformation due to crystallographic slip and the separation deformation due to crack opening.

\[ \dot{F} = \dot{F}^{e} F^{p} \dot{F}^{\alpha}, \]

where \( \dot{F}^{e} \) is the elastic deformation gradient, \( \dot{F}^{p} \) is the plastic deformation gradient and \( \dot{F}^{\alpha} \) is the separation deformation, respectively. The velocity gradient is expressed as the additive decomposition as follows:

\[ \dot{I} := \dot{F} F^{-1} = \dot{I}^{e} + \dot{I}^{p} + \dot{I}^{\alpha}, \]

where the velocity gradients due to elastic deformation \( \dot{I}^{e} \), crystallographic slip \( \dot{I}^{p} \) and crack opening \( \dot{I}^{\alpha} \), which are respectively defined as

---

*Received: 2016.10.17
**Member, Department of Engineering, Information and Systems, University of Tsukuba
***Member, International Research Institute of Disaster Science, Tohoku University
****Member, Jointing and Welding Research Institute, Osaka University
2.2 Flow rule for crystallographic slip

The flow rule for a crystal plasticity model is given as

\[ \dot{\mathbf{F}} = \sum_{\alpha=1}^{N^p} \left( \mathbf{m}^{(\alpha)} \otimes \mathbf{s}^{(\alpha)} \right) h^{(\alpha)}, \tag{4} \]

where \( N^p \) is the number of slip systems of crystal lattice of a metal, \( \mathbf{s}^{(\alpha)} \) is the slip rate in slip system \( \alpha \), and \( \mathbf{m}^{(\alpha)} \) and \( \mathbf{s}^{(\alpha)} \) are the unit vectors that define the slip direction and the normal direction of the slip plane of system \( \alpha \) after elastic deformation. The evolution law of \( \dot{\mathbf{F}} \) is given as the following equation, which was proposed by Asaro et al.\(^5\)

\[ \dot{\mathbf{F}} = \sum_{\alpha=1}^{N^p} \left( \mathbf{m}^{(\alpha)} \otimes \mathbf{s}^{(\alpha)} \right) h^{(\alpha)} \dot{\mathbf{F}}^{(\alpha)} \tag{5} \]

where \( \dot{\mathbf{F}}^{(\alpha)} \) is the slip resistance of slip system \( \alpha \) and \( \dot{\mathbf{F}}^{(\alpha)} \) is a parameter that controls the strain rate dependency. The evolution equation of \( \dot{\mathbf{F}}^{(\alpha)} \), is give as

\[ \dot{\mathbf{F}}^{(\alpha)} = \sum_{\beta=1}^{N^p} h_{\alpha\beta} \dot{\mathbf{F}}^{(\beta)} \tag{6} \]

where \( h_{\alpha\beta} \) represents the hardening modulus. The hardening function is defined as

\[ \begin{align*}
  h_{\alpha\alpha} &= h_0 \text{sech}^2 \left( \frac{h_0 \gamma}{\tau_0 - \gamma_0} \right) \\
  h_{\alpha\beta} &= q h_{\alpha\alpha} \quad (\alpha \neq \beta)
\end{align*} \tag{7} \]

where \( h_0 \) and \( \gamma_0 \) are the self-hardening and latent hardening moduli, respectively and \( q \) is the ratio of the latter to the former. Also, \( h_0 \), \( \gamma_0 \) and \( \tau_0 \) are the initial hardening modulus, the initial critical resolved shear stress and the stage-I (saturation) stress, respectively.

2.3 Flow rule for crack opening

The flow rule for a crack opening is obtained as

\[ \dot{\mathbf{F}}^c = \sum_{\alpha=1}^{N^c} \left( \mathbf{m}^{(\alpha)} \otimes \mathbf{s}^{(\alpha)} \right) h^{(\alpha)} + \left( \mathbf{m}^{(\alpha)} \otimes \mathbf{s}^{(\alpha)} \right) \dot{h}_{s}^{(\alpha)} \tag{8} \]

where \( N^c \) is the number of cracks of crystal lattice of a metal, \( \mathbf{m}^{(\alpha)} \) is the normal component of the material separation rate on cleavage plane \( \alpha \) and \( \mathbf{s}^{(\alpha)} \) is the tangential component, \( \mathbf{h}^{(\alpha)} \) is characteristic length of a material, and \( \mathbf{m}^{(\alpha)} \) and \( \mathbf{s}^{(\alpha)} \) are defined as the unit vector representing the normal and tangential direction of cleavage plane after elastic and plastic deformation.

More specifically, it is well known the cleavage failure occurs on a \{100\} plane in a body-centered cubic metal.

Under the equilibrium state, the cohesive traction \( t_n^{(\alpha)} \) and \( t_s^{(\alpha)} \) should be equivalent to the stress vector in normal and tangential direction. The two conditional equations for such a state are given as

\[ \begin{align*}
  g_n^{(\alpha)} (w_n^{(\alpha)}, w_s^{(\alpha)}) &= \sigma : (\mathbf{m}^{(\alpha)} \otimes \mathbf{s}^{(\alpha)}) - t_n^{(\alpha)} = 0 \\
  g_s^{(\alpha)} (w_n^{(\alpha)}, w_s^{(\alpha)}) &= \sigma : (\mathbf{m}^{(\alpha)} \otimes \mathbf{s}^{(\alpha)}) - t_s^{(\alpha)} = 0
\end{align*} \tag{9} \]

in each cleavage plane \( \alpha \). These conditional equations are nonlinear due to the cohesive traction which is expressed as exponential function, while it can be easily solved by the Newton-Raphson method.

3. Cohesive zone model for cleavage failure

The CZM represents the separation process of a continuum body into two or more parts, with controlling the release of the internal stress. At the atomic scale, the material separation is characterized by the relation between the atomic force and the distance between the crack surfaces, which is generally given by the universal binding energy relation (UBER)\(^7\). Since the atomic separation takes place in the brittle fracture under the ideal condition such that neither microscopic defects nor inclusions exist, Rice and Wang\(^6\) employed UBER in order to realize the process of the brittle fracture. The cohesive potential is given as

\[ \Psi(w^{(\alpha)}) = G_c \left[ 1 - \left( 1 + \frac{w^{(\alpha)}}{W_c} \right) \exp \left( \frac{-w^{(\alpha)}}{W_c} \right) \right], \tag{10} \]

where \( G_c \) is the critical energy release rate. The effective opening displacement \( w^{(\alpha)} \) represents the material separation width on the cleavage plane \( \alpha \), which is defined as

\[ w^{(\alpha)} = \sqrt{\left( \frac{w_n^{(\alpha)}}{\beta} \right)^2 + \left( \frac{w_s^{(\alpha)}}{\beta} \right)^2}, \tag{11} \]

where \( W_c \) is the critical value of \( w^{(\alpha)} \). Here, \( w_n^{(\alpha)} \) is the normal component of the material separation on cleavage plane \( \alpha \), \( w_s^{(\alpha)} \) is the tangential component, and \( \beta \) is the weighting coefficient to control the effect of the tangential opening displacement. It is,
However, to be noted that this separation displacement is recognized as an apparent one, as $G_c$ is defined as a fracture toughness of a material point involving sufficient number of atoms. Also, $G_c$ is defined as

$$G_c = \int_0^\infty \rho^{(a)} \, du^{(a)} = c t_c W_c,$$

(12)

where $t_c$ is the maximum value of the effective cohesive traction $t^{(a)}$ at $W_c$ and $c$ is the base of natural logarithm. $t^{(a)}$ is the effective cohesive traction, which is obtained as

$$t^{(a)} = \sqrt{t_n^{(a)}} + \frac{1}{\beta} t_s^{(a)}.$$  

(13)

The cohesive tractions in the normal and tangential directions, $t_n^{(a)}$ and $t_s^{(a)}$ are given as the derivatives of the potential with respect to the normal and tangential opening displacements $W_n^{(a)}$ and $W_s^{(a)}$, respectively, as

$$t_n^{(a)} = \frac{\partial \mathbb{P}}{\partial W_n^{(a)}} = \frac{G_c}{w_c} \left( \frac{w_n^{(a)}}{w_c} \right) \exp \left( -\frac{w_n^{(a)}}{w_c} \right),$$

(14)

$$t_s^{(a)} = \frac{\partial \mathbb{P}}{\partial W_s^{(a)}} = \frac{\beta G_c}{w_c} \left( \frac{w_s^{(a)}}{w_c} \right) \exp \left( -\frac{w_s^{(a)}}{w_c} \right).$$

(15)

According to the idea of CZM, a new crack surface is gradually formed after $t^{(a)}$ reaches $t_c$ at a material point. In the unloading process, the stiffness is smaller than the original and defined by a line connecting the point just before unloading to the origin; see Fig. 2. and Reference 4.

4. Result and discussion

4.1 Anisotropic tensile-softening behavior by proposed damage constitutive law

The performance of the proposed damage constitutive law is demonstrated by two sets of numerical simulations of the anisotropic tension-softening behavior under uniaxial loading. The uniaxial loadings are applied to a single element with a single crystalline grain. The material used here is assumed to be isotropic linear elastic; Young modulus of 206 GPa and Poisson’s ratio of 0.3. The initial critical resolved shear stress is set as the enough large value to prevent crystallographic slip on purpose to clarify the capability of our model; $\tau_0 = 1.0 \times 10^5$ MPa.

At the first set of numerical simulation, we assume the material constants of CZM as $G_c = 5.4$ kJ/mm$^2$, $w_c = 0.01$ mm and $\beta = 1.0$. It is here noted that $\beta = 1.0$ represents the tangential component of the critical cohesive traction is same as the normal one. The crystal orientation is rotated in three directions $\phi = 0, 15, 30^\circ$, which is defined between the normal direction to the cleavage plane $\{100\}$ and the loading direction. Figure 3 shows the obtained curves of the stress versus strain in the loading direction. As can be seen from the figure, the tensile strength decreases along with the increase of $\phi$ since the normal component of the stress traction on the cleavage plane decreases.

According to the idea of CZM, a new crack surface is gradually formed after $t^{(a)}$ reaches $t_c$ at a material point. In the unloading process, the stiffness is smaller than the original and defined by a line connecting the point just before unloading to the origin; see Fig. 2. and Reference 4.

Our model is capable to realize the anisotropic tensile strength due to the microstructure of the crystalline grain.

At the second set, we change the weight coefficient of the CZM to demonstrate the performance of our proposed model; $\beta = 0.5, 1.0, 2.0$. The direction of the crystal orientation is fixed at $\phi = 30^\circ$ in all cases. Figure 4 shows the obtained curves of the stress versus strain. As can be seen from the figure, the tensile strength decreases with the increase of $\beta$ which indicates the ratio of the tangential component of the critical cohesive traction to normal component. Note here that, even if the crystal orientation is set as $\phi = 0^\circ$, the tensile strength doesn’t change since $\beta$ doesn’t contribute to the normal component. The results show that our model provides us to control the anisotropic tensile strength by $\beta$.

Therefore, our proposed model enables us to represent the anisotropic tensile-softening behavior attributed from not only the microstructure of the single crystalline grain but also the difference between the normal and tangential component of...
critical cohesive traction.

4.2 Crack propagation in a single grain with different crystal orientations

Using our proposed anisotropic damage constitutive law, we conduct two sets of the crack initiation and propagation analyses in the specimen of a single crystalline grain. The specimen has a spatial dimension of 0.7×0.5×0.1mm and is given a sharp initial crack whose size is 0.1mm as shown in Fig. 5. To realize bending condition, imposed displacements from -0.025 to 0.275mm are given on the upper and lower surface of the specimen. We assumed the crystal orientations as $\phi = 0^\circ$, $30^\circ$ and the same material constants as in the Reference4), i.e., $G_c = 15000$N/m, $t_c = 2.0$GPa and $\beta = 2.0$.

The distributions of the ratio of the material separation width to its critical value, $w^{(1)}/w_c$, are shown in Fig. 6 respectively, in which the direction of a new crack growth from the pre-crack is clearly recognized. Here, $\alpha = 1$ indicates the maximum value of the separation width in all cleavage planes. As can be seen from Fig. 6(a), the crack in the single crystalline grain of $\phi = 0^\circ$ goes straight along with the cleavage plane. On the other hands, the crack in $\phi = 30^\circ$ propagates in the slant direction to the pre-crack as shown in Fig. 6(b), although the loading direction is the same as previous one. Thus, our proposed model enables us to realize the material separation on the cleavage plane as it is called cleavage failure.

The overall responses of these results are shown in Fig. 7, respectively. Here, we have defined the apparent stress as the areal average of the nodal forces at the upper surface and the apparent strain as the ratio of the displacement at the upper surface divided by the initial length along z axis of the specimen. As can be seen from the figure, the crack propagation in the case of $\phi = 0^\circ$ is apparently unstable, since the maximum value of stress is lower than that of $\phi = 30^\circ$ and dramatically drops down.

5. Conclusions

We have proposed a new anisotropic damage constitutive law in which the cohesive traction is embedded for a cleavage failure that incorporates an exponential type of CZM with a slip plane defined in the conventional crystal plasticity model. The proposed model enables us to realize the crack propagating in arbitrary directions in a single crystal grain due to the cleavage failure whereas the conventional CZM with the standard FEM is subjected to meshing. It is noted that the proposed damage constitutive law enables us to represent the anisotropic characteristics of both the elastic-plastic deformation and tensile strength depending on the lattice orientations in a crystal grain.

Acknowledgements

This work was supported by JSPS KAKENHI Grant Numbers JP17K17627, JP16H02137 and University of Tsukuba Basic Research Supported Program Type S.

Reference

1) R. Ritchie, J. Knott and J. Rice: On the relationship between critical tensile stress and fracture toughness in mild steel, J. Mech. Phys. Solids, 21(1973), 395-410.
2) A. Pineau, A.A. Benzerga and T. Pardo: Failure of metals: Brittle and ductile fracture, Acta Mater. 107(2016), 424-483.
3) F. Terasaki: Cleavage failure and deformation behavior of single crystal of pure iron under low temperature (in Japanese), Bulletin of the Japan Institute of Metals, 9(1970), 147-155.
4) A. Pandolfi, P.R. Gaduru, M. Ortiz and A.J. Rosakis: Three dimensional cohesive-element analysis and experiments of dynamic fracture in C300 steel, Int. J. Sol. Struct., 37(1999), 3733-3760.
5) J. R. Asaro: Cystal plasticity. J. Appl. Mech., 50(1983), 921-934.
6) J. Rice and J. Wang: Embrittlement of interfaces by solute segregation, Mater. Sci. Eng. A102(1989), 23-40.
7) J. H. Rose and J. R. Smith: Universal binding energy curves for metals and bimetallic interfaces, Phys. Rev. Lett., 47(1981), 675-678.