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Theoretical and Applied Fracture Mechanics 47 (2007) 244–259
theoretical and applied fracture mechanics
www.elsevier.com/locate/tafmec

Validation of component assembly model and extension to plasticity

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Available online 13 March 2007

Abstract

Material potential energy is well approximated by "pair-functional" potentials. During calculating potential energy, the orientational and volumetric components have been derived from pair potentials and embedding energy, respectively. Slip results in plastic deformation, and slip component has been proposed accordingly. Material is treated as a component assembly, and its elastic, plastic and damage properties are reflected by different components respectively. Material constitutive relations are formed by means of assembling these three kinds of components. Anisotropy has been incorporated intrinsically via the concept of component. Theoretical and numerical results indicate that this method has the capacity of reproducing some results satisfactorily, with the advantages of physical explicitness, etc.

Keywords: Elastic; Plastic; Damage; Fracture; Continuum damage mechanics; Anisotropy; Pair-functional; Pair potentials; Orientational/volumetric/slip component; Component assembly model

1. Introduction

Material made up of a large number of atoms can be regarded as a many-body system, and the binding forces among atoms determine the material structures and its intrinsic mechanical and electromagnetic properties [1–4]. Microscopically, material properties are not unalterably determined by their average chemical composition but they are to a large extent influenced by their microstructure. Material deforms under external agencies, and its microstructures change accordingly. With external loads continually increasing, microdefects such as microcracks and microvoids begin to nucleate and grow, and the mechanical properties of materials degrade accordingly. The process of material degrading has been researched by damage mechanics [5–18]. Meantime, the other kind of microdefects, dislocations move, interact, proliferate and pileup, etc. Dislocations and their interactions determine the material strength in the absence of other internal defects, and they tend to self-organize in the form of patterns, resulting into a heterogeneous field of deformation at microscale although the overall macroscopic field is thought to be homogeneous [19–37]. As the collective motion of large

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doi:10.1016/j.tafmec.2007.01.003

number of dislocations, plastic flow and hardening have been researched in plastic theories [29,38]. The damage constitutive relation is difficult to derive and the corresponding formulations can be complex, if anisotropic damage and dissipative potentials and internal variables are considered.

Component assembly model [39] has been derived from pair-function potentials [2,4,40–42]. Material potential energy due to deformations has been written as the sum of pair-functional potentials. In which, pair potentials has been grouped according to discrete directions which are determined by the interactions among atoms, and each group has been represented by an orientational component, i.e., the sum of pair potentials in material parallel to the direction is the energy of the corresponding orientational component and the stiffness contribution of these atomic bonds is its stiffness. Meanwhile, the other kind of component – the volumetric one has been proposed from embedding energy. As the main plastic deformation mechanism, slip has been investigated in the presentation and slip component has been set up accordingly. Material has been treated as a component assembly, and its constitutive relations have been formed by means of assembling the response functions of these three kinds of components.

The remainder of this paper is organized as follows. In part 2, the component assembly model is reviewed briefly. In which, the orientational and volumetric components are derived from pair potentials and embedding energy respectively. Breaking of atomic bonds results in macroscopic damage and fracture and it changes components' property gradually, and this material degrading process is investigated in part 3. In part 4, the third kind of component – the slip one is also introduced, and the elasto-plast-damage constitutive equations have been formed by assembling these three kinds of components. In the last part, the differences between the proposed model and continuum damage models, microplane theory [43–46], quasi-continuum (QC) model [47,48], virtual internal bonds (VIB) model [49] and cohesive zone one [50] have been discussed briefly, and a concise conclusion has also been given.

2. Introduction of the component assembly model

The principal view of pair-functional potentials is that the cohesive energy of an atom is determined by the local electron density at the site into which that atom is placed [51–53]. The embedded atom method posits a total energy of the form,

$$E_{\text{exact}}(\{\mathbf{R}_i, \mathbf{r}_n\}) \to E_{\text{approx}}[\rho(\mathbf{r}), \{\mathbf{R}_i\}] = \frac{1}{2}\sum_{ij}^{i\neq j}\phi(R_{ij}) + \sum_i F(\rho_i), \tag{1}$$

where, the term $\phi(R_{ij})$ describes a pairwise isotropic interatomic potential function which is essentially repulsive and depends only on the atomic spacing $R_{ij} = |\mathbf{R}_i - \mathbf{R}_j| = R^{(i,j)}$, $(i \neq j)$, $\mathbf{R}_i$ is the position of the ith nuclear and r_n is the position vector of the nth electron. $F(\rho)$ is referred to as the embedding energy (function), modeling the attractive interaction as a function of the local electron density ρ into which the considered atom is placed. The above equations may include various parameters and these parameters can be obtained by fitting equations to intrinsic material parameters such as the elastic constants, crystal structure and cohesive energy, etc.

In practice, our interest is in excursions about the equilibrium positions, it is convenient to define zero of energy at initial equilibrium positions. Expanding Eq. (1) by Taylor series, further progress can be made in trimming down the first term $\frac{\partial E_{\text{tot}}}{\partial \mathbf{R}} \cdot \delta\mathbf{R}$ by recognizing that the expansion is built around the equilibrium configuration, and the first term can be eliminated since we have $\frac{\partial E_{\text{tot}}}{\partial \mathbf{R}} \cdot \delta\mathbf{R} \equiv 0$ at equilibrium. Thus, potential energy due to deformation (strain energy) can be expressed in the form (the third and higher derivatives excluded):

$$U = \frac{1}{4}\sum_{(\alpha,\beta)}^{\alpha\neq\beta}\phi''\left(R^{(\alpha,\beta)}\right)\left[\delta R^{(\alpha,\beta)}\right]^2 + \frac{1}{4}\sum_{(\alpha,\beta)}^{\alpha\neq\beta}\phi'\left(R^{(\alpha,\beta)}\right)\delta^2 R^{(\alpha,\beta)} + \frac{1}{2}\sum_{\alpha}F''\left(\rho^{(\alpha)}\right)\left[\delta\rho^{(\alpha)}\right]^2 + \frac{1}{2}\sum_{\alpha}F'\left(\rho^{(\alpha)}\right)\delta^2\rho^{(\alpha)}. \tag{2}$$

Here, it should be emphasized that in component assembly model pair potentials are grouped according to discrete directions not to the quantities of interatomic potential in QC. Pair potentials are grouped according to directions, and microstructures and their evolutions are embodied on energy changing in different

directions. Furthermore, an orientational component has been set up to represent each group of atomic bonds. In addition, considering the change of electronic density is the function of the volume change, another kind of component, the volumetric one has also been proposed to represent the contribution of embedding energy. Evidently, the orientational component works like a bar and the volumetric one responds only to volume changes. Material is treated as a component assembly. By energy equivalence, and comparing with continuum mechanics [38], yields the result:

$$C_{ijkl} = \sum_s H^s m_i^s m_j^s m_k^s m_l^s + K\delta_{ij}\delta_{kl}, \tag{3}$$

herein H^s denotes the elastic modulus of the sth orientational component, and K the bulk modulus of the volumetric one. δ_{ij} denotes the second-order identity. Due to simple deformation of the orientational and volumetric components, their response functions are much simpler than the constitutive in continuum mechanics, and they can be expressed as follows:

$$\sigma^s = \sigma^s(\varepsilon^s) = \sigma^s\left(\varepsilon_{ij} m_i^s m_j^s\right) (= H^s \varepsilon^s), \tag{4}$$

and

$$\sigma_{\mathrm{V}} = \sigma_{\mathrm{V}}(\varepsilon_{\mathrm{V}}) = \sigma_{\mathrm{V}}(\varepsilon_{ii}) (= K\varepsilon_{ii}), \tag{5}$$

where σ^s and ε^s denote the stress and the strain of the sth orientational component respectively, σ_{V} and ε_{V} the (hydrostatic) stress and the (volumetric) strain of the volumetric one respectively. In addition, the elasticity tensor in component assembly model satisfies the Voigt symmetry, $C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij}$. Due to the volumetric component, it gets rid of the constraint of the Cauchy relation, $C_{ijkl} = C_{ikjl}$.

Once pair-functional potentials have been specified and the crystal structure is known, material properties can be derived directly. Actually, materials are always inhomogeneous and anisotropic, but many materials demonstrate macroscopic isotropy, such as most metals. In particular, for homogeneous material (the observing length is much larger than characteristic length), there is

$$C_{ijkl} = \int_0^{\frac{\pi}{2}} \int_0^{2\pi} H(\theta,\varphi) m_i(\theta,\varphi) m_j(\theta,\varphi) m_k(\theta,\varphi) m_l(\theta,\varphi) \sin\theta \mathrm{d}\theta \mathrm{d}\varphi + K\delta_{ij}\delta_{kl}. \tag{6}$$

For changes of electronic density relate only to volumetric strain, and infinitesimal deformation is considered, the bulk modulus can be treated as a constant:

$$K(\theta,\varphi) \equiv K. \tag{7}$$

Eq. (6) is the constitutive equation for homogeneous materials. In particular, for macroscopic homogeneous and isotropic materials, the orientational components have the same modulus:

$$H(\theta,\varphi) \equiv H. \tag{8}$$

Integrating Eq. (6) on the up half a unit sphere, and yields:

$$C_{ijkl} = \left(\frac{2\pi}{15}H + K\right)\delta_{ij}\delta_{kl} + \frac{2\pi}{15}H(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \tag{9}$$

Comparing with traditional continuum mechanics, yields the result

$$\begin{cases} H = \frac{15}{2\pi}\mu \\ K = \lambda - \mu \end{cases}, \tag{10}$$

herein, λ and μ are Lame's coefficients. Figs. 1 and 2 are the typical configurations of planar and spatial discrete orientational components respectively.

For orthotropic material, it has nine independent material constants. The integral of Eq. (6) will be transformed to discrete summation in numerical computing, and the selected directions turn into discrete orientational component's directions, it has the same form as Eq. (3). Anisotropy is embodied intrinsically in the different moduli of orientational components. Concretely, the component's stiffness can be derived by means of least square method,

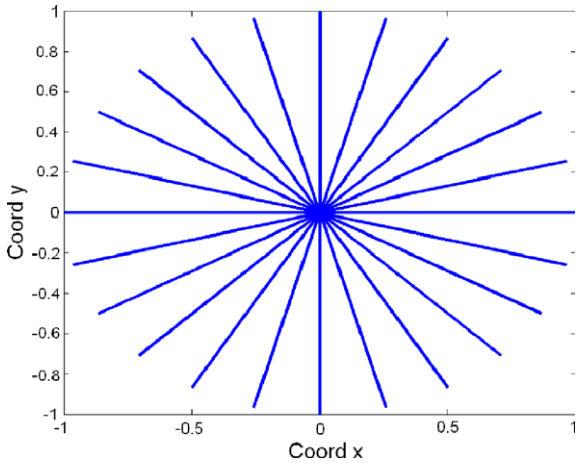

Fig. 1. The configuration of planar discrete orientational components.

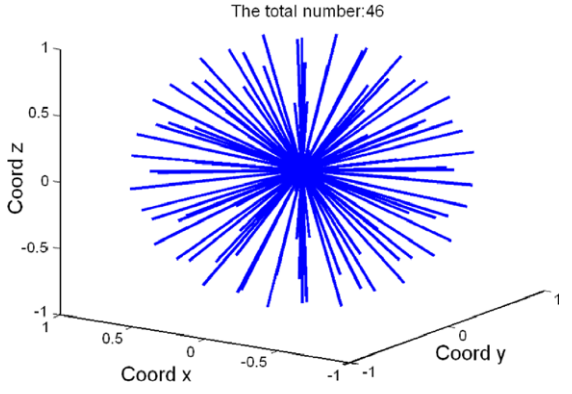

Fig. 2. The configuration of spatial discrete orientational components.

$$\begin{aligned}\Psi &= \left\{ C_{ijkl} - \left[\sum_s H^s m_i^s m_j^s m_k^s m_l^s + K\delta_{ij}\delta_{kl} \right] \right\}^2 \\ &= \left\{ C_{1111} - \left[\sum_s H^s m_1^s m_1^s m_1^s m_1^s + K \right] \right\}^2 + \cdots + \left\{ C_{2222} - \left[\sum_s H^s m_2^s m_2^s m_2^s m_2^s + K \right] \right\}^2 + \cdots \\ &\quad + \left\{ C_{3131} - \left[\sum_s H^s m_3^s m_1^s m_3^s m_1^s \right] \right\}^2 + \cdots + \left\{ C_{1212} - \left[\sum_s H^s m_1^s m_2^s m_1^s m_2^s \right] \right\}^2, \end{aligned} \tag{11}$$

from $\frac{\partial \Psi}{\partial H^t} = 0,\ t = 1, 2, \ldots$, there is,

$$m_i^t m_j^t m_k^t m_l^t \left\{ \sum_s m_i^s m_j^s m_k^s m_l^s \cdot H^s + \delta_{ij}\delta_{kl} \cdot K \right\} = m_i^t m_j^t m_k^t m_l^t \cdot C_{ijkl}. \tag{12}$$

In addition, for $\frac{\partial \Psi}{\partial K} = 0$, there is

$$\delta_{ij}\delta_{kl} \sum_s m_i^s m_j^s m_k^s m_l^s \cdot H^s + 9\mathrm{K} = \delta_{ij}\delta_{kl} C_{ijkl}. \tag{13}$$

In the above three equations, *ijkl* may be equal to 1111, 1122, 1133, 2211, 2222, 2233, 3311, 3322, 3333, 2323, 3131 and 1212 for orthotropic materials. Consider the symmetry to all orientational components to simplify the solution. Finally, the equations for components are written as

$$[A]\begin{Bmatrix} H \\ K \end{Bmatrix} = \{b\}. \tag{14}$$

In general, the coefficient matrix $[A]$ is not a square one, and the above equations can be solved by means of MINRES and its variants, e.g., GMRES [54,55].

3. Damage in the proposed model

Fracture of engineering structures [56–62] is often preceded by considerable changes in the microstructures of the material they are made of. Accurate failure predictions can only be obtained if this microstructural damage is taken into account in the fracture modeling. This requirement has led to the development of so-called local or continuum approaches to fracture, in which fracture is regarded as the ultimate consequence of the material degradation process [7,17,63]. In these methods, the degradation is often modeled using continuum damage mechanics [5–14,63]. Continuum damage theories introduce a set of field variables (damage variables) which explicitly describe the local loss of material integrity. A crack is represented by that part of the material domain in which the damage has become critical, i.e., where the material cannot sustain stress anymore. Redistribution of stresses results in the concentration of deformation and damage growth in a relatively small region in front of crack tip. It is the growth of damage in this process zone which determines in which direction and at which rate the crack will propagate. Crack initiation and growth thus follow naturally from the standard continuum theory, instead of from separate fracture criteria.

It is true that, microstructures changing and damage and fracture, they all are the changing and breaking of atomic bonds. As an abstract of atomic bonds, when atomic debonding emerges, the corresponding orientational component changes its mechanical properties, e.g., stiffness. The more atomic debonding occurs and the more stiffness changes:

$$D = 1.0 - \frac{H}{H_0}, \tag{15}$$

where H_0 and H denote the initial and instantaneous (damaged) secant stiffness of the component respectively, D its damage factor. A scalar value is enough for a $1 - D$ component, it is a microscopic value (however, for material, its constitutive is a typical fourth order tensor, as the following Eq. (26)). Meantime, as a typical $1 - D$ component, the orientational one has simple constitutive relation, it is expressed as follows:

$$\sigma^s = (1 - D^s)H_0^s\varepsilon^s = (1 - D^s)H_0^s\varepsilon_{ij}m_i^s m_j^s, \tag{14'}$$

and its rate form is

$$\dot{\sigma}^s = (1 - D^s)H_0 m_i^s m_j^s \dot{\varepsilon}_{ij} - H_0 m_i^s m_j^s \varepsilon_{ij}\dot{D}^s. \tag{14''}$$

The stress contribution of single orientational component is written as

$$\sigma_{ij} = \sigma^s m_i^s m_j^s. \tag{16}$$

Meanwhile, the hypothesis that damage is never healed up has been adopted:

$$\dot{D} \geqslant 0. \tag{17}$$

The damage of the orientational component has been treated as a function of its deformation history ε_h (the maximum/minimum strain in whole deformation process):

$$D = D(\varepsilon_h). \tag{18}$$

It admits the notation

$$\left\langle \frac{\mathrm{d}D}{\mathrm{d}\varepsilon_h} \right\rangle = \begin{cases} \frac{\mathrm{d}D}{\mathrm{d}\varepsilon_h}, & \text{when } \varepsilon = \varepsilon_h \text{ and } \varepsilon\dot{\varepsilon} > 0; \\ 0, & \text{other conditions.} \end{cases} \tag{19}$$

It follows that,

$$\dot{D}^s = \left\langle \frac{\mathrm{d}D}{\mathrm{d}\varepsilon_h} \right\rangle^s \dot{\varepsilon}^s = \left\langle \frac{\mathrm{d}D}{\mathrm{d}\varepsilon_h} \right\rangle^s m_i^s m_j^s \varepsilon_{ij}. \tag{20}$$

From another point of view, since the orientational component is derived from pair potentials, its property can be investigated directly by the interatomic potentials. For example, the Lennard-Jones potential [40,41] has the following form

$$U(R_{ij}) = a\left[\left(\frac{b}{R_{ij}}\right)^{12} - 2\left(\frac{b}{R_{ij}}\right)^{6}\right]. \tag{21}$$

The stiffness of the orientational component has been gotten from Eq. (21), $H \propto U'' = \frac{a}{b^2}\left[156(\frac{b}{R_{ij}})^{14} - 84(\frac{b}{R_{ij}})^{8}\right]$, Fig. 3 is the curve of the orientational component's stiffness versus the length.

Embedding energy is essentially a kind of Coulomb potential. For the conservation of electric charge, there is $\rho V = \text{const}$, and it indicates $\dot{\rho} = -\frac{\rho}{V}\dot{V} \propto (-\dot{\varepsilon}_{ii})$. On the other hand, the attractive force between the atom and electronic gas is proportional to ρ. Considering K an representative of the intensity of the force, there are $K \propto \rho$ and $\dot{K} \propto (-\dot{\varepsilon}_{ii})$, it implies $\ln\frac{K}{K_0} \propto (-\ln\frac{V}{V_0})(\approx -\varepsilon_{ii})$ or $\ln\frac{K}{K_0} = -\omega\varepsilon_{ii}$, ω is a material parameter. Fig. 4 displays the linear relation between $\frac{1}{\omega}\ln\frac{K}{K_0}$ and ε_{ii}.

Furthermore, it can simply be expressed as

$$\dot{K} = -\omega K\dot{\varepsilon}_{ii} = -\omega K\dot{\varepsilon}_V, \tag{22}$$

Eq. (22) indicates that the damage factor of the volumetric component D_V is

$$D_V = \omega\varepsilon_{ii} = \omega\varepsilon_V, \tag{23}$$

and its rate form

$$\dot{D}_V = \omega\dot{\varepsilon}_{ii}, \tag{24}$$

Followed by Eq. (5), there is

$$\sigma_V = (1 - D_V)K_0\varepsilon_{ii}, \tag{5'}$$

where K_0 denotes the initial bulk modulus. Its rate form is expressed as follows:

$$\dot{\sigma}_V = (1 - D_V)K_0\dot{\varepsilon}_{ii} - K_0\varepsilon_{ii}\dot{D}_V = (1 - 2\omega\varepsilon_{ii})K_0\dot{\varepsilon}_{ii}. \tag{5''}$$

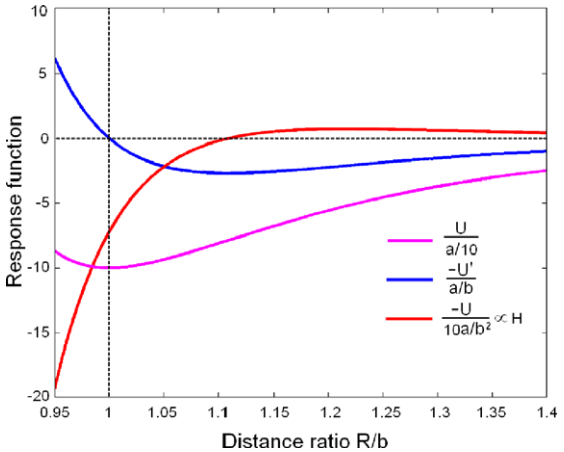

Fig. 3. The curve of H versus R.

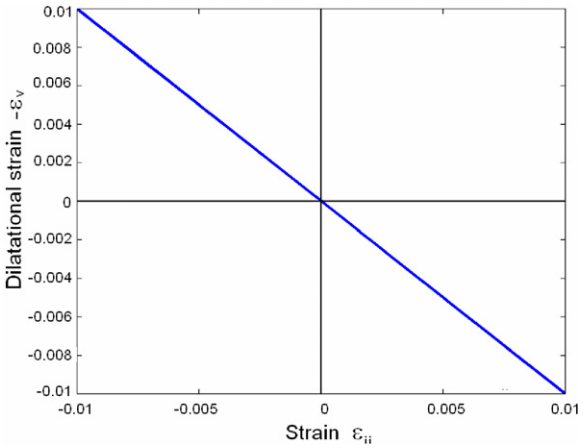

Fig. 4. The curve of $\frac{1}{\omega}\ln\frac{K}{K_0}$ versus ε_{ii}.

Eqs. (5′), (5″) and (22)–(24) imply that damage heals up as soon as deformation is removed. Certainly, it is very easy to consider the hypothesis that damage is never healed up. It is also very easy to consider the quasi-lateral condition in component assembly model, for this condition is embodied on each simple deformed component. Finally, there yields the elasto-damage constitutive equations,

$$\dot{\sigma}_{ij} = \left\{ \sum_{s=1}^{N} \left[(1-D^s)H_0^s - H_0^s \varepsilon^s \left\langle \frac{\mathrm{d}D}{\mathrm{d}\varepsilon_h} \right\rangle^s \right] m_i^s m_j^s m_k^s m_l^s + (1-2\omega\varepsilon_{ii})K_0\delta_{ij}\delta_{kl} \right\} \dot{\varepsilon}_{kl}, \tag{25}$$

where N denotes the total number of the orientational components. The elasto-damage elasticity tensor is given by

$$C_{ijkl}^{\mathrm{ed}} = \sum_{s=1}^{N} \left[(1-D^s)H_0^s - H_0^s \varepsilon^s \left\langle \frac{\mathrm{d}D}{\mathrm{d}\varepsilon_h} \right\rangle^s \right] m_i^s m_j^s m_k^s m_l^s + (1-2\omega\varepsilon_{ii})K_0\delta_{ij}\delta_{kl}. \tag{26}$$

The orientational and volumetric components have been derived from pair functional theory, and they indicate different deformation mechanisms. Material is treated as a component assembly, and it means that material change its state so soon as any component changes its state. For simplicity, the bulk modulus of the volumetric component can be treated as a constant, $\omega \equiv 0$. Fig. 5 illustrates the construction of material damage surface from component.

If the effective Poisson's ratios are defined as

$$\tilde{v}_{21} = \left| \frac{\varepsilon_2}{\varepsilon_1} \right| \tag{27}$$

and

$$\tilde{v}_{31} = \left| \frac{\varepsilon_3}{\varepsilon_1} \right|, \tag{28}$$

where $\varepsilon_i, i = 1,2,3$ is the principal strain. Under uniaxial tension, there is

$$\begin{Bmatrix} \sigma_1/\varepsilon_1 \\ 0 \\ 0 \end{Bmatrix} = \left\{ \sum_{s=1}^{N} (1-D^s)H_0^s \begin{bmatrix} m_1^4 & m_1^2 m_2^2 & m_1^2 m_3^2 \\ m_1^2 m_2^2 & m_2^4 & m_2^2 m_3^2 \\ m_1^2 m_3^2 & m_2^2 m_3^2 & m_3^4 \end{bmatrix} + K \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \right\} \begin{Bmatrix} 1 \\ -\tilde{v}_{21} \\ -\tilde{v}_{31} \end{Bmatrix}, \tag{29}$$

and the effective Poisson's ratios can be gotten by solving Eq. (29).

The wedge splitting test, shown in Fig. 6, is a recent experimental technique introduced in [64] to determine some softening properties of a quasibrittle material. Displacement control is applied to concrete specimen

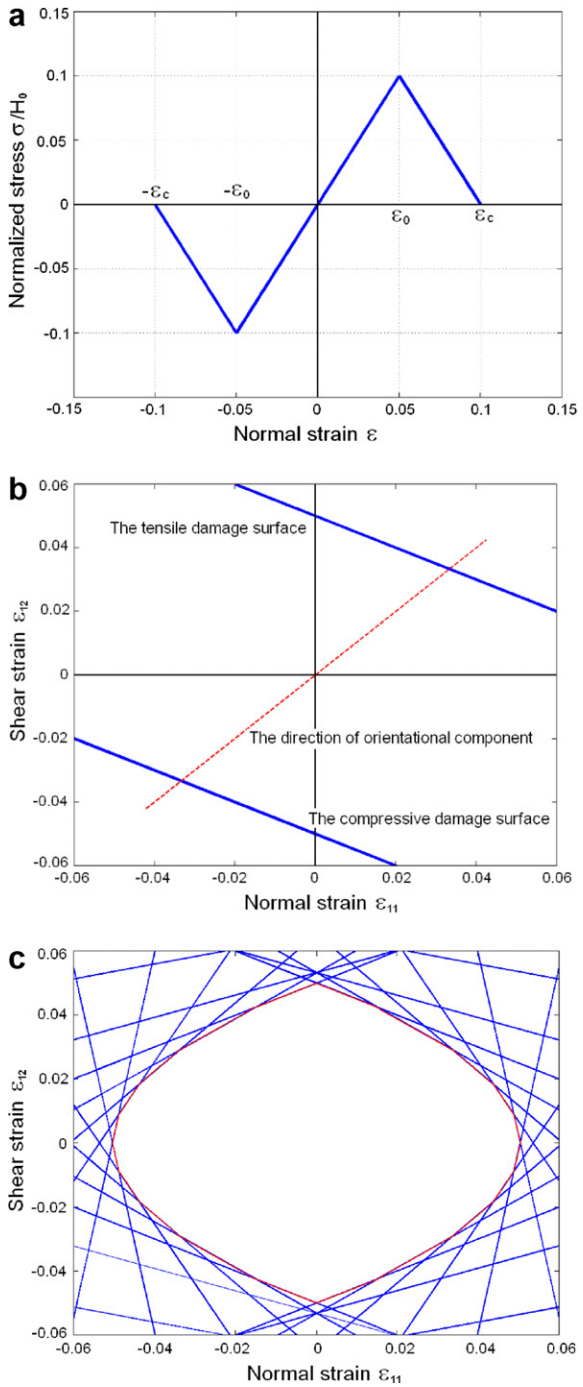

Fig. 5. The response function (a) and the damage surface (b) of the orientational component, and the material damage surface (c).

through the downward movement of a wedge placed between rollers creating a splitting action. The wedge splitting test results of experiments can be used for the parameter identification problem. Considering the compression strength of concrete much larger than the tensile one, the response function of orientational components is chosen in Figs. 7 and 8 is the corresponding damage factor versus strain curve. In addition, for simplicity, the stiffness of volumetric component is treated as constant. The spatial discretization of orientational components is shown in Fig. 2. Fig. 9 shows that the numerical result comparing to experiment data

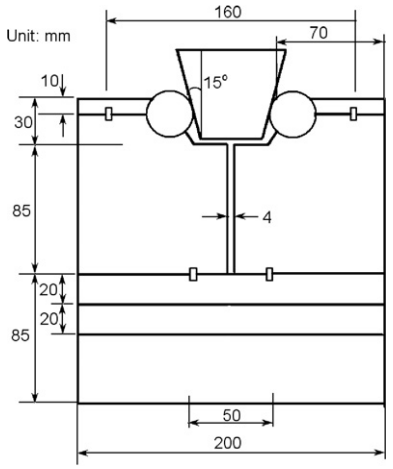

Fig. 6. The configuration of wedge splitting.

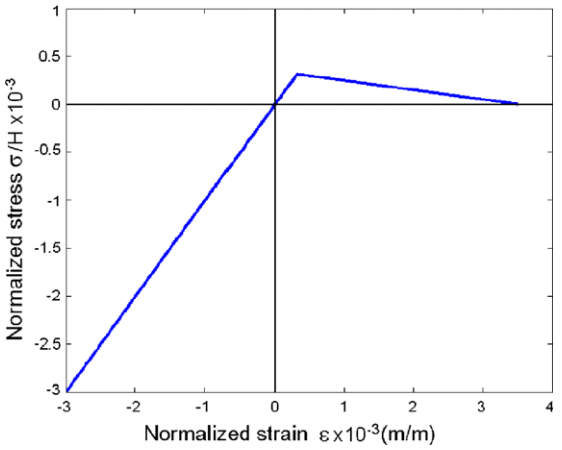

Fig. 7. The response function.

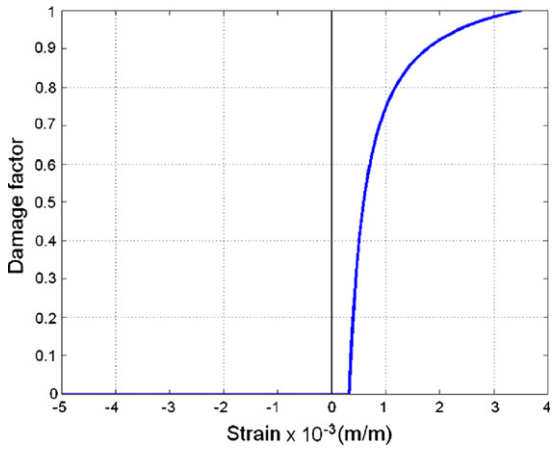

Fig. 8. The damage versus strain curve.

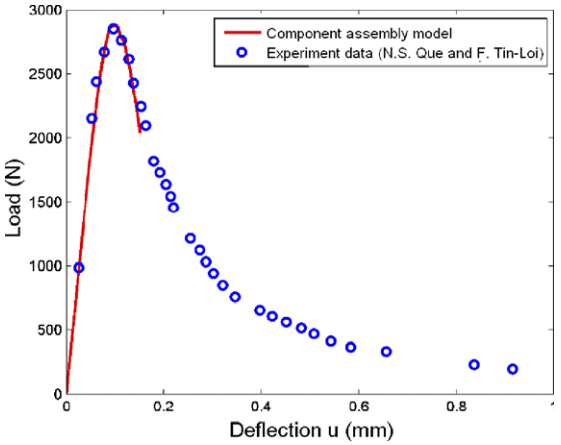

Fig. 9. The load–displacement curve.

[50]. For fitting the whole experiment data, the more sophisticated response function is needed, e.g. three-branch piecewise linear one. Moreover, for fitting experiment data better, material failure criteria have been needed, however, it is not included in this example.

4. Plasticity in the components assembly model

Due to not changing the length of bonds, atomic movement perpendicular to atomic bond can not be modelled by simple pair-functional potentials, as dislocations, etc. The introduction of the concept of dislocations in [20,22] and several others [23,24] marked the first decisive step in explaining the phenomenon of plastic deformations. Dislocation slip is the main plastic deformation mechanism in most metals.

Slip is a typical two dimensional movement, it results in plastic deformation. As the basic research element, and for embodying the concept of the component of plastic deformations, slip system can be called as the "slip component". Its kinematic and kinetic variables are the slip quantity γ and the resolved shear stress τ, respectively. During the gliding process, the critical resolved shear stress τ_{cr} and the slip quantity γ have the following relation

$$\dot{\tau}^{(\alpha)} = \dot{\tau}_{cr}^{(\alpha)} = \sum_{\beta=1}^{n} h_{\alpha\beta}\dot{\gamma}^{\beta}, \quad \text{for } \dot{\gamma}^{\beta} > 0, \tag{30}$$

herein $h_{\alpha\beta}$ is the hardening modulus, $\alpha = \beta$ denotes the self-hardening and $\alpha \neq \beta$ the latent hardening. α and β indicate the αth and the βth slip components respectively. $\mathbf{b}^{(\alpha)}$ and $\mathbf{n}^{(\alpha)}$ are the unit vectors in the referential slip and normal directions of the αth slip component. A 2-order tensor is defined accordingly,

$$\mathbf{P}^{(\alpha)} = \frac{1}{2}\left(\mathbf{n}^{(\alpha)} \otimes \mathbf{b}^{(\alpha)} + \mathbf{b}^{(\alpha)} \otimes \mathbf{n}^{(\alpha)}\right). \tag{31}$$

For infinitesimal deformation, the resolved shear stress and stress field have the relation

$$\tau^{(\alpha)} = P_{ij}^{(\alpha)}\sigma_{ij}. \tag{32}$$

Similarly, the plastic strain can be expressed by these slip components

$$\varepsilon_{ij}^{p} = \sum_{\alpha=1}^{n} \gamma^{(\alpha)} P_{ij}^{(\alpha)}. \tag{33}$$

Finally, the relation between the plastic strain and the stress is given by

$$\dot{\varepsilon}_{ij}^{p} = S_{ijkl}^{p}\dot{\sigma}_{kl}, \tag{34}$$

where $\mathbf{S}^{\mathrm{p}}$ is the material plastic compliance tensor. For infinitesimal deformation, it is expressed in the form

$$S^{p}_{ijkl} = \sum_{\alpha=1}^{n}\sum_{\beta=1}^{n} \tilde{h}_{\alpha\beta} P^{(\alpha)}_{ij} P^{(\beta)}_{kl}, \tag{35}$$

herein $\tilde{h}_{\alpha\beta}$ is the inversion of $h_{\alpha\beta}$. The above equation is the sum of (continuous) slipping components. Supposing the elastic property not changing during slipping, from Eq. (25), there is

$$\dot{\varepsilon}^{\mathrm{e}}_{ij} = S^{\mathrm{ed}}_{ijkl}\dot{\sigma}_{kl}. \tag{25'}$$

where $\mathbf{S}^{\mathrm{ed}}$ is the elasto-damage compliance tensor, $\mathbf{S}^{\mathrm{ed}} = [\mathbf{C}^{\mathrm{ed}}]^{-1}$. Combining Eqs. (25′) and (35), and considering the relation:

$$\varepsilon_{ij} = \varepsilon^{\mathrm{e}}_{ij} + \varepsilon^{\mathrm{p}}_{ij}, \tag{36}$$

the elasto–plasto-damage constitutive equations are given by

$$\dot{\varepsilon}_{ij} = \left(S^{\mathrm{ed}}_{ijkl} + S^{\mathrm{p}}_{ijkl}\right)\dot{\sigma}_{kl} = S^{\mathrm{epd}}_{ijkl}\dot{\sigma}_{kl}, \tag{37}$$

herein $\mathbf{S}^{\mathrm{epd}}$ denotes the elasto–plasto-damage compliance tensor. Fig. 10 illustrates the proposed method.

The material yield surface and its evolution can be predicted by these slip components. Material yield surface and its evolution are constructed by means of intersecting these slip components', and Fig. 11 illustrates the constructing procedure for isotropic materials. τ^{0}_{cr} denotes the initial resolved shear stress. The Bauschinger Effect, isotropic and kinematic hardening, etc., [29,35,38] can be recurred easily by this construction of yield and loading surfaces, if slip components have different hardening properties. Moreover, for the strain of the slip component always perpendicular to its yield or loading surfaces, and considering material yield and loading surfaces are the internal enveloping surfaces of slip components' surfaces, the Illiushin Hypothesis is always sound. In addition, material loading surfaces can be independent or interdependent if the slip components' surfaces are independent or not.

The above derivations imply that the correlation between plasticity and damage is excluded. In this application, the authors show the feasibility of the proposed work to metals. The constitutive model is demonstrated here through the degradation of the material stiffness due to both the plastic deformation and damage. The metal investigated here is the aluminum alloy 2024-T3 [8], and plane stress situation is assumed. Orientational components bear elasto-damage deformation, and their discretization configuration is shown in Fig. 1. Slip component discretization is set that one has per 15^{0} in the whole plane. The response function of the orientational component is two-branch law, and the damage threshold (elastic) and failure strains are set as $\varepsilon^{\mathrm{e}}_{0} = 0.00727$ and $\varepsilon^{\mathrm{e}}_{c} = 0.0727$, respectively. For simplicity, the latent hardening is excluded in this example, and the self-hardening stiffness of all slip components is chosen as $h_{\alpha\alpha} = 1500$ (MPa), the initial critical

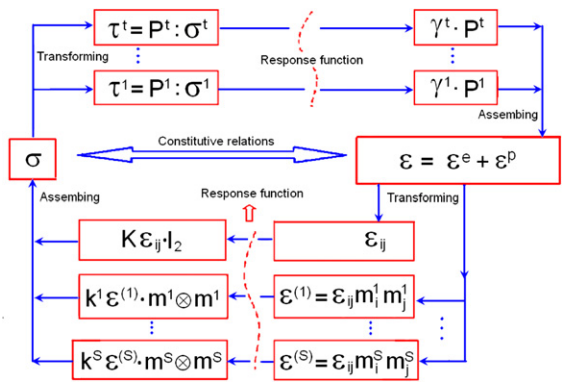

Fig. 10. The procedure of components assembly.

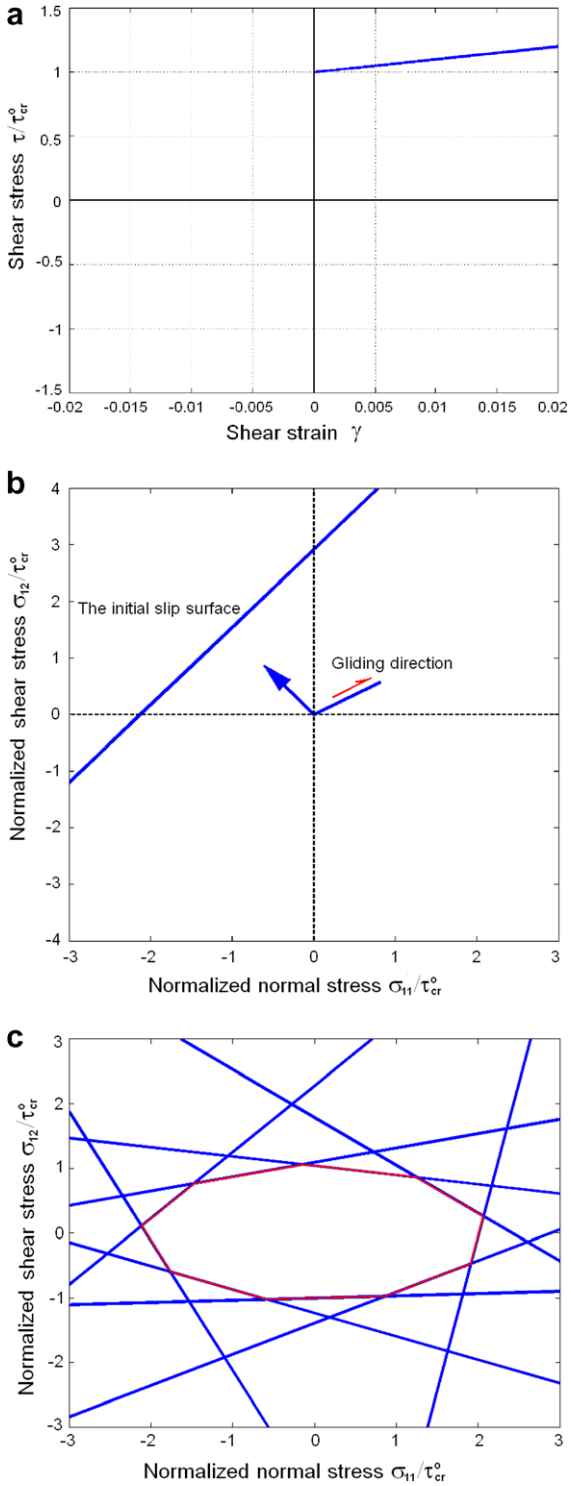

Fig. 11. The response function (a) and the yield surface (b) of the slip component, and the material yield surface (c).

resolved shear stress is $\tau^0_{cr} = 171.28$ (Mpa). The results are shown in Fig. 12. In which, the red line is the result of the component assembly model.

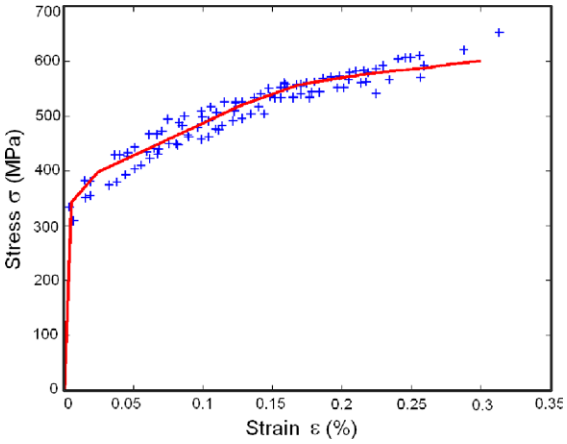

Fig. 12. Uniaxial stress–strain curve for aluminum alloy 2024-T3 (comparison with experiment data [8]).

5. Discussion

5.1. Comparing with classic anisotropic damage models

In the anisotropic damage models, the effective tensor $\bar{\sigma}$ is related to the stress tensor σ by the following linear transformation [16]:

$$\bar{\sigma}_{ij} = M_{ikjl}\sigma_{kl}, \tag{38}$$

where **M** is a fourth-order linear transformation operator called the damage effect tensor. Depending on the form used for **M**, it is very clear from the above equation that the effective stress tensor $\bar{\sigma}$ is generally not symmetric. Using a nonsymmetric effective stress tensor as given by Eq. (38) to formulate a constitutive model will result in the introduction of the Cosserat and a micropolar continuum [65,66]. However, the use of such complicated mechanics can be avoided if the proper fourth-order linear transformation tensor is formulated in order to symmetrize the effective stress tensor. Such a linear transformation tensor called the damage effect tensor is obtained in [15,18,67]:

$$M_{ikjl} = (\delta_{ik} - \phi_{ik})^{-\frac{1}{2}}\left(\delta_{jl} - \phi_{jl}\right)^{-\frac{1}{2}}, \tag{39}$$

$$M_{ikjl} = \frac{1}{2}\left[(\delta_{ik} - \phi_{ik})^{-1}\delta_{jl} + \delta_{ik}\left(\delta_{jl} - \phi_{jl}\right)^{-1}\right], \tag{40}$$

$$M_{ikjl} = 2\left[(\delta_{ik} - \phi_{ik})\delta_{jl} + \delta_{ik}(\delta_{jl} - \phi_{jl})\right]^{-1} \tag{41}$$

and

$$M_{ikjl} = (I_{ikjl} - \psi_{ikjl}), \tag{42}$$

where I_{ijkl} is the fourth-order identity tensor. However, it is very difficult to solve matrix inversion and square root, e.g., $(\delta_{ik} - \phi_{ik})^{-\frac{1}{2}}$. Alternatively, it is not easy to characterize physically the fourth-order damage tensor ψ_{ijkl} as opposed to the second-order damage tensor ϕ_{ij}. On the contrary, the component assembly model has the intrinsically symmetric elasto-damage stiffness, and the artificially symmetrical treatments in classic anisotropic damage models are no longer needed.

In classic anisotropic damage models, the plastic and dissipative potentials and the internal variables have been assumed at the representative volume element (RVE), and the choice of functions and variables is artificial to some extent. However, the basic research elements in component assembly model are three kinds of components, their deformations are simple. In addition, the constitutive equations (response functions) can be gotten physically especially in crystals, e.g., the response functions of the orientational and volumetric components from interatomic potentials and the response function of the slip one from crystal plasticity.

5.2. Comparing with microplane model

Just like microplane model [43–46], the basic research element is not RVE. The basic element in microplane model is discrete microplanes, and the stress–strain relations are defined independently on planes of all possible orientations in the microstructure, no matter what elasticity, plasticity and damage. Moreover, the microplane stresses or strains are constrained kinematically or statically to the macroscopic stress or strain tensors in a weak sense.

There are three basic research elements in the component assembly model, and they are the orientational component, the volumetric and slip ones, respectively. Actually, these components are re-divisions of RVE according to different deformation mechanisms. In which, as a 1D bar, the orientational component only bears the tensile or compressive loads. As a typical 2D component, the slip one can bear shear loads. The 3D volumetric component bears the hydrostatic stresses. Material is treated as a component assembly, and its constitutive equations have been formulated by assembling all kinds of components' response functions. Anisotropy has been incorporated naturally via component concept. Meanwhile, material damage and yield have been reflected via different components.

5.3. The relation between QC, VIB, cohesive zone and the proposed model

QC, VIB and the component assembly model have the same physical foundation, and they all are from interatomic potentials. In QC, the atoms are grouped according to the quantities of interatomic potentials, by means of combining with continuum mechanics (QC is used near crack tips or in slip bands and continuum mechanics is used in other regions). In component assembly model, the atoms are grouped according to the directions, and material is treated as a component assembly. VIB model is derived from pair potentials and has simple form. In which, due to not considering the embedding energy, it is constrained by the Cauchy relation, $C_{ijkl} = C_{ikjl}$.

Cohesive zone model has been used to simulate fracture process extensively. Material fracture work is expressed by cohesive zone models constitutive. Actually, material damage and fracture processes are atomistic bonds change and break continually, and the cohesive zone models constitutive can be gotten from interatomic potentials. Certainly, cohesive zone models constitutive can be gotten from components response functions by means of energy equivalence. Actually, material damage and its microstructure evolutions are occurred in space not plane.

Theoretical analysis indicates that the proposed method has the capacity of re-expressing the generalized Hooke's Law (Eq. (3)) and reproducing some results satisfactorily [68,69], preliminary computations show that component assembly model has the capacity of simulating material damage process, with the advantages of great conceptual simplicity, physical explicitness and intrinsic induced anisotropy etc.

Acknowledgements

This research work was sponsored by National Natural Science Foundation of China through Grant Nos. 10572140 and 10232050, and also partly by Ministry of Science and Technology Foundation No. 2002CB412706.

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