Discrete element model for crack propagation in brittle materials

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SUMMARY

We propose a discrete element model for brittle rupture. The material consists of a bidimensional set of closed-packed particles in contact. We explore the isotropic elastic behavior of this regular structure to derive a rupture criterion compatible to continuum mechanics. We introduce a classical criterion of mixed mode crack propagation based on the value of the stress intensity factors, obtained by the analysis of two adjacent contacts near a crack tip. Hence, the toughness becomes a direct parameter of the model, without any calibration procedure. We verify the consistency of the formulation as well as its convergence by comparison with theoretical solutions of tensile cracks, a pre-cracked beam, and an inclined crack under biaxial stress. Copyright © 2015 John Wiley & Sons, Ltd.

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1. INTRODUCTION

Real materials may present complex structure and uncountable flaws (cracks, property discontinuities, voids, etc.) which define their mechanical behavior. Theoretical approaches simplify the material description based on model parameters. In continuum mechanics, isotropic linear elasticity is described by only two parameters (e.g., Poisson's ratio ν and Young's modulus E) relating stresses to strains. If the elastic behavior is restrained to a certain range of stresses and strains, and no stress is conceivable outside this range, a quasi-brittle failure can be therefore associated. Under low stress (and strain) gradients, the rupture behavior depends basically on the strength of the material, which may be limited by some stress condition like in Rankine, Mohr–Coulomb, and Von Mises materials. On the other hand, under very high-stress gradients (e.g., induced by existing cracks), the rupture behavior is well described by fracture mechanics formulation. Crack propagation is mostly based on the evaluation of the energy release rate, which may be limited by the fracture energy of the material.

Various numerical methods from continuum mechanics have been adapted to study the fracture behavior of materials like the Barenblatt–Dugdale cohesive zone crack model [1, 2] in the early 1960s, special finite elements (finite element method) proposed by Henshell and Shaw [3] in the 1970s, and more recently the work of Belytschko with the extended finite element method [4–6]. These widely used methods present very good results, while the number of cracks is relatively limited. For very complex systems of cracks, presenting fragmentation patterns (e.g., induced by very large strains or cyclic loading), discrete approaches become more competitive options.

The discrete element method (DEM) [7] was originally developed for modelling granular and particulate systems [8–13]. Further developments have adapted the method to study the fracture of quasi-brittle materials such as concrete and rocks [14–18]. DEM is not based on continuum

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Figure 1. (a) Periodic compact distribution of particles to a discrete model and (b) the associated unit cell.

mechanics; materials are assimilated to assemblies of particles in contact (Figure 1). The constitutive parameters of these contacts (e.g., stiffness, strength, etc.) influence the behavior of the whole model at the macroscopic scale. These parameters are usually identified (calibrated) using some kind of optimization [19–21] intending to describe the expected behavior of the material (obtained experimentally, for example). This procedure allows the analysis of a specific range of experiments (or practical situations) previously considered during calibration (e.g., a sample under a bending moment should be calibrated considering tensile and compression tests). Despite the good concordance of discrete models with experimental results, it remains difficult to define the expected error of a prediction when no reference experimental data are available for the comparison. It is usually the case, because discrete element models are normally not conceived to present a convergent behavior associated with a systematic evolution of the discretization (as in continuum models), but an approximative behavior for a given sample configuration.

We aim to associate the advantages of continuous approaches like theoretical background and convergence toward a unique solution to a discrete approach. Recent works [22, 23] present analytical expressions which relate directly DEM contact parameters to elastic continuous solid parameters (i.e., Young's modulus and Poisson's ratio). Based on the existence of a relation between discrete and continuous models in elasticity, we propose a DEM approach for brittle materials. The concordance with classical theories (continuum mechanics) exempts us of any previous calibration of the model parameters in order to obtain convergent results.

This paper begins with a presentation of the contact law used in our discrete model and its relation with the material elasticity (Section 2). In Section 3, we present the theoretical elements of our discrete approach based on fracture mechanics. We compare our numerical results to classical cases of tensile fracture (mode I), shear fracture (mode II), and mixed mode in Section 4. Finally, we present the conclusions of our work.

2. STRESS AND STRAIN ANALOGY IN ISOTROPIC ELASTICITY

While cracks are not propagating, we can suppose that brittle materials present an elastic behavior. For a given problem, comparable results between continuous and discrete approaches must present similar stress and strain distributions. Let us consider a homogeneous (elastic and isotropic) material as an assembly of particles in contact, following the dense pack pattern shown in Figure 1(a). All mechanical properties of these particles are defined at the contact level (a local scale). The forces are transmitted through contacts, while material strain depends on particles translational and rotational motions.

2.1. Contact model

We adopt a linear relation between contact forces and relative particle position which can be seen as a simplified version of Hertz contact model (Figure 1). Let us define $\mathbf{n}_{ij}$ as the normal vector pointing from the center of i to the center of j and $\mathbf{t}_{ij}$ as the tangential vector, orthogonal to $\mathbf{n}_{ij}$ and positively oriented shown in Figure 2.

The contact force (applied by a particle j over a particle i) is decomposed in normal and tangential components (Figure 2), respectively $\mathbf{N}_{ij} = \mathbf{N}_{ij}^e + \mathbf{N}_{ij}^v$ and $\mathbf{T}_{ij} = \mathbf{T}_{ij}^e + \mathbf{T}_{ij}^v$, both depending on two contributions.

Figure 2. Normal displacement (a), tangential displacement, (b) and contact forces associated (c) between two particles i and j .

The normal component is the sum of two contributions $\mathbf{N}_{ij} = \mathbf{N}_{ij}^e + \mathbf{N}_{ij}^v$. The elastic one, defined as $\mathbf{N}_{ij}^e = k_n \delta_n \mathbf{n}_{ij}$, depends on the normal displacement δ_n and the normal stiffness k_n . The inelastic one, defined as $\mathbf{N}_{ij}^v = c_n \dot{\delta}_n \mathbf{n}_{ij}$ depends on a viscous damping parameter c_n and the time derivative of the normal deflection $\dot{\delta}_n$.

Similarly, the elastic term of the tangential force, $\mathbf{T}_{ij}^e = k_t \delta_t \mathbf{t}_{ij}$ depends only on tangential relative displacement δ_t and tangential stiffness k_t . The inelastic term of the tangential force, $\mathbf{T}_{ij}^v = c_t \dot{\delta}_t \mathbf{t}_{ij}$ is based on a tangential viscous damping parameter c_t and on the time derivative of the tangential displacement $\dot{\delta}_t$. The latter contribution is only introduced to stabilize the numerical integration scheme. We choose c_n, c_t as a small fraction of $\sqrt{mk_n}$ (where m is the particle mass), which guarantees a negligible inelastic effect.

2.2. Particle displacement and elastic behavior

Our numerical approach is based on DEM like in [7, 13] alternating the computation of all contact forces and the application of Newton's second law to the particles. The discrete particle motion equations are solved by Gear's order three predictor–corrector algorithm [24]. We adopt a 2D close-packing distribution of particles, as shown in Figure 3(a), to represent a linear elastic isotropic material (Figure 3(b)). With a discrete approach, the relation between relative position of the particles and contact forces is analogous to strain and stress relation in a continuous approach. The balance of the contact forces gives rise to a macroscopic stress tensor. Equivalence between continuous and discrete approaches [22, 25] has shown that normal and tangential stiffness (k_n and k_t , respectively) can be directly related to elasticity parameters of the continuous solid (Young's modulus E and Poisson's ratio ν , for example) as follows (in-plane stress):

$$\begin{cases} k_n = \frac{E}{\sqrt{3}(1-\nu)}, \\ k_t = \frac{1-3\nu}{1+\nu} k_n = \frac{1-3\nu}{\sqrt{3}(1-\nu^2)} E. \end{cases} \quad (1)$$

The relations expressed in Equation (1) were deduced for homogeneous stress and strain conditions. In more general conditions, where stress and strain gradients may be observed, they indicate asymptotic limits. Better correlations between continuous and discrete approaches are naturally obtained for materials described by smaller particles, which represent a more precise discretization.

Figure 3. (a) Periodic structure of the discrete material and (b) continuous equivalence.

3. STRESS INTENSITY FACTORS AND CRACK PROPAGATION ANALOGY FOR BRITTLE MATERIALS

The convergence similarity between discrete and continuous approaches in elasticity allows us to analyze the singular stress field at the vicinity of a crack (Figure 4) in order to extend the notion of stress intensity factors [26] and crack propagation to the discrete approach.

3.1. Stress field near a crack tip and crack propagation

Based on the polar coordinate system placed at the crack tip (Figure 4), the stress components can be written for $r > 0$ as [27] follows:

$$\begin{cases} \sigma_{rr}(r, \theta) = \frac{K_{rr}(\theta)}{\sqrt{2\pi r}}, & \text{with } K_{rr}(\theta) = K_I \cos \frac{\theta}{2} \left(1 + \sin^2 \frac{\theta}{2}\right) + K_{II} \left(-\frac{5}{4} \sin \frac{\theta}{2} + \frac{3}{4} \sin \frac{3\theta}{2}\right); \\ \sigma_{\theta\theta}(r, \theta) = \frac{K_{\theta\theta}(\theta)}{\sqrt{2\pi r}}, & \text{with } K_{\theta\theta}(\theta) = K_I \cos \frac{\theta}{2} \left(1 - \sin^2 \frac{\theta}{2}\right) + K_{II} \left(-\frac{3}{4} \sin \frac{\theta}{2} - \frac{3}{4} \sin \frac{3\theta}{2}\right); \\ \sigma_{r\theta}(r, \theta) = \frac{K_{r\theta}(\theta)}{\sqrt{2\pi r}}, & \text{with } K_{r\theta}(\theta) = K_I \sin \frac{\theta}{2} \cos^2 \frac{\theta}{2} + K_{II} \left(\frac{1}{4} \cos \frac{\theta}{2} + \frac{3}{4} \cos \frac{3\theta}{2}\right). \end{cases} \quad (2)$$

The parameters K_I and K_{II} are the so-called stress intensity factors. K_I is associated with crack opening mode, while K_{II} is associated with shear mode. Their values, which depend on loading and crack shape, quantify the strength of the singularity. For brittle materials (in the domain of linear elastic fracture mechanics), they are directly associated with the energy release rate during crack extension [26]. Some crack propagation criteria for brittle materials take advantage of this principle, relating the stress intensity factors to the material toughness K_{IC} . K_{rr} , $K_{r\theta}$, and $K_{\theta\theta}$ are the effective stress intensity factors, and θ is the relative angle defined by the tangent direction at the crack tip. A free surface condition imposes in reality $\sigma_{rr}(0, \theta) = 0$ and $\sigma_{r\theta}(0, \theta) = 0$; consequently, $\sigma_{\theta\theta}(0, \theta)$ is a principal stress.

One of the simplest criteria of crack propagation in mixed mode was proposed by Erdogan *et al.* [28], which is based on the maximum circumferential tensile stress. This theory states that crack propagates perpendicularly to the direction of the greatest tension, following θ_0 . Considering the terms of Equation (2), that is to say $K_{\theta\theta}(\theta_0) = \max K_{\theta\theta}(\theta)$, and consequently $K_{r\theta}(\theta_0) = 0$. For a given stress distribution, the stability of the crack depends therefore on the structure material. As long as $K_{\theta\theta}(\theta_0) < K_{IC}$, the crack remains stable, otherwise it propagates [27].

In the discrete medium, the efforts are transmitted by the contact forces between the particles. In the next section, we present the equivalence between the contact force (discrete medium) and the principal stresses (continuous medium). From the values of the principal stresses acting near the crack, we complete the construction of the model with a definition of the stress intensity factors for the discrete medium.

3.2. Discrete crack analysis

3.2.1. Mean stresses and strains in the discrete medium. We determine mean values of the components of the stress and strain tensor based on the behavior of one pair of contacts associated with three particles (i , j , and k) in contact: ki and kj (Figure 5(a)), near a crack under a given loading

Figure 4. Crack tip and stresses near a crack tip.

Figure 5. (a) The adjacent contacts at the crack tip in a (b) discrete medium.

Figure 6. (a) Contact forces and (b) their resultants for an adjacent pair of contacts.

(Figure 5(b)). We define a local coordinate system $(n; t)$, where t virtually connects both contacts for which n is an orthogonal axis.

The distribution of contact forces on the pair of contacts is shown in Figure 6(a); it has normal components (N) and tangential components (T). The components of the resultant contact force in $(n; t)$ coordinate system (f_n and f_t , respectively; Figure 6(b)) can be written as follows:

$$\begin{cases} f_n = \frac{1}{2} (N_{ik} \sqrt{3} + T_{ik} + N_{jk} \sqrt{3} - T_{jk}) , \\ f_t = \frac{1}{2} (-N_{ik} + T_{ik} \sqrt{3} + N_{jk} + T_{jk} \sqrt{3}) . \end{cases} \quad (3)$$

We can associate mean stresses to these forces, considering the length of a particle diameter d :

$$\begin{cases} \bar{\sigma}_n = f_n/d , \\ \bar{\sigma}_t = f_t/d . \end{cases} \quad (4)$$

The contacts ki and kj may present normal and tangential displacements (δ_{nik} and δ_{tik} ; $\delta_{nj k}$ and δ_{tjk} , respectively). Mean strain values $\bar{\varepsilon}_{nn}$ and $\bar{\varepsilon}_{tt}$ (Figure 7(a)) can be derived from these contact displacements, considering the dimensions of the particle structure (Figure 7(b)):

$$\begin{cases} \bar{\varepsilon}_{nn} = \frac{1}{2} (\delta_{nik} \sqrt{3} + \delta_{nj k} \sqrt{3} + \delta_{tik} - \delta_{tjk}) \frac{2}{d \sqrt{3}} , \\ \bar{\varepsilon}_{tt} = \frac{1}{2} (\delta_{nik} + \delta_{nj k} - \delta_{tik} \sqrt{3} + \delta_{tjk} \sqrt{3}) \frac{2}{d} , \end{cases} \quad (5)$$

3.2.2. Principal stresses and strains. The complete stress tensor (in 2D) can be expressed by the principal stresses $\bar{\sigma}_I$ and $\bar{\sigma}_{II}$ and their orientation. Let us call β the angle between $(n; t)$ and the coordinate system associated with the principal stresses (Figure 8(a)). This principle can be extended

Figure 7. (a) Contact displacements, mean strains, and (b) associated dimensions of the particle structure.

Figure 8. (a) Mean stresses $\bar{\sigma}_n$ and $\bar{\sigma}_t$, and (b) their relation to the stress field of an equivalent continuous medium.

Figure 9. Mohr's circle associated on stress state $\bar{\sigma}_n$ and $\bar{\sigma}_t$.

to the mean stress values on the discrete medium (Figure 8(b)). After a force balance, the principal stresses may be calculated as

$$\begin{cases} \bar{\sigma}_I = \bar{\sigma}_n + \bar{\sigma}_t \tan(\beta), \\ \bar{\sigma}_{II} = \bar{\sigma}_n - \bar{\sigma}_t / \tan(\beta). \end{cases} \quad (6)$$

In the Mohr plane (Figure 9), we observe the infinite number of circles associated with a pair of stress values $\bar{\sigma}_n$ and $\bar{\sigma}_t$. For this reason, it is imperative to know the angle β for the determination of mean principal stresses $\bar{\sigma}_I$ and $\bar{\sigma}_{II}$.

For a homogeneous material, the elastic behavior can be written as a function of Young's modulus E and Poisson's ratio ν

$$\underline{\underline{\varepsilon}} = \frac{1}{E} \left[(1 + \nu) \underline{\underline{\sigma}} - \nu \text{tr}(\underline{\underline{\sigma}}) \underline{\underline{I}} \right], \quad (7)$$

where $\underline{\underline{\varepsilon}} = \begin{bmatrix} \bar{\varepsilon}_I & 0 \\ 0 & \bar{\varepsilon}_{II} \end{bmatrix}$ is the mean stresses tensor (in 2D); $\underline{\underline{\sigma}} = \begin{bmatrix} \bar{\sigma}_I & 0 \\ 0 & \bar{\sigma}_{II} \end{bmatrix}$ is the mean strains tensor (in 2D); $\bar{\varepsilon}_I$ and $\bar{\varepsilon}_{II}$ are mean principal strains; $\bar{\sigma}_I$ and $\bar{\sigma}_{II}$ are mean principal stresses; and $\underline{\underline{I}}$ is identity matrix. The principal stresses are directly related to principal strains by the expression:

$$\begin{bmatrix} \bar{\varepsilon}_I & 0 \\ 0 & \bar{\varepsilon}_{II} \end{bmatrix} = \frac{1 + \nu}{E} \begin{bmatrix} \bar{\sigma}_I & 0 \\ 0 & \bar{\sigma}_{II} \end{bmatrix} - \frac{\nu}{E} (\bar{\sigma}_I + \bar{\sigma}_{II}) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \quad (8)$$

Any shear deformation is observed in the direction associated with the principal stresses. Therefore, β also defines the direction of the mean principal strains (Figure 10).

The unit vectors that define the coordinate (n, t) with principal coordinate (Figure 6(a)) can be written as a function of β as: $\underline{n} = (\cos \beta, -\sin \beta)$ and $\underline{t} = (\sin \beta, \cos \beta)$. The mean strains $\bar{\varepsilon}_{nn}$ and $\bar{\varepsilon}_{tt}$ are related to the mean principal strains by the relations $\bar{\varepsilon}_{nn} = \underline{n} \cdot \underline{\underline{\varepsilon}} \cdot \underline{n}$ and $\bar{\varepsilon}_{tt} = \underline{t} \cdot \underline{\underline{\varepsilon}} \cdot \underline{t}$, we have

$$\begin{cases} \bar{\varepsilon}_{nn} = \bar{\varepsilon}_I \cos^2 \beta + \bar{\varepsilon}_{II} \sin^2 \beta, \\ \bar{\varepsilon}_{tt} = \bar{\varepsilon}_I \sin^2 \beta + \bar{\varepsilon}_{II} \cos^2 \beta. \end{cases} \quad (9)$$

Like the principal stresses, the determination of β is necessary to define the mean principal strains $\bar{\varepsilon}_I$ and $\bar{\varepsilon}_{II}$ from a pair of strains values $\bar{\varepsilon}_{nn}$ and $\bar{\varepsilon}_{tt}$ acting on a pair of contacts.

3.2.3. Determination of β . We can determine the value of β by associating the information from mean strains and stresses at a pair of contacts. From the equations system 8 and 9, we can write the trace of the strain tensor from the trace of the stress tensor

$$\bar{\varepsilon}_{nn} + \bar{\varepsilon}_{tt} = \frac{1 - \nu}{E} (\bar{\sigma}_I + \bar{\sigma}_{II}). \quad (10)$$

From the expressions of the mean principal stresses Equation (6), Equation (10) can be written simply as follows:

$$\bar{\varepsilon}_{nn} + \bar{\varepsilon}_{tt} = \frac{1 - \nu}{E} (\bar{\sigma}_n + \bar{\sigma}_t \tan \beta + \bar{\sigma}_n - \bar{\sigma}_t / \tan \beta). \quad (11)$$

Figure 10. (a) Mean strain in a discrete medium and (b) in a continuous medium.

We can simplify Equation (11) by isolating

$$\tan \beta - \frac{1}{\tan \beta} = -\frac{2}{\tan(2\beta)} = \frac{A}{\bar{\sigma}_t}, \quad (12)$$

where $A = \frac{E}{1-\nu}(\bar{\varepsilon}_{nn} + \bar{\varepsilon}_{tt}) - 2\bar{\sigma}_n$. Finally, the value of β can be obtained

$$\beta = -\frac{1}{2} \arctan\left(\frac{2\bar{\sigma}_t}{A}\right). \quad (13)$$

From the values of $\bar{\sigma}_n$ and $\bar{\sigma}_t$ Equation (4) and β Equation (13), the stress $\bar{\sigma}_I$ can be determined by applying Equation (6) ($\bar{\sigma}_I = \bar{\sigma}_n + \bar{\sigma}_t \tan \beta$). But, for the stress $\bar{\sigma}_{II}$, it is sensitive with small values of β . By introducing the values of the mean strains $\bar{\varepsilon}_{nn}$ and $\bar{\varepsilon}_{tt}$ Equation (5) and the value of σ_I in Equation (10), we obtain

$$\bar{\sigma}_{II} = \frac{E}{1-\nu}(\bar{\varepsilon}_{nn} + \bar{\varepsilon}_{tt}) - \bar{\sigma}_I. \quad (14)$$

3.2.4. Failure criterion – calculation of effective stress intensity factor $K_{\theta\theta}$. The stress intensity factor $K_{\theta\theta}$ must be obtained for a certain direction θ_0 , orthogonal to the direction of the principal stress. The maximum circumferential tensile stress $\bar{\sigma}_{\theta\theta}(\theta_0)$ is then defined as (Figure 10) follows:

$$\begin{cases} \bar{\sigma}_{\theta\theta}(\theta_0) = \bar{\sigma}_I, & \text{if } |\beta| \leq \pi/4, \\ \bar{\sigma}_{\theta\theta}(\theta_0) = \bar{\sigma}_{II}, & \text{if } |\beta| > \pi/4, \end{cases} \quad (15)$$

where $\bar{\sigma}_I$ and $\bar{\sigma}_{II}$ are the mean principal stresses acting on two adjacent contacts (Figure 8(b)).

From the value of stress $\sigma_{\theta\theta}(r, \theta_0)$ close to a crack Equation (2), its mean value over a distance $0 < r < d$ can be written of a function of $K_{\theta\theta}(\theta_0)$ as

$$\bar{\sigma}_{\theta\theta}(\theta_0) = \frac{1}{d} \int_0^d \sigma_{\theta\theta}(r, \theta_0) dr = \frac{1}{d} \int_0^d \frac{K_{\theta\theta}(\theta_0)}{\sqrt{2\pi r}} dr = \sqrt{\frac{2}{\pi d}} K_{\theta\theta}(\theta_0). \quad (16)$$

Using the value of $\bar{\sigma}_{\theta\theta}(\theta_0)$ obtained by the study of the forces on two contacts Equation (15), the value of the effective stress intensity factor $K_{\theta\theta}(\theta_0)$ is simply calculated (depending on the result of Equation (16) as

$$K_{\theta\theta}(\theta_0) = \bar{\sigma}_{\theta\theta}(\theta_0) \sqrt{\frac{\pi d}{2}}. \quad (17)$$

In practice, we calculate the stress intensity factor $K_{\theta\theta}(\theta_0)$ for each pair of neighbor contacts. The analysis of all contact pairs eliminates any difficulty of finding crack tips. When $K_{\theta\theta}(\theta_0)$ reaches the value of the material toughness K_{IC} , the cohesion forces of the most tensioned contact of the pair are set to zero, giving rise to the propagation of the crack at the proximity of this contact.

3.3. Isotropic behavior

The structure used in our discretization presents an angular period of $\pi/3$ radians (Figure 11). However, this geometrical anisotropy describes coherent isotropic elasticity [22]. Our approach in fracture mechanics is based entirely on elasticity results. We may expect the same coherence on the crack analysis, with eventually some difference with the convergence. In a rough discretization, cracks may be described slightly differently considering the direction of the discrete structure. These differences tend to disappear with the refinement of the model.

Figure 11. $\pi/3$ geometrical periodicity.

4. COMPARISON WITH CLASSICAL RESULTS

In this section, we compare our numerical results to continuous solutions of fracture mechanics of brittle materials. Three situations are analyzed: pure tensile fracture, mixed mode beam crack, and biaxial fracture. The load intensity in all examples is driven by imposed displacements, which allow us to keep the crack propagation in quasi-static regime.

We suppose, for simplicity, that the particle diameter d also corresponds to the thickness of the simulated plane stress geometries without loss of generality. The units of length and mass are respectively d and the particle mass m . This implies (for a given material toughness K_{IC}) $T = \sqrt{m/(K_{IC}\sqrt{d})}$ as time unit and $K_{IC}/\sqrt{d}$ as stress unit. Small strain is modeled taking $k_n = 10^4 K_{IC}/\sqrt{d}$ as normal stiffness. The ratio between tangential and normal stiffness $k_t/k_n = 0.5$ (directly related to Poisson ratio) has no fundamental effect in plane stress results. We adopt a small value of viscous damping $c_n = 0.65\sqrt{mK_{IC}\sqrt{d}}$.

4.1. Tension panel

We present the results for two pre-cracked samples: middle-crack tension panel (Figure 12(a)) and double-edge notch tension panel (Figure 12(b)), which are classical examples of tensile (mode I) crack. A vertical displacement induces a mean tensile stress Σ to the sample. We measure the maximum stress value $\Sigma^{\max}$ supported by the structure before complete fracture of the panel. The panels have a rectangular shape with height equal to three times width L to avoid eventual boundary effects.

Figure 12. Tensile test: (a) middle-crack panel and (b) double-edge notch panel. The discrete samples correspond to $L/d = 11$.

Our numerical results of $\Sigma^{\max}$ are compared with the following expressions [29]:

- middle-crack tension panel

$$\Sigma^{\max} = \frac{K_{IC}}{\sqrt{\pi a}} \sqrt{\cos \frac{\pi a}{L}} [1 - 0.1(a/L)^2 - 0.96(a/L)^4]^{-1}, \quad (18)$$

- double-edge notch tension panel

$$\Sigma^{\max} = \frac{K_{IC}}{\sqrt{\pi a}} \sqrt{1 - \frac{2a}{L}} [1.122 - 1.122(a/L) - 0.82(a/L)^2 + 3.768(a/L)^3 - 3.04(a/L)^4]^{-1}. \quad (19)$$

In both cases, four different crack lengths a/L were tested: 3/22, 4/22, 5/22, and 6/22. The maximum stress $\Sigma^{\max}$ supported by the panels before fracture propagation decreases when crack length grows as shown in Figure 13. The systematic variation of the ratio L/d allows the analysis of the discrete approach convergence. Higher values of L/d are associated with more precise descriptions of the crack zone inducing better results whatever the crack type. We observe an error of 10–15% for $L/d = 11$, which decreases to less than 5% for $L/d = 22$ and keep decreasing for subsequent increase of L/d .

A consistent isotropic description is supported by the results obtained with a discretization presenting an angular offset of $\pi/6$ rad for $L/d = 88$ (as discussed in Section 3.3, this offset corresponds to half of the angular period of $\pi/3$ rad of the discrete structure). This absence of the effect of the orientation of the discrete structure for two extreme cases ($\varphi = 0$ and $\varphi = \pi/6$ radians) is a strong indicator of isotropic behavior described by the failure criterion, and this is confirmed with the study of crack propagation in mixed mode in the following sections.

Figure 13. Normalized maximum stress $\Sigma^{\max} \sqrt{L}/K_{IC}$ as a function of the crack length a/L for the (a) middle-crack panel and (b) double-edge notch panels with different discretizations: ($\square$) $L/d = 11$, ($\circ$) $L/d = 22$, ($\triangle$) $L/d = 44$, (∇) $L/d = 88$, and ($\blacktriangledown$) $L/d = 88$ with an angular offset of the particle structure of $\pi/6$ radians. The continuous lines indicate the reference expressions for $\Sigma^{\max}$ corresponding to Equations (18) and (19).

Figure 14. (a) Pre-cracked beam setup and (b) collapsed structure for $L/d = 22$.

4.2. Pre-cracked beam

The crack tip of the pre-cracked beam in Figure 14(a) is under mixed mode (I and II). The stress intensity factors can be written as $K_I = 8.76M\sqrt{\pi a}/L^2$ and $K_{II} = 1.39V\sqrt{\pi a}/L$ [30], where L is the beam height, $a = 0.5L$ is the crack length, M and V are the bending moment and the shear force, respectively. According to Figure 14(a), $M = 0.1875LP$ and $V = 0.625P$, both are proportional to the force per unit of length P , applied over the beam thickness by imposed displacements. Following the maximum circumferential tensile stress, the limit $K_{\theta\theta}(\theta_0) = K_{IC}$ imposes a maximum value for P , $P_{\max} \approx 0.37K_{IC}\sqrt{L}$ before the collapse of the structure, shown in Figure 14(b) for a rough discretization. The crack propagation angle associated $\theta_0 \approx 41.4^\circ$ Equation (A.3) corresponds nearly to the path from the crack tip until the loading force P .

We have tested three different discretizations L/d : 22, 44, and 88. We obtain a limit load of $90\%P_{\max}$ with the first (and roughest) one. The two other leads respectively to 95% and 98% of $P_{\max}$, indicating a good convergence to the theoretical value.

4.3. Biaxial fracture

As previously seen for the pre-cracked beam, shear stress may induce crack deflection. Let us consider a square plate (side length L) under biaxial stresses (lateral compression Σ_x and vertical tension Σ_y – controlled by the displacements of non-frictional moving walls) with an initial inclined crack of length a (Figure 15(a)). Depending on the initial crack angle α , a pure shear stress condition (in α direction) can be obtained if $\Sigma_x/\Sigma_y = \tan^2 \alpha$. Following the maximum circumferential tensile stress criterion (Section 3.1), for pure shear stress ($K_I = 0$), the angle which maximizes $\sigma_{\theta\theta}$ (Equation (A.3) in Appendix A) is $\theta_0 \simeq 70.5^\circ$ (relative to α). The crack deflection angle θ_0 is only a prediction of the initial crack propagation. The general tendency of the crack is to become horizontal, orthogonal to stress tensile direction.

The results of the simulation of an inclined crack with $\alpha = 60^\circ$, $a/L = 0.41$, $L/d = 176$ are shown in Figure 15(a) and (b). The crack propagation presents a coherent path tending slightly to a

Figure 15. (a) Square plate with an inclined crack under biaxial loading. The dotted lines indicate the crack propagation path. (b) Simulated inclined crack under biaxial load. In detail, (c) the theoretical prediction of the crack branching.

horizontal direction (Figure 15(a)). In detail, in Figure 15(b), the theoretical prediction of the initial crack deflection is fairly obtained.

5. CONCLUSIONS

We propose in this paper a DEM approach in fracture mechanics adapted to the analysis of isotropic brittle materials, which is entirely compatible with continuum classical theory. Based on the equivalence between discrete and continuum approaches in elasticity, we determine the tensors of stress and strain as a function of the forces and displacements of two adjacent contacts. It allows us to calculate the stress intensity factor $K_{\theta\theta}$ (in polar coordinates) and introduce the toughness of the material as a model parameter without any previous calibration, which represents an important feature for DEM models.

The consistency of the formulation is verified by numerical simulations; the DEM approach is first applied to two tensile cracks (mode I) and a pre-cracked beam (mixed mode). In these cases, the maximum load before the collapse of the structures is compared with theoretical solutions, wherein a fast monotone convergence as function of the discretization (particle size) is observed.

A usual drawback of discrete approaches is the anisotropy due to the particle structure adopted on the models, specially for regular patterns [25]. This undesirable effect on the study of isotropic materials is avoided in our formulation as shown by the results in mode I; two different orientations of the structure produce similar results. The biaxial test of the sample with an initial inclined crack under pure shear stress (mode II) also indicates a reduced effect of the particle structure on the crack branching, which follows the theoretical prediction. An isotropic behavior (despite the anisotropic structure of the discrete model) is essential to extend the scope to crack initiation and associate the strength of the material as a model parameter, as shown by Le [31].

APPENDIX: θ_0 AS FUNCTION OF K_I AND K_{II} FOR THE MAXIMUM CIRCUMFERENTIAL STRESS CRITERIUM

The angle θ_0 can be derived for known stress intensity factors K_I and K_{II} . Based on Equation (2) and considering the maximum circumferential stress criterion ($K_{r\theta}(\theta_0) = 0$), we can write

$$\frac{K_{II}}{K_I} = \frac{-\sin \frac{\theta_0}{2} \cos^2 \frac{\theta_0}{2}}{\frac{1}{4} \cos \frac{\theta_0}{2} + \frac{3}{4} \cos \frac{3\theta_0}{2}} = \frac{\sin \theta_0}{1 - 3 \cos \theta_0}. \quad (\text{A.1})$$

Equation (A.1) can be directly solved for θ_0 by numerical methods or developed analytically as follows.

If we expand Equation (A.1) and divide the whole expression by $\sqrt{K_I^2 + (3K_{II})^2}$, we have

$$\sin \theta_0 \cos \phi + \cos \theta_0 \sin \phi = \sin(\theta_0 + \phi) = \frac{K_{II}}{\sqrt{K_I^2 + (3K_{II})^2}}, \quad (\text{A.2})$$

where $\cos \phi = K_I / \sqrt{K_I^2 + (3K_{II})^2}$ and $\sin \phi = 3K_{II} / \sqrt{K_I^2 + (3K_{II})^2}$.

Finally, the exact value of θ_0 can be obtained by the inversion of Equation (A.2) as

$$\theta_0 = \arcsin \left(\frac{K_{II}}{\sqrt{K_I^2 + (3K_{II})^2}} \right) - \phi, \quad (\text{A.3})$$

where $\phi = \arccos \left(K_I / \sqrt{K_I^2 + (3K_{II})^2} \right) = \arcsin \left(3K_{II} / \sqrt{K_I^2 + (3K_{II})^2} \right)$.

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