Numerical Simulation of Elastic Behaviour and Failure Processes in Heterogeneous Material

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Abstract: A general numerical approach is developed to model the elastic behaviours and failure processes of heterogeneous materials. The heterogeneous material body is assumed composed of a large number of convex polygon lattices with different phases. These phases are locally isotropic and elastic-brittle with the different lattices displaying variable material parameters and a Weibull-type statistical distribution. When the effective strain exceeds a local fracture criterion, the full lattice exhibits failure uniformly, and this is modelled by assuming a very small Young modulus value. An auto-select loading method is employed to model the failure process. The proposed hybrid approach is applied to plane stress problems with fracture patterns and effective loaddisplacement curves presented to illustrate the full failure process.

keyword: Heterogeneous materials; Weibull distribution; Elastic-brittle model; Failure process; Finite element method.

1 Introduction

Heterogeneous materials (such as composites, polymer blends, ceramics, concrete, etc) are used more and more in many modern structures, because their mechanical properties of strength, stiffness and toughness have significantly improved. During loading of these materials, micro-mechanical failure mechanisms, such as matrix cracking, void formation and fibre-matrix debonding, are frequently encountered, requiring a numerical simulation for their determination. Moreover, when developing new materials, the relations between the micro-mechanical failure mechanisms and the microscopic deformation behaviour are necessary to predict macroscopic properties of the microstructure.

Heterogeneity implies material properties vary spatially.

It is difficult to observe and/or to simulate the spatial pattern of material heterogeneity from micro to macro scales. The irregular and complex nature of spatial variability of material properties deny a precise quantitative description of the microstructure geometry because of uncertainties due to insufficient detail information. Therefore, a statistical model is an attractive alternative mathematical framework to describe heterogeneity.

Many statistical theories have been developed to achieve this goal. For example, the homogenization method developed for heterogeneous materials with periodic microstructures. In this model the material is assumed statistically homogeneous with local material properties treated as constant when averaged over a representative volume element (RVE). The real heterogeneous material is therefore replaced by a homogeneous one, in which the local material properties are determined from the averages of the representative volume elements in the original material. Hashin (1983) and Nemat-Nasser and Hori (1993) present comprehensive reviews of the RVE analysis. Based on this mathematical framework, many significant contributions developing the model have been produced, for example, by Hollister and Kikuch (1992), Ghosh, Lee and Moorthy (1995, 2005 Raghavan), Boutin (1996), van der Sluis, Vosbeek, Schreurs and Meijer (1999, 2000), Terada, Hori, Kyoya and Kikuchi (2000), Ganser, Fischer and Werner (2000), Kouznetsova, Geers and Brekelman (2002), Ostoja-Starzewski (1999, 2002), Fish and Chen (2003). These authors and others have successfully applied the method to determine the effective elastic properties of various heterogeneous materials with periodic microstructures. However, in practical problems, many heterogeneous materials exhibit significant randomness in their geometrical configurations and even a periodic distribution of a single cell is seldom observed. Moreover, the homogenization method is unsuitable to simulate the failure processes in heterogeneous materials.

Finite element methods have been used to simulate the

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failure processes of homogeneous materials (see, for example, Mackerle 2000, Zienkiewicz and Taylor 2000). However, such approaches are not as numerically efficient for heterogeneous materials as homogenous materials because of difficulties arising from mesh generation, mesh restructuring and stiffness matrix evaluations, which are often required in simulations of crack initiation and propagation. The spring network method, borrowed from material physics, provides an efficient approach to simulate the failure processes of heterogeneous materials. This method models the properties of the heterogeneous medium by assigning the spring constants to model the spring bonds of all lattices according to the local phase properties. The approach allows cracks to be created in the material by simply removing the spring bonds. Various studies relating to the application of the spring network method to the fracture simulation of heterogeneous media are described by Herrmann and Roux (1990), Grah, Alzebdeh, Sheng, Vaudin, Bowman, and Ostoja-Starzewski, (1996), Krajcinovic (1996), Alzebdeh, Jasiuk, and Ostoja-Starzewski (1998), Ostoja-Starzewski and colleagues (see, 1989, 1996a, 1996b, 1997a, 1997b, 1998).

In the present study, a numerical approach is developed to model the behavior of three-dimensional heterogeneous brittle materials for both compressive and tensile cases by Chen, Y. H., Yao Z. H., and Zheng X. P. (2002, 2003). This hybrid method is based on the conventional displacement finite element method incorporating techniques from the spring network method and the volume average concept in RVE, thus effectively reducing the computational complexity associated with such micromechanical simulations. A more general approach is now developed to model the elastic behaviours and failure processes of two-dimensional heterogeneous materials. Lattice model and statistical approaches are used to simulate initial heterogeneity of the material. A simple elastic-brittle constitutive law and breaking rule in every lattice is employed. In each load-step stage the problem is treated as linear allowing use of an auto-select loading method to model a realistic failure process. When the effective strain exceeds the local fracture criterion, the full lattice is considered to fail uniformly. This is implemented by taking a very small Young modulus value. The specimen is considered totally fractured if its resultant force on any cross-section tends to zero or a prescribed small value under displacement- control loading. Finally, the proposed theoretical is applied to plane stress problems with fracture patterns and effective loaddisplacement curves presented to illustrate the full failure process.

2 Basic Equations

Consider a heterogeneous material body Ω composed of a large number of convex polygon lattices Ω_k with different phases, such that $\Omega = \bigcup_k \Omega_k$. We assume: (1) these different phases are perfectly bonded, so that the displacements and the tractions are continuous across the interface boundaries; (2) the phase in each sub-domain Ω_k is taken locally homogeneous, isotropic and elastic-brittle; (3) the size of these sub-domains Ω_k is sufficiently large at microscale and sufficiently small at macroscale. Assumption (3) is similar to the requirement introduced in the representative volume element (RVE) analysis. In the proposed model, heterogeneity is implemented by simply taking the material constants, such as Young modulus, Poisson ratio and failure criteria as random fields.

For linear elastic problems in the absence of body forces, the basic governing equations in a Cartesian coordinate reference system (i, j = 1, 2, 3) are the equilibrium equations

$$\sigma_{ij,j} = 0 \quad \text{in}\,\Omega,\tag{1}$$

the geometrical (strain-displacement) equations

$$\varepsilon_{ij} = \frac{1}{2} \left(u_{i,j} + u_{j,i} \right) \quad \text{in}\,\Omega,\tag{2}$$

and the constitutive equations

$$\sigma_{ij} = \frac{E^{(k)}}{1 + \mathbf{v}^{(k)}} \left[\varepsilon_{ij} + \frac{\mathbf{v}^{(k)}}{1 - 2\mathbf{v}^{(k)}} \varepsilon_{kk} \delta_{ij} \right] \quad \text{in} \Omega_k.$$
(3)

Here σ_{ij} , ε_{ij} and u_i represent the Cartesian stress tensor, strain tensor and displacement vector respectively; δ_{ij} denotes the Kronecker delta; $E^{(k)}$ and $v^{(k)}$ indicate Young modulus and Poisson ratio in sub-domain Ω_k . It is noted that even though this is only a piecewise-constant model, a very wide class of material microstructures can be modelled by changing the distribution of Young modulus, and/or by adjusting the shape and size of lattices. For example, by increasing the value of Young modulus creates a very stiff inclusion, and by decreasing its value a very soft inclusion is achieved thus simulating a hole. The set of equations (1)-(3) is completed by introducing the boundary conditions:

Displacement boundary conditions (Dirichlet)

$$u_i = \overline{u}_i \quad \text{on}\,\Gamma_u;\tag{4}$$

Traction boundary conditions (Neumann)

$$\sigma_{ij}n_j = \overline{t}_i \quad \text{in}\,\Gamma_t,\tag{5}$$

where n_j denotes direction cosines of the unit normal on boundary Γ , and $\Gamma = \Gamma_u \cup \Gamma_t$.

Equations (1)-(5) define a linear elasticity boundary value problem for a heterogeneous material. However, to simulate the damage initiation and propagation in heterogeneous material, a local fracture criterion is required to supplement equations (1)-(5).

In micro-mechanics analysis, it is usual (see, for example, Boutin 1996, van der Sluis et al. 1999, Terada et al. 2000) to introduce a macroscopic stress tensor $\hat{\sigma}_{ij}^{(k)}$ and strain tensor $\hat{\epsilon}_{ij}^{(k)}$ in sub-domains Ω_k . These are defined as the volume averages of the corresponding microscopic fields

$$\begin{cases} \hat{\sigma}_{ij}^{(k)} = \frac{1}{V_k} \int_{\Omega_k} \sigma_{ij} dV \\ in \, \Omega_k \\ \hat{\varepsilon}_{ij}^{(k)} = \frac{1}{V_k} \int_{\Omega_k} \varepsilon_{ij} dV \end{cases}$$
(6)

where V_k denotes the volume of sub-domains Ω_k .

A brittle failure criterion, together with the elastic constitutive equations (3), are expressed as follows

$$\begin{cases} \sigma_{ij} = \frac{E^{(k)}}{1 + \nu^{(k)}} \left[\epsilon_{ij} + \frac{\nu^{(k)}}{1 - 2\nu^{(k)}} \epsilon_{kk} \delta_{ij} \right] & \text{if } f^{(k)}[\hat{\epsilon}_{ij}^{(k)}] < 0 \\ \sigma_{ij} = 0 & \text{if } f^{(k)}[\hat{\epsilon}_{ij}^{(k)}] \ge 0 \\ & \text{in } \Omega_k, \end{cases}$$
(7)

where $f^{(k)}[\hat{\mathbf{\epsilon}}_{ij}^{(k)}]$ is the criterion function. Equations (7) describe an elastic-brittle mode, in which the stress and strain retain a linear relation when the effective strain is under the local fracture criterion and otherwise the full lattice fails uniformly. In this study, the maximum principal strain theory (see, for example, Ugural and Fenster 1987) is employed, in which the criterion function is defined as follows

$$f^{(k)}[\hat{\mathbf{\epsilon}}_{ij}^{(k)}] = \max\left\{ \left| \hat{\mathbf{\epsilon}}_{1}^{(k)} \right|, \left| \hat{\mathbf{\epsilon}}_{2}^{(k)} \right|, \left| \hat{\mathbf{\epsilon}}_{3}^{(k)} \right| \right\} - \boldsymbol{\epsilon}_{c\,\mathbf{\Gamma}}^{(k)} \quad \text{in}\,\Omega_{k}. \tag{8}$$

Here, $\hat{\varepsilon}_1^{(k)}$, $\hat{\varepsilon}_2^{(k)}$ and $\hat{\varepsilon}_3^{(k)}$ represent the principal strains of the macroscopic strain tensor $\hat{\varepsilon}_{ij}^{(k)}$, $\varepsilon_{cr}^{(k)}$ is the tensile failure strain for phase Ω_k . Criterion (8) is suitable for a wide class of isotropic elastic-brittle materials.

3 Weibull Distribution

The Weibull distribution is a popular representation of time to failure. This model is used also to deal with such problems as reliability, life testing of material, etc (see, for example, Weibull 1961 and Abernethy 1996). The Weibull distribution is adopted here to describe the properties of material (e.g. elasticity, strength, etc). Since all such parameters are positive, the two-parameter Weibull model is employed with probability density function

$$p(r) = \begin{cases} 0 & r < 0\\ \frac{m}{R} \left(\frac{r}{R}\right)^{m-1} e^{-\left(\frac{r}{R}\right)^m} & r \ge 0 \end{cases}$$
(9)

where R > 0, m > 0 are scale and shape parameters respectively. This probability density function is used for its simplicity though, if required, it may be replaced by a generalized Gamma function (see, for example, Andrew and Price, 1979).

The corresponding distribution function is given by

$$P(r) = \int_{-\infty}^{r} p(t)dt = \begin{cases} 0 & r < 0\\ 1 - e^{-\left(\frac{r}{R}\right)^{m}} & r \ge 0 \end{cases}$$
(10)

with mean α

1

$$\alpha = \int_{-\infty}^{+\infty} rp(r)dr = R\Gamma(1 + \frac{1}{m}), \qquad (11)$$

and variance β

$$B = \int_{-\infty}^{+\infty} (r - \alpha)^2 p(r) dr$$
$$= R^2 \left\{ \Gamma(1 + \frac{2}{m}) - \left[\Gamma(1 + \frac{1}{m}) \right]^2 \right\}.$$
(12)

Thus, once *R* and *m* are specified, the Weibull distribution is completely determined. Alternatively, if only α and β are specified, the transcendental equations (11)-(12) require solution to obtain the parameters *R* and *m*. Figure 1 shows the variations of the mean and variance





Figure 1 : Variation of mean and variance values with shape parameter m(R=1)

with different values of the shape parameter m when R=1. This figure indicates that the parameter m has little effect on the mean, but it significantly affects the variance. The variance decreases rapidly as m increases implying a more homogeneous material for larger shape parameter m.

Let us assume that the heterogeneous material body Ω is composed of *N* convex polygon lattices, and the Young modulus *E* over all Ω_k has a Weibull-type statistical distribution defined by parameters *R* and *m*. The semi-axis $0 \le r < +\infty$ is divided into *N* equal-probability intervals, such that the mid-point $r_k(k = 1, 2, \dots, N)$ of the *k*th interval is defined by the following distribution

$$P(r_k) = \frac{2k - 1}{2N} \quad k = 1, 2, \dots N.$$
(13)

By solving equation (13) and taking $E_k = r_k$, it follows that

$$E_k = r_k = R \sqrt[m]{\ln\left(\frac{2N}{2N-2k+1}\right)} \quad k = 1, 2, \dots N.$$
 (14)

This provides the Weibull-type statistical distribution expression for Young modulus E_k and Figure 2 illustrates this form for m=2. When these E_k values are distributed into lattice Ω_k in a random way, a model of a heterogeneous material body is derived. Figure 3 illustrates an example of a plane heterogeneous material with uniform square lattices. The different colours show the space distribution of Young modulus with black indicating high



Figure 2 : Weibull distribution representation of Young modulus E (m=2)



Figure 3 : Space distribution of Young modulus *E* (*m*=2)

value and white low value. In the same way, we can obtain the Weibull-type statistical distribution expression for Poisson ratio $v^{(k)}$ and failure strain $\varepsilon_{cr}^{(k)}$.

4 Finite Element Formulation

A finite element method is used to implement the numerical simulations described previously. Since the size of all sub-domains Ω_k in Ω is assumed sufficiently small at the macroscale level, the domain decomposition $\Omega = \bigcup_{k} \Omega_k$ is taken as the finite element mesh discretization. The displacement finite element method produces a system of algebraic equations in the form

$$\mathbf{K}\mathbf{a} = \mathbf{f},\tag{15}$$

where the stiffness matrix \mathbf{K} and the nodal load vector \mathbf{f} are defined by

$$\begin{cases} \mathbf{K} = \sum_{k} \mathbf{K}^{(k)} = \int_{\Omega_{k}} \mathbf{B}^{\mathrm{T}} \mathbf{D}^{(k)} \mathbf{B} \, dV \\ \mathbf{f} = \sum_{k} \mathbf{f}^{(k)} = \int_{\Gamma_{k}} \mathbf{N}^{\mathrm{T}} \mathbf{\bar{t}} \, ds \end{cases}$$
(16)

In this expression, **B** is the strain matrix, $\mathbf{D}^{(k)}$ is the constitutive matrix and **N** is the vector of displacement shape functions. In comparison with the conventional finite element methods, here the constitutive matrix $\mathbf{D}^{(k)}$ for homogenous materials can take different values for different elements. From the constitutive equation (3), the constitutive matrix $\mathbf{D}^{(k)}$ is given by the expression

After imposing the necessary geometric boundary conditions, the displacements at all the element nodes are obtained by solving equation (15). Thus, the microscopic stress and strain components are computed at any location within an element by using the following equations

$$\begin{cases} \sigma^{(k)} = \mathbf{D}^{(k)} \mathbf{B} \mathbf{a}^{(k)} \\ \epsilon^{(k)} = \mathbf{B} \mathbf{a}^{(k)} \end{cases}$$
(18)

Strain and stress are not constant through the element, but by choosing simple shape functions, the relevant average strain and stress parameters in an element are easily determined. From equations (6) and (18), the macroscopic stress and strain components over element Ω_k are given as follows

$$\begin{aligned}
\hat{\mathbf{\sigma}}^{(k)} &= \frac{1}{V_k} \mathbf{D}^{(k)} \left[\int_{\Omega_k} \mathbf{B} dV \right] \mathbf{a}^{(k)} \\
& in \, \Omega_k. \end{aligned} \tag{19}$$

$$\hat{\mathbf{\epsilon}}^{(k)} &= \frac{1}{V_k} \left[\int_{\Omega_k} \mathbf{B} dV \right] \mathbf{a}^{(k)}
\end{aligned}$$

For linear elastic problems, equations (15)-(19) can be applied directly to determine the effective elastic properties of the heterogeneous materials. However, to simulate damage initiation and propagation in these materials, an efficient computing scheme must be devised. In this paper, an incremental or stepwise procedure is constructed to model the non-linear behaviour of the damage initiation and propagation in heterogeneous materials. This approach provides a relatively complete description of the load-deformation behaviour and is created as follows:

- 1. A small initial load step (i.e. force-load or displacement-load) is applied to the heterogeneous material body. The linear algebraic equation (15) is solved to calculate the macroscopic stress and strain components given by equation (19).
- 2. Since in each load-step stage the problem remains linear, an auto-select loading method is designed to allow modelling of a realistic failure process. From the determined strain levels of all lattices, the lattice, which is most likely to fail (i.e. reach ε_{cr}) under an increasing global strain, can been selected by equation (7). Without making many small steps, the strain level of this lattice and corresponding load level are directly determined causing the lattice exactly to fail.
- 3. This failing lattice is excluded from the heterogeneous material body by choosing the Young modulus of the lattice to be very small. This process, therefore, represents the damage initiation and propagation in the heterogeneous material body, causing a renewal of its geometric configuration. The system must now be re-examined for the same load level and the linear algebraic equation (15) solved again for the updated geometric configuration. If

any of the remaining lattices exhibit failure, this process is repeated, and the system re-examined again. This iterative procedure continues until no lattices fail at this load level. A range of failure possibilities exist in the sense that either just one lattice needs removing at a given load level or a number fail and are removed with the system retaining a load-carrying capability and able to withstand further straining.

4. The incremental load is increased, and steps 2 and 3 repeated until a continuous crack path is formed through the whole specimen. The end occurs when the specimen has no load-carrying capability left, implying that the resultant force over any cross-section of specimen reaches a value tending to zero or close to zero.

This proposed approach allows the simulation of fracture events, i.e. the simultaneous growth of many cracks, through discarding lattices not satisfying local failure criteria, as well as accounting for stress redistribution throughout the lattice medium. Moreover, it is worth noting that no remeshing of the domain is required as the fracture simulation proceeds.

5 Numerical Results and Discussion

Figure 4 shows an example of a square plate under plane stress. It is investigated to illustrate the applications of the present method. The square plate is subject to an uniaxial displacement-control compression in the x-direction. The boundary conditions of the square plate are expressed in equation (20). That is, the top and bottom sides are traction free; the left side is the frictionless surface fixed in the horizontal direction; the right side is also the frictionless surface subject to horizontal displacement; and the point (x=0 and y=0) is fixed in both of the horizontal and vertical direction.

$$\begin{cases} \sigma_{yy} = 0, \ \sigma_{xy} = 0 & \text{on} \quad y = \pm b/2 \\ u = 0, \ \sigma_{xy} = 0 & \text{on} \quad x = 0 \\ u = \Delta \overline{u}, \ \sigma_{xy} = 0 & \text{on} \quad x = a \\ u = 0, \ v = 0 & \text{at} \quad x = 0, \ y = 0 \end{cases}$$
(20)

Figure 5 illustrates a square plate specimen uniformly discretized into 50×50 square lattices. The initial heterogeneity of modulus and strength are simulated by



Figure 4 : Geometry and boundary conditions of the square plate



Figure 5 : Weibull distribution of Young modulus

the Weibull distribution. The numerical simulations discussed herein use four-node square finite elements, with displacement represented by bilinear interpolation. An auto-select loading method (displacement-control load) is employed so that a realistic failure process is simulated.

The effective stress-strain curves describing *heterogeneous-stiffness materials* are shown in Figures 6 and 7, where the Young modulus is modelled by a Weibull-type statistical distribution with $mean[E^{(k)}]=100$ GPaPoisson ratiov^(k)= 0.3 and the fail-



Figure 6 : Equivalent stress-strain curves for different parameter *m*



Figure 8 : Equivalent stress-strain curves for different parameter *m*

ure strain $\varepsilon_{cr}^{(k)} = 0.2\%$ assumed constant over all lattices. Figure 6 illustrates the effective stress-strain curves for different values of shape parameter m. The results show that both the equivalent Young modulus and failure strength increase with an increase of the shape parameter *m*. That is, the greater homogeneity occurring in the stiffness of the materials, the better the effective stiffness and strength. Figure 7 shows realisations of the effective stress-strain curves for various random samples for prescribed *m*. These findings demonstrate that although the value of the equivalent Young modulus are similar, the resulting failure strengths and paths are different. This implies that even though the Young modulus has the same statistical distribution, the different space configurations cause different failure strengths and paths.



Figure 7 : Equivalent stress-strain curves for various random samples



Figure 9 : Equivalent stress-strain curves for various random samples

The effective describing stress-strain curves heterogeneous-strength materials are shown in Figures 8 and 9, where the failure strain is modelled a Weibulltype statistical distribution with mean $[\epsilon_{cr}^{(k)}]=0.2\%$, and Poisson ratiov^(k)= 0.3 and Young modulus $E^{(k)}$ = 100GPa assumed constant over all lattices. Figure 8 illustrates the effective stress-strain curves for different values of shape parameter m. The results show that the values of the equivalent Young modulus are similar for different m, and the failure strength increases with increase of shape parameter m. That is, the more homogeneous the distribution of strength in the materials, the better the effective strength. Figure 9 shows realisations of the effective stress-strain curves for various random samples for prescribed *m*. Again values of the equivalent Young modulus remain similar in magnitude, but the failure strengths and paths are different. This implies that even though the failure strain obeys the same statistical distribution, because of different space configurations different failure strengths and paths occur.

Figures 6-9 also illustrate the occurrence of some nonlinear phenomena, such as strain softening, pre-peak and post-peak. The characteristic of strain softening phenomenon is that the stress decreases with increasing of the strain in the stress-strain curves. A pre-peak phenomenon is observed due to the fall in stress-strain curve occurring prior to reaching maximum stress strength and similarly, a post-peak phenomenon is because a fall in the stress-strain curves occurs after the maximum stress strength is reached. These nonlinear phenomena have been discovered in many experiments using the heterogeneous materials, as described by Karsan and Jirsa (1969), and Read and Hegemier (1984).

Figure 10 illustrates several appearances of fracture patterns, selected from a failure simulation using the whole heterogeneous specimen. A black lattice in these figures implies a failure of the lattice bonds. From this sequence of patterns derived by the mathematical model simulation described previously, the full fracture procedure of the heterogeneous specimen is observed, including crack initiation, crack propagation and ultimate fracture. Moreover we observe in the sequence that the expectancy of failure in the lattice is likely to take place in the neighborhood of the previous-failed lattices, especially at the tip of the crack.

6 Conclusions

A general numerical approach is developed to model the elastic behaviour and failure processes of heterogeneous materials. Although a two-parameter Weibull statistical distribution is used to simulate initial heterogeneity of materials, the model can be modified to use multiparameter Weibull distributions or other suitable statistical distributions (see, for example, Andrew and Price, 1979). Since the techniques developed in spring network method and the volume average concept (RVE) are employed, the proposed method simulates crack initiation and propagation without significant computational complexity. Moreover, by adopting a displacement-type finite element method, the described method is well suited for easy implementation in standard finite element codes. A selection of applications of the present method to plane stress problems is presented. The numerical results indicate that the method is very suitable to simulate strain softening, pre-peak and post-peak nonlinear phenomena occurring in the failure process of heterogeneous materials. The results also indicate that the more homogeneous the stiffness or strength of the materials at the microscale level, the better effective stiffness and strength occur at the macroscale level. Furthermore, even though the same statistical distribution is taken to describe stiffness or strength in heterogeneous materials, because of the different space configurations of properties different failure strengths and paths occur in the materials.

The present approach, after suitable modification, provides a method to investigate effective properties of various practical heterogeneous materials, optimize and design ingredients and space configurations in composite materials, etc. It also allows examination of nonlinear phenomena in the structures or materials by combining simple constitutive relations and heterogeneous model in contrast to the more conventional approach by combining complicated constitutive model and homogeneous model. In this respect, the presented approach more really describes realistic materials.

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(a)





(b)





(e)





(f)







(i)

(j)

Figure 10 : Full fracture procedure of the heterogeneous specimen

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