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A stochastic model of damage accumulation in complex microstructures

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A statistical approach for modeling fracture in brittle materials is presented. In particular, a microstructural-based finite element code called OOF is used in conjunction with a stochastic representation of failure that relies on the Weibull law. The OOF code, which maps materials microstructures onto finite element meshes, enables to calculate the local stress states; these stresses are used along with the statistical criterion for brittle fracture in order to determine microcrack formation and propagation. Computer simulations are performed on several microstructures of different materials types, e.g., laminates, particulate composites and polycrystals. The damage accumulation due to microcracking is characterized by the stereological measure of failed material and is investigated in order to assess the effect of microstructural features on the failure mechanism. Moreover, the approach allows to analyze the influence of the characteristic parameters for brittle materials on damage evolution.

1. Introduction

Materials used in engineering applications often have complex microstructures or composite architectures designed to enhance macroscopic properties. Requirements for mechanically reliable and damage-tolerant devices have stimulated the investigation of composite materials and heterogeneous microstructures that increase fracture energies by spatially distributing damage. The accumulation of damage in a composite or a microstructure has stochastic aspects associated with distribution of defects within phases or interfaces. Damage accumulation also has deterministic aspects associated with distribution of stress within a material as a function of loading, material geometry, and the spatial distribution of elastic properties. However, when considering similar materials, stochastic effects appear for a given load and geometry because of the large variety of spatial elastic property distributions within a set of "similar" microstructures or because composite processing uncertainties also produce micromechanical variability.

Local microstructural features can affect macroscopic mechanical response to a prescribed loading condition, especially with regard to mechanical reliability. Damage accumulation in a matrix, inclusions, or at their interface, in the case of matrix-reinforcement debonding, is strongly affected by microstructural size scales and topology (e.g., inclusion shape, size and volume fraction). Predictive micromechanical models that incorporate microstructural details will foster the design of optimal microstructures in complex materials. Ensuing models that treat stochastic aspects of microstructures will provide means to assess the reliability of designed microstructures.

In this paper, we describe a method that directly incorporates microstructural features and indirectly treats the statistical aspects of damage accumulation through parameters that define a failure probability that depends on localized microstructural stresses. The method is combined with public domain software, OOF [1] and serves as a means to gain insight of the role that microstructure plays in reliability. To establish the microstructural role, several prototypical microstructural case studies are presented below.

One existing method for calculating microstructural stresses, the unit cell method, is based on the assumption that a representative volume element (RVE) can be used to represent the mean behavior for an entire microstructure. The RVE method may suffice for predictions of linear properties or the occurrence of first failures, but it is not able to account for effects due to microstructural variability or correlated failure events. It is questionable whether the RVE method can be successfully extended to heterogenous materials and complex microstructures. Moreover, it is difficult to define an appropriate RVE to treat inhomogeneous materials.

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Alternative approaches have been proposed to account for microstructural heterogeneity and randomness. Ghosh, Lee and coworkers developed a multilevel computational model for multi-scale damage analysis [2]. This approach performs both the macroscopic analysis with a conventional FEM code and the microscopic analysis by using the Voronoi Cell Finite Element Method (VCFEM). This model is able to track the incidence and propagation of microstructural damage in composites and has been tested for different heterogeneous microstructures. The same authors applied VCFEM to a variety of microstructural classes such as composites and porous microstructures [3–5], composites of ductile matrix with brittle elastic inclusions [6, 7]. Stochastic models were introduced in an extension of the VCFEM model in which discretely reinforced materials were analyzed with a Weibull distribution to account for the size effect in particle cracking and hence flaw size and distribution [8]. Experimental data were combined with a computational approach to develop a damage evolution technique that was applied to microscopic damage within SiC particle reinforced aluminum alloys [9]. Three dimensional modeling and characterization of particle reinforced matrix composites was developed by the same group [10, 11]. The authors demonstrated that it was possible to characterize damage as a function of stereological measures, i.e., for materials with different volume fractions and reinforcing particle size.

Other groups have investigated microstructural effects on brittle materials behavior. Zavattieri *et al.* studied polycrystalline ceramic microstructures by simulating microcracking at grain boundaries and presented a micromechanical model that accounts for interface parameters, grain size and grain morphology [12]. Zhao and Yu presented a model for damage of materials combining macroscopic mechanical properties with microstructural parameters [13]. Fischer-Cripps used a finite element method to calculate the indentation response of a mica-containing glass-ceramic: the finite element modeling is performed at the microscale in order to assess the connection between the macroscopic behavior of the material and damage events on a microstructural scale [14]. Fitoussi *et al.* investigated the damage mechanism for SMC composites, introducing into the micromechanical model a local interface failure criterion [15]. Landis *et al.* investigated the strength distributions of unidirectionally reinforced fiber composites with a micromechanical model and Weibull statistics as a function of fiber strength [16].

In this paper, we develop a method to investigate the effects of microstructure, statistics, and stress-flaw correlations for accumulating damage in brittle materials. Our method couples a finite element approach that directly derive from microstructures with a stochastic criterion for brittle fracture. Previously, we utilized two methods to evaluate probability of first failure in complex microstructures [17]. These methods relied on assumption of linear elasticity and a Weibull model for the local probability of failure determined by the individual properties of the microstructural constituents or features. The methods allowed the determination of the reliability of a perfectly brittle microstructure. In this paper, we extend the model to damage accumulation. Our method extends an object-oriented microscale finite element analysis (OOF) and allows determination of evolution of the complex stress state in heterogeneous material with gradually failing components. This tool is used in conjunction with the Weibull law for brittle fracture, in order to track the incidence and propagation of microstructural damage. This approach allows investigation of arbitrary microstructures of complex materials. The paper describes this technique which provides a method for analysis of heterogeneous structures undergoing damage in two-dimensional representations of real microstructures.

2. Method

We represent a microstructure as a finite element model with mesh properties that derive from a two dimensional image. Stochastic behavior is incorporated into each element through a probabilistic failure model that depends on element type and on local stress conditions. In this paper, we employ a local Weibull model for sequential element failure and a finite element analysis is performed via OOF [1], an image based computational tool. In fact, real microstructure images of selected materials may be digitized and used as input for the preprocessor, PPM2OOF. This preprocessor is able to map materials micrographs onto finite element meshes that can be refined as appropriate. Materials properties are defined, inside the preprocessor, corresponding to the different parts of the image. PPM2OOF creates triangular elements for which local materials properties can be used for adaptive mesh refinement. OOF performs a finite element solution for user-specified loading conditions for meshes that are produced by PPM2OOF. In such a way, the “actual” microstructure of a material is analyzed through its image and the effect of particular microstructural features can be analyzed from their macroscopic response. We extend OOF to probabilistic models of sequential failure in quasi-brittle materials (i.e., those that can sustain sequential, but limited, failure from isolated defects).

OOF has been adopted to model microstructural effects on residual stress distribution, damage and fracture in several different materials classes, including composites. For example, it has been utilized to determine residual stresses in plasma-sprayed thermal barrier coatings [18, 19], to study the effect of interface properties on microcracking of iron titanate [20] and the stresses in aluminum-silicon alloys [21]. Moreover, the code was employed to determine residual stress distributions in ceramics caused by thermal expansion anisotropy, using polycrystalline alumina as a model system [22] and the fracture of a textured anisotropic ceramic [23] and to predict residual stresses in polycrystalline alumina and spontaneous microcracking upon cooling from the processing temperature [24]. Hsueh *et al.* studied the stress transfer in platelet-reinforced composites by considering a two-dimensional model system constituted of an elongated platelet embedded in a matrix [25]. Other brittle matrix composites were investigated [26–28] . Cannillo and Carter [17] adopted OOF to determine reliability of composite microstructures, by including both effects of microstructural heterogeneity and of arbitrary loading conditions. Zimmerman *et al.* [29] examined damage evolution during microcracking due to thermal expansion and elastic anisotropy in random polycrystalline microstructures. The authors adopted the Griffith criterion to describe failure and damage accumulation due to microcracking of brittle materials.

In this paper, we extend the analysis to reliability and damage accumulation in complex microstructures of brittle materials by introducing a stochastic approach as a failure criterion. Observations of failures from specimens of nominally the same material show that failure strengths are distributed for identical specimen geometries. The distribution of failure strengths derives from microstructural variations and from distributions in the size and spatial arrangement of defects. Material reliability can be characterized with a failure probability, rather than with a single average strength. The failure probability is empirically related to the specimen volume and the stress state in the specimen. A widely used model of probabilistic failure is the well-known Weibull's equation [30]

$$P(\sigma, \Delta V; \sigma_\circ, m, V_\circ) = 1 - \exp\left[-\left(\frac{\sigma}{\sigma_\circ}\right)^m \frac{\Delta V}{V_\circ}\right] \quad (1)$$

that correlates the probability of failure to the stress state σ in a volume ΔV and to two Weibull parameters (a shape factor m and a scale parameter $\sigma_\circ$). Equation 1 is incorporated into a new OOF element that fails (by reducing element stiffness in the direction of maximum tensile load) with probability P in an element of size ΔV.

An image of a microstructure in the form of a two-dimensional array of pixels, obtained either by scanning a micrograph or through a microstructural simulation algorithm, is taken as input to PPM2OOF. Reliability parameters (i.e., m and $\sigma_\circ$) and thermoelastic properties (e.g., Young's modulus, thermal expansion tensor, etc.) are specified with user-identified regions in the image. A two-dimensional triangular finite element mesh is generated from the specified underlying image properties. The mesh is adaptive and can automatically refine itself in subregions where the underlying properties change at a fine scale, or where large gradients develop in the stress or strain—such as at interfaces that separate regions with differing properties. A microstructure is thus generated from an image and local properties are mapped onto a set of finite elements where each element e_i has thermoelastic properties and Weibull moduli m_i and σ_{oi} inherited from its location on an image. Each element, e_i, has an area ΔA_i that is used to determine the volume ΔV_i in Equation 1 through a characteristic thickness w: $\Delta V_i = w \Delta A_i$.

The microstructure's reliability is simulated with Monte Carlo processes that utilize a discrete representation of Equation 1 and local stresses to "fracture" elements sequentially. The microstructural grid is analyzed with finite element solver (OOF) and discrete approximations to the stress and strain fields are calculated for a specified loading condition, L. A failure probability $P_{\text{fail } i}(L)$ is computed in every element from equation 1, using the maximum principal stress as σ [17]. Each element is randomly assigned a *test* probability $P_{\text{test } i}$ from a uniform distribution in the interval [0, 1]. An element, e_i, fractures if $P_{\text{fail } i}(L) > P_{\text{test i}}$. Element fracture is simulated by an anisotropic reduction of the stiffness tensor—the tensor is rotated so that one direction is coincident with the direction of maximum principle stress and the components stiffness values in that direction are reduced by two orders of magnitude and all other values are reduced by knockdown parameter set to $1/5$.

Damage is accumulated during the sequential Monte Carlo/FEM process. As local damage occurs at a load L, a new equilibrium stress state and a new set of $P_{\text{fail } i}(L)$ are computed. Local failures tend to redistribute stress to neighboring elements. Other failures may occur due to this stress redistribution, and if so other elements fail and the process is iterated until no more failures occur at L.

In this way, it is possible to determine the locations and correlations of first, second, third, and subsequent failures. This approach simulates damage evolution and its direct relation to microstructure. Moreover, it is possible to study the effect of the characteristic parameters for brittle materials, such as the Weibull moduli, with damage evolution.

It is worth observing that the method presumes that the Weibull moduli may be applied discretely to small uniform elements in a microstructure. Thus, it is implicitly assumed that sub-microscopic flaws are distributed within each finite element, i.e., the finite element discretization is coarse enough to average over a distribution of pre-existing flaws which are very small compared to the characteristic element size.

A Weibull model is usually employed for the probability of first failure and would therefore be an appropriate choice for weakest link failure of a material specimen. In this study, the Weibull distribution is employed for damage accumulation as a matter of convenience and comparison to experiments in quasi-brittle materials. Using the same Monte Carlo scheme, differing probability distributions (that depend on local elastic field conditions) could be easily substituted for Equation 1. *Which* probability distribution and methods for its empirical determination could be examined by extension of the method described in this paper.

It should be noted that the Griffith condition of crack growth based on the global energy balance is not necessarily satisfied by a damage event. Enforcing the Griffith criterion has not been done in this work and remains a topic for future modeling.[1]

Moreover, as regards fracture initiation, it is assumed that there is an existing unknown distribution of flaws in each element. As described, using a Monte Carlo process, an element may fail following Weibull statistics. Therefore, cracks are forced to initiate in terms of a prescribed length defined by the element length.

[1] The authors are grateful to a reviewer of this manuscript for this suggestion.

(a)

(b)

Figure 1 (a) The onset of critical damage in a homogeneous specimen, with Weibull modulus $m = 25$. The mesh is uniformly triangular. (b) The first failures in a homogeneous specimen, with Weibull modulus $m = 5$ illustrating the distribution of damage associated with smaller values of Weibull modulus.

The use of an atomistic approach to describe fracture initiation could be an extension of the present work.

2.1. Effect of Weibull parameters on damage evolution in monolithic structures

To gain an understanding of the role of m and $\sigma_\circ$ in damage evolution, the trivial case of a uniform material that can be characterized by a single Weibull law is considered. The simulation of such a monolithic material would apply to the case of an amorphous material without an intrinsic length scale—and may apply to a material with a microstructure that is considered homogeneous at the length scale of the finite element mesh. In the latter case, the critical load L_c at which a cluster of failed elements suffice to propagate across an entire mesh could be used as a means to determine the particular Weibull moduli as a function of specimen geometry and loading. A method of homogenizing a microstructure's reliability characteristics is one purpose of this paper and is described in the following sections.

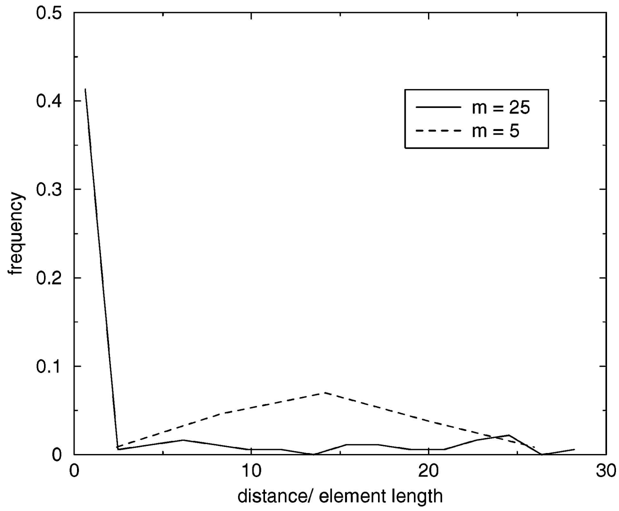


Figure 2 Distribution of distances of second failures from first (normalized by the element length) for $m = 25$ and $m = 5$.

A homogeneous specimen is considered with the following thermoelastic properties: $E = 150$ GPa, $\nu = 0.25$, $m = 25$, $\sigma_\circ = 0.1$ GPa, assuming that the Weibull moduli are the same in each element of the mesh. The sample is loaded in a uniform stress state by application of a fixed strain with no shear components at the "grips." The stress field is computed under plane stress conditions and subjected to the Monte Carlo process described above. The sequence of elements failing simulates crack propagation in the sample, and, as illustrated in Fig. 1a, subsequent failures are highly correlated, i.e., an element breaking is likely to be close to one that failed in the previous iteration.

The same experiment is then repeated for a sample with the same thermoelastic and fracture properties, but a Weibull modulus of 5. Failures, as reported in Fig. 1b, are much less correlated than in the previous case. These computations illustrate how the Weibull modulus m affects fracture (or local correlation) behavior of the material. The numerical experiments can be repeated to obtain a distribution of fracture behaviors for a fixed Weibull parameter. In Fig. 2 these distributions are illustrated, as obtained with 100 cases. While for $m = 25$ the failures are highly correlated, i.e., a second failure is likely to occur next to the first one, for $m = 5$ the fracture events are much more dispersed. This confirms that the value of m has a strong influence on the correlation of subsequent failures and the distance between them.

To gain a deeper insight into the role of the m parameter, different specimen characterized by values of m equal to 2, 5, 10, 15, 20 and 25 respectively are considered and the average distance of the second failure from the first one is calculated over 100 samples for each case. Fig. 3 illustrates that this distance decreases with increasing Weibull moduli, i.e. the events are more correlated with high values of m. Similar behavior is then found for the distances of the subsequent failures (third to second, fourth to third, $(i + 1)$th to ith).

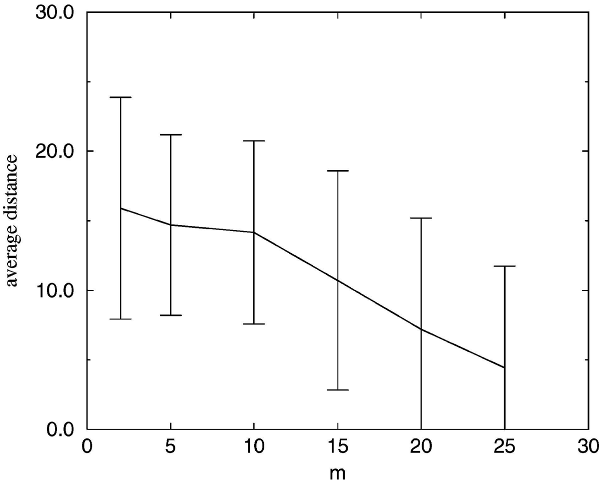


Figure 3 Distribution of distances of second failures from first (normalized by the element length) and standard deviations as obtained with 100 experiments for $m = 2, 5, 10, 15, 20, 25$. The standard deviation is appropriate for a normal distibution. As the average distance must be positive, the distribution cannot be normal and thus the deviations are more meaningful at smaller values of m.

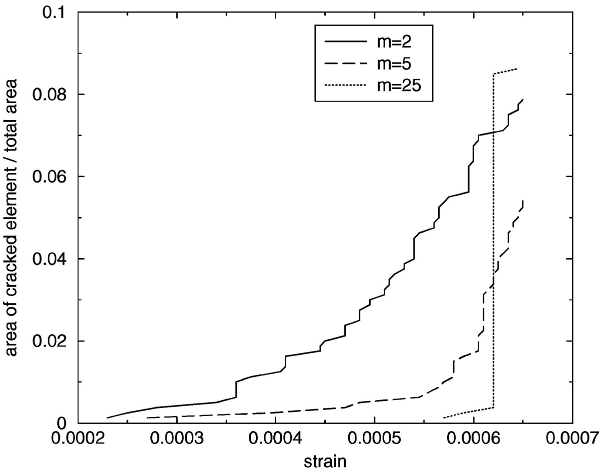


Figure 4 Evolution of the damage parameter for different values of m.

The Weibull moduli of brittle materials such as ceramics are known to display a large range of values (typically $m \in (2, 30)$) [31–35]. Furthermore, m may depend on the test method [36]. The range of values of Weibull modulus in Fig. 3 and the associated correlative behavior thus spans the expected behaviors of real materials.

2.2. Damage accumulation

To quantify the microstructural damage accumulation, we introduce a damage parameter

$$d = \frac{\text{area of cracked elements}}{\text{total area}} \tag{2}$$

This parameter can be calculated and plotted for samples with different values of m as a function of the applied strain (or load). In a preliminary study, various fixed strain increments $\Delta\epsilon$ were used to determine a strain increment that is small enough to al-

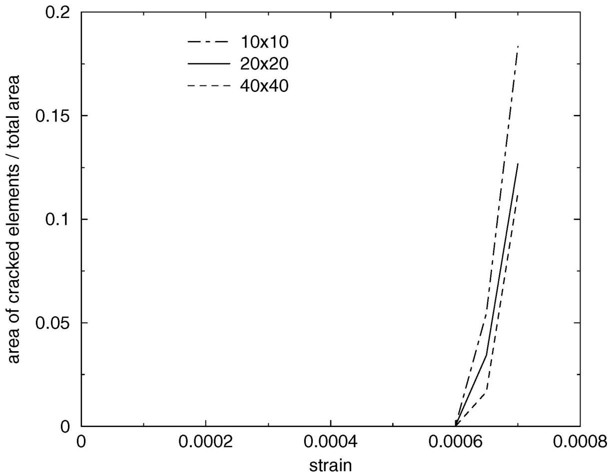


Figure 5 Damage parameter for different discretizations.

low enough data to be obtained before critical failure (i.e., one or few element failures per strain increment) and thus allow determination of damage accumulation curve's shape. This increment is used in the rest of the paper.

In Fig. 4 the damage parameter is plotted as a function of applied strain, for three different simulations corresponding to values of m equal to 2, 5, 25. As can be inferred from the picture, damage progresses stably for low values of m. However, for large values of m there is an onset of critical damage levels over a narrow range of strains near the characteristic stress $\sigma_\circ$. The damage curve becomes more non-linear with increase of m.

Thus, the Weibull modulus plays a critical role in determining the rate of damage. If $m \to 2$ the fraction of cracked material depends weakly on applied stress. Otherwise, if $m \to \infty$ the damage parameter would remain zero until the average stress reaches $\sigma_\circ$ [38]. In fact, the Weibull parameter $\sigma_\circ$ determines the critical load at which the sample is likely to fail: $\sigma_\circ$ strongly correlates with the strain at which the damage parameter increases rapidly, and becomes singular as m increases.

For the initial (i.e., with no failed elements) homogeneous sample, the elastic solution is insensitive to mesh refinement.[2] However, because each failed element occupies a finite region, the progression of damage will be sensitive to discretization. To investigate the effects of discretization length scale on the Monte Carlo algorithm, a homogeneous sample is considered and three different discretizations are analyzed: meshes of 10×10, 20×20 and 40×40 elements (Fig. 5). For each mesh, 20 runs were performed and damage curves were recorded. Average damage curves were then calculated over 20 runs for each discretization. Fig. 5 illustrates that the results are consistent for finer discretizations (20×20 and 40×40), and the damage parameter seems sensitive to discretization if mesh is coarse (10×10).

[2] If the microstructure has a characteristic length scale, then the elastic solution would depend on mesh size. This effect is considered below.

3. Case studies

The combined FEM-Monte Carlo reliability and damage accumulation method described above is applied to three prototypical two-dimensional microstructures: laminated composites, single-phase polycrystals, and particulate composites.

The results obtained for laminated composites (bilayers of two homogeneous materials with differing elastic and intrinsic reliability characteristics) demonstrate a homogenization method for a material with anisotropic reliability characteristics with underlying orthorhombic symmetry with respect to loading axes. The homogenization results in a model of a single phase material that has orientation dependent reliability.

The results of this anisotropic homogenization are applied to a case of single phase two-dimensional polycrystal where the orientation of each grain is used to simulate a system of orientation-dependent Weibull moduli.

3.1. Laminated composites

A lamellar composite of two elastically isotropic materials is considered. The two layers display the same thermo-elastic constants, but different Weibull moduli, $m = 5$ and $m = 25$. The sample initially in a stress-free state is loaded under uniaxial tension as described above. Two loading conditions—parallel and perpendicular to the lamellae—suffice to model the anisotropic characteristics of damage evolution. 'Greased' grip conditions are applied so the stress singularity at the corners from fixed grip conditions does not arise.

The applied strain is incremented up to the critical value for which fracture occurs. Fig. 6 illustrates the phase difference of damage accumulation in the cross laminate loaded sample. The material with $m = 5$ has failures distributed throughout, while the material with $m = 25$ displays highly correlated damage accumulation. However, because the lower modulus phase is likely to fail first for similar $\sigma_{\circ}$, the location of correlated damage in the higher modulus phase is correlated with location of failures in the lower modulus material.

Figure 6 Damage in a lamellar composite with two different Weibull moduli (5 (darker gray) and 25).

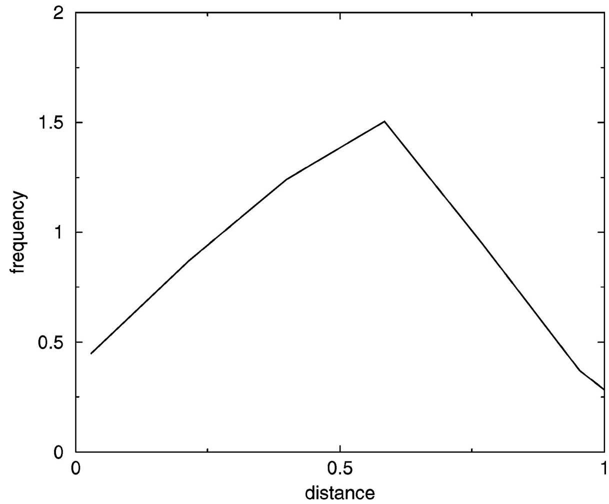


Figure 7 Distances from subsequent failures—for the entire specimen. The specimen length width is set equal to 1.

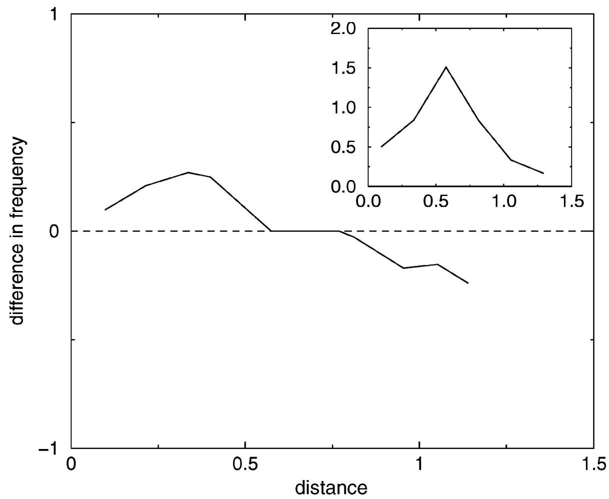
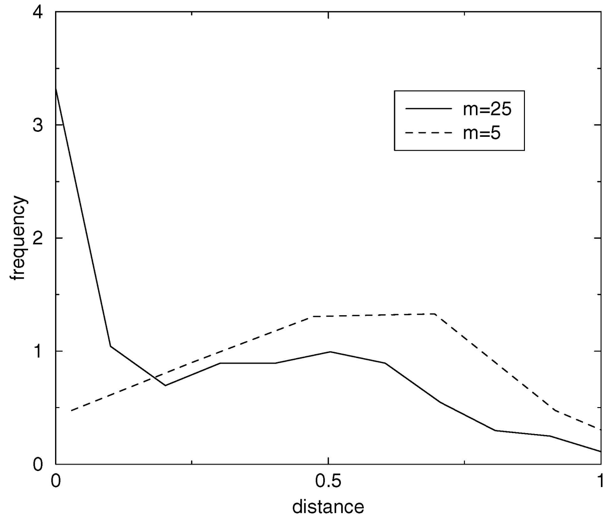


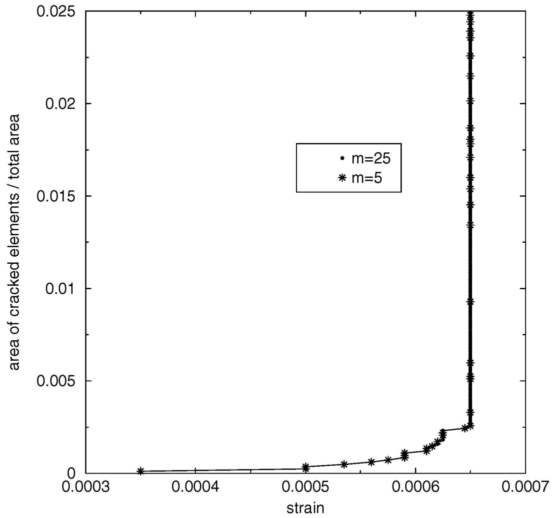
Figure 8 Difference of the distribution of distance of failures for the specimen (from the previous picture) and that of perfectly random failures (also illustrated in the top corner).

The correlation between subsequent fracture events can be analyzed with the distance between first and second failures. Fig. 7 shows the distribution of distances of second failure (i.e., the second element failing according to the fracture criterion chosen) from the first one, obtained by repeating the experiment 100 times. The failures appear not to be correlated because they occur both in the phase with $m = 5$ and $m = 25$. This distribution can be compared with that of a perfectly random set of failures. Fig. 8 illustrates the difference of the two distributions: the distribution of distance from failures in the laminated samples behaves similarly to the random case. However, if the failures are divided into two sets characterized by the material in which they fail, Fig. 9a is obtained: this graph shows that failures in the phase with $m = 25$ are likely to occur one next to the other.

Moreover, the damage accumulation curve can be plotted, according to Equation 2. Fig. 9b illustrates that the damage begins to occur in the phase with Weibull modulus equal to 5 at relatively low applied strain. Then, at a critical value of strain, cracks develop in

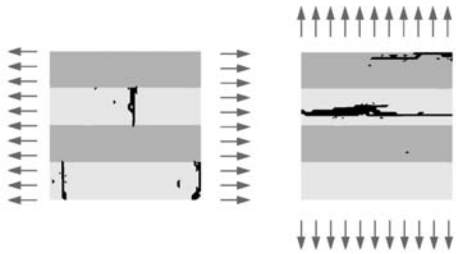


(a)

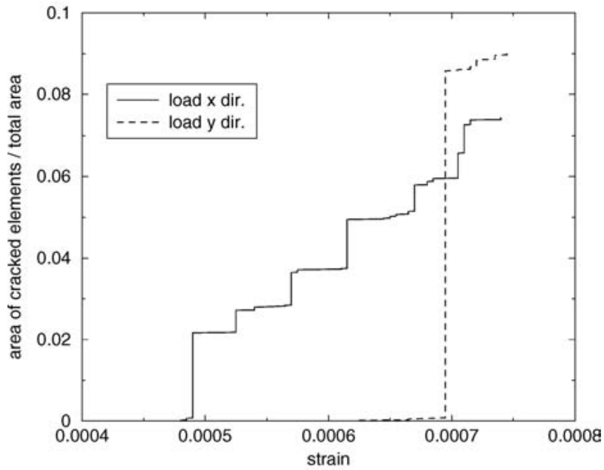


(b)

Figure 9 (a) Distances from subsequent failures for the two phases. The specimen length width is set equal to 1. (b) Damage evolution for the lamellar composite.



(a)



(b)

Figure 10 (a) Effect of loading direction on damage evolution in a lamellar specimen. Dark gray corresponds to $E = 100$ GPa, light gray corresponds to $E = 200$ GPa. (b) Effect of the loading direction on damage accumulation.

the phase with high Weibull modulus, with a marked increment in the fraction of broken material over a very narrow range of strain.

This case study can be extended to investigate the effect of applied load direction with respect to an underlying orthorhombic symmetry for families of constituent thermoelastic and reliability behavior. For loading perpendicular to the lamellae with arbitrary differences in thermoelastic moduli, the attributed homogeneous Weibull moduli would be approximately equal to that of the phase with the largest component.

For the case of loading parallel to the lamellae, the stresses in each phase scale with that phase's elastic stiffness. To study this case, the Young's moduli are set to 100 GPa in first ($\sigma_\circ = 0.1$ GPa) phase and 200 GPa in the second ($\sigma_\circ = 0.1$ GPa) phase. The difference in damage character is illustrated in Fig. 10a. The loading condition is such that the stress is double in one phase compared to the other one—failures occur where the ratio of stress to $\sigma_\circ$ is larger. The corresponding damage parameters for these two cases can be computed: Fig. 10b illustrates damage evolution, where each "step" in the curve corresponds to the opening of one crack along the lamellae.

Moreover, the layer size provides a microstructural length scale against which the mesh size can be compared and provides a means to study the mesh size dependence of computational accuracy. Finite element grids, with differing refinements, were created for the same microstructure. The average distance of the second element failing from the first one (normalized to the element length) is investigated as a function of the number of elements within a lamellar layer. As plotted in Fig. 11, the distance is affected more by the value of the Weibull modulus than by the mesh refinement. This suggests that results are consistent and the numerical convergence is relatively insensitive to the finite element length as long as there are more than approximately fifteen elements for any microstructural feature.

3.2. Polycrystalline microstructures

The approach presented in this paper is applicable to any two-dimensional microstructure and most useful for those microstructures in which direct calculation of the stress state is not straightforward. Consider a heterogeneous microstructure that is generated by a Voronoi tessellation of a Poisson point process as a representative polycrystalline material (Fig. 12). The properties of each grain can be set independently; here, each grain is assigned the same elastic constants and $\sigma_\circ$, but a random value of the Weibull modulus m, picked from a uniform distribution $m \in (5, 25)$. This case is analyzed

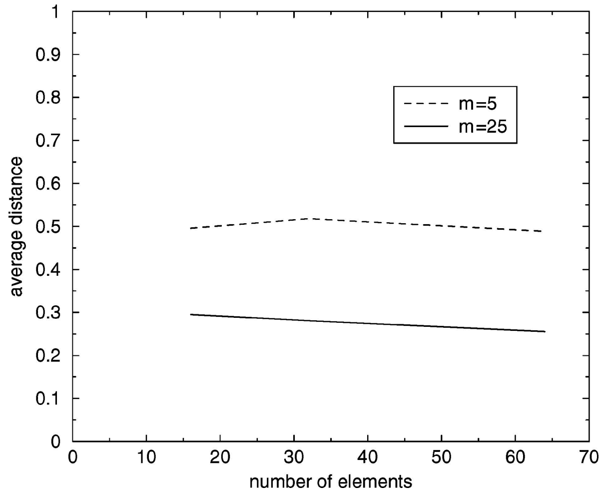


Figure 11 Mesh refinement effect on the average distance between subsequent failures: number of elements on the specimen width (i.e. the mesh has n^2 elements) vs. average distance of second failure from first.

in order to assess the effect of local probabilities of failures on the behavior of the complex material.

In order to minimize the effect of finite length of an element, a mesh was created so that approximately 15 elements spanned an average grain according to the estimate produced in the previous section. The sample was stressed in tension and the FEM solution was obtained under plane stress conditions. Until a finite amount of applied strain is reached, no fracture events occur. As the applied internal load increases above a certain level, fracture typically initiates in grains with low Weibull modulus. Fig. 12 illustrates the damage evolution for a particular polycrystal. Damage evolves with increasing applied strain nonlinearly. At larger values of applied strain, damage is produced in grains with higher Weibull modulus. The cracks apparently follow paths connecting grains with high Weibull modulus (i.e., with further increase of load, cracks tend to connect high Weibull moduli grains).

The fracture behavior of this polycrystal can be analyzed with Fig. 13 in which the grains are divided in four groups depending on the value of the Weibull modulus. As illustrated in Fig. 13a, the distance between subsequent failures decrease with increasing Weibull moduli, thus confirming that cracks tend to create paths along high Weibull moduli grains conforming to the accumulation illustrated in Fig. 13b.

This model simulates the evolution of fracture patterns in complex microstructures, accounting for stress relaxation due to microcracking. This is in contrast to models that treat microstructural elements (e.g., a grain in a polycrystal or a fiber in a composite) as either intact or failed.

3.3. Particulate composites

The third class of heterogenous microstructures considered in this study is that of particulate composites. Random microstructures were generated by means of an algorithm where circular inclusions, with radii picked randomly from a limited uniform size distribution, were placed sequentially in a matrix by a Poisson hard-sphere placement until a specified volume fraction of inclusions was achieved. An example of such a microstructure is illustrated in Fig. 14. The elastic and reliability properties of the matrix and of the inclusions are assigned independently.

In the first case considered, the matrix and the inclusions have Young moduli of 100 and 400 GPa respectively and the same Weibull moduli ($m = 25$, $\sigma_\circ = 0.1$ GPa). Due to the elastic mismatch, an applied load results in a distribution where stress tends to be larger in the particles, and thus failures are likely to occur in the particles. Fig. 15a illustrates the cumulative fraction of elements failing in the matrix and in the inclusions, confirming that most cracks develop in the particles. Fig. 15b illustrates the progression of damage for increasing applied strain: the damage evolves nonlinearly. Most damage occurs in the particles and each finite damage increment in the curve corresponds to the complete failure of a single particle at that applied strain.

The same microstructure and elastic properties were examined, but with the particles and matrix assigned to $m = 5$. Depending on the particle's Weibull modulus, two different behaviors can be observed in Fig. 16. For $m = 25$ subsequent failures occur in the same particle; in the case $m = 5$ the failures are more randomly

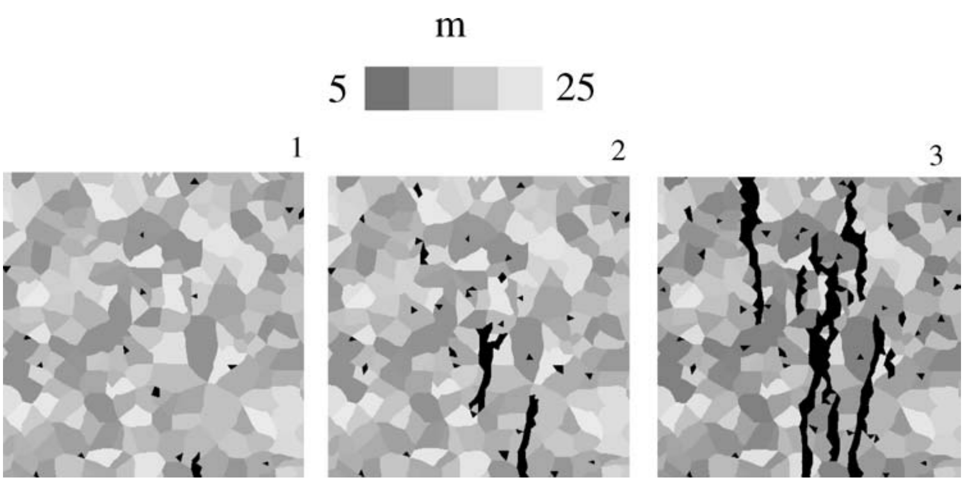
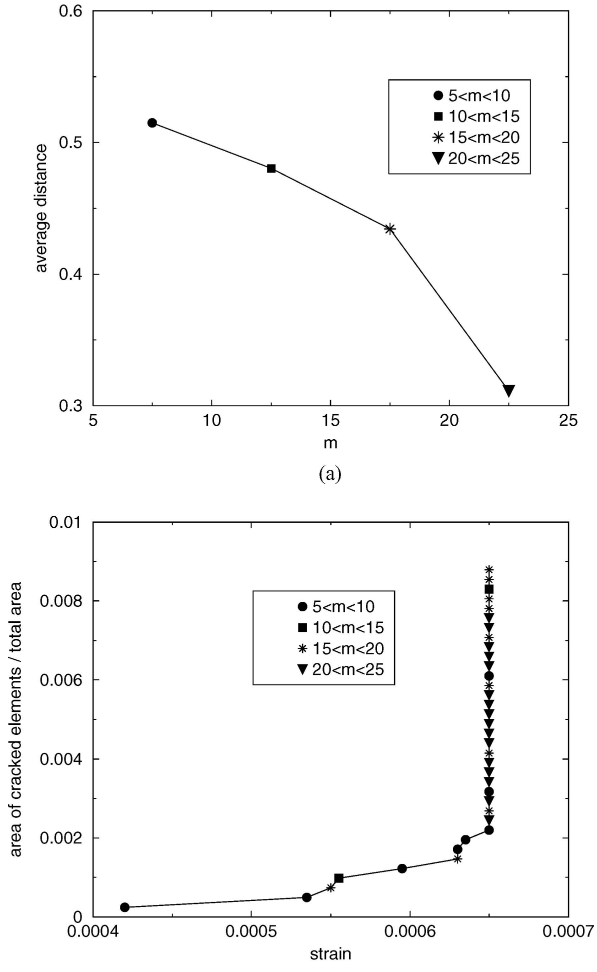


Figure 12 Damage evolution in a polycrystal.



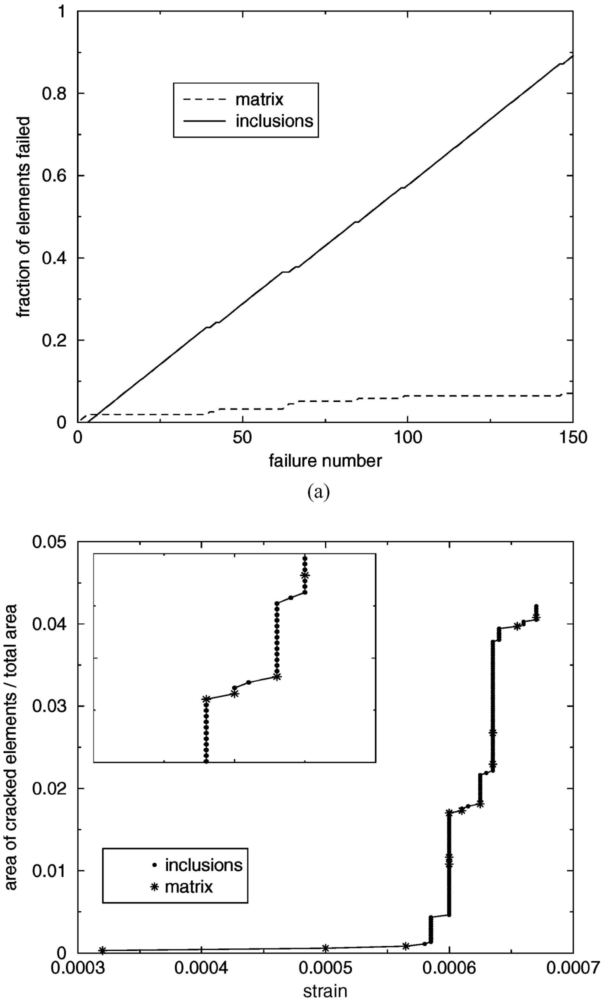
(a)

(b)

Figure 13 (a) Distance from subsequent failures (second to first) for a polycrystal. (b) Damage evolution in a polycrystal

Figure 14 Particulate composite microstructure.

distributed. Distribution of distances for subsequent failures are illustrated in Fig. 17a: as mentioned, the failures are correlated for high Weibull modulus, and are spatially distributed for a low m. Fig. 17b reports the damage parameter as a function of the applied strain for the two different cases. The damage is greater with high Weibull modulus because this corresponds to the failure of an entire particle.



(a)

(b)

Figure 15 (a) Fraction of elements failing in the matrix and in the inclusions for a particulate microstructure. (b) Damage evolution in a particulate microstructure (and zoom in the top-left corner).

The effect of volume fraction on the behavior of the particulate composite is studied by considering four different microstructures with increasing volume fraction of particles ($E_{\text{matrix}} = 100$ GPa, $E_{\text{particle}} = 400$ GPa). The length scale of the finite element grid is fixed while the microstructure is different for each simulation, (i.e., by increasing volume fractions with a Poisson point process). Analyzing the damage behavior of these microstructures in Fig. 18, the microstructures with higher volume fraction of hard particles seem to be more susceptible to damage caused by brittle fracture. Moreover it can also be observed that larger particles are more likely to break than smaller ones; in fact experimental results, i.e., micrographs of damaged composites, indicate that larger inclusions tend to fracture at lower loads than smaller inclusions, and this is also confirmed by other authors by means of theoretical or numerical models [2, 9, 11, 38].

Nevertheless some larger particles which should have a higher propensity to crack at relatively low applied strain may not break due to rupture of neighboring particles and hence stress redistribution, as pointed out also in [2]. Thus, the effect of the evolving microstructural topology on the damage accumulation is evident.

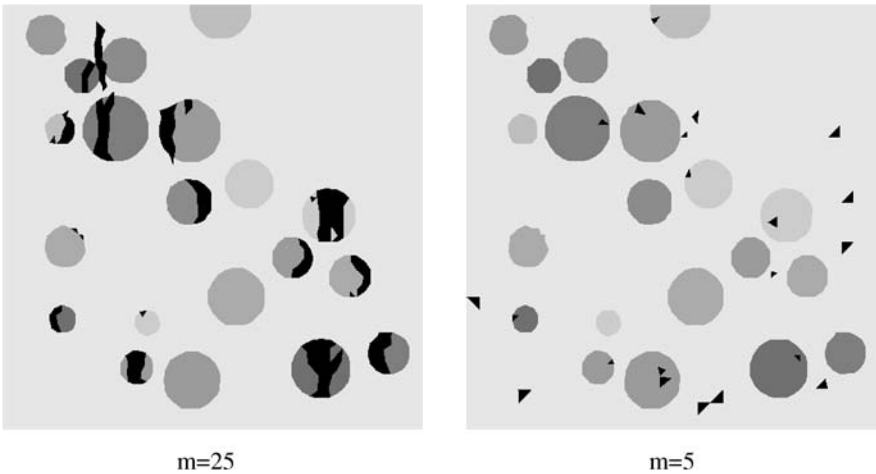


Figure 16 Illustration of effect of reliability parameters on the damage progression in the same particulate microstructure.

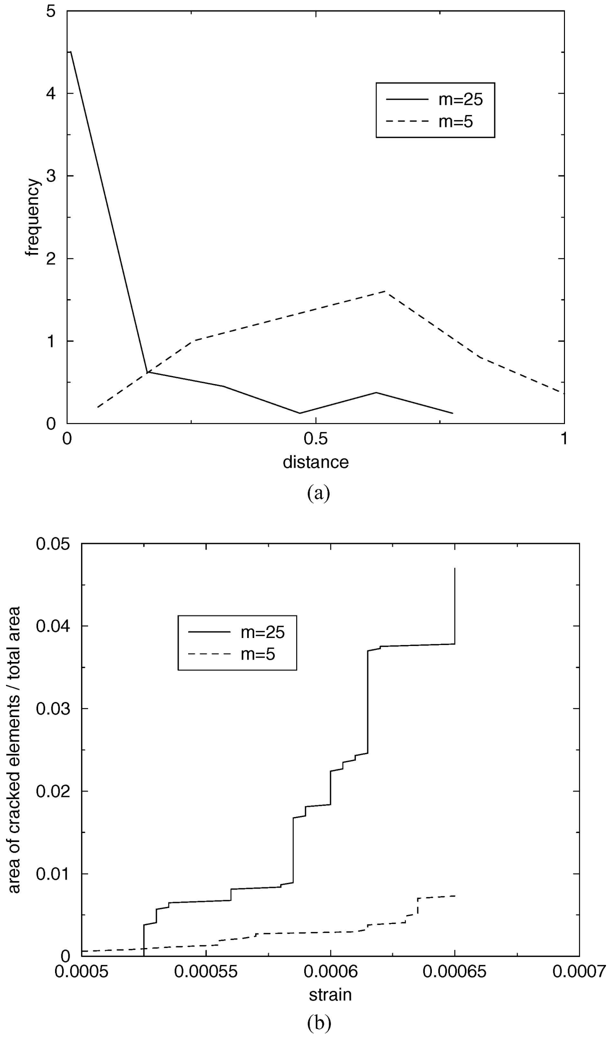


Figure 17 (a) Frequency plot correlating distance of second failure from the first one in particulate microstructures. (b) Damage evolution in particulate microstructures.

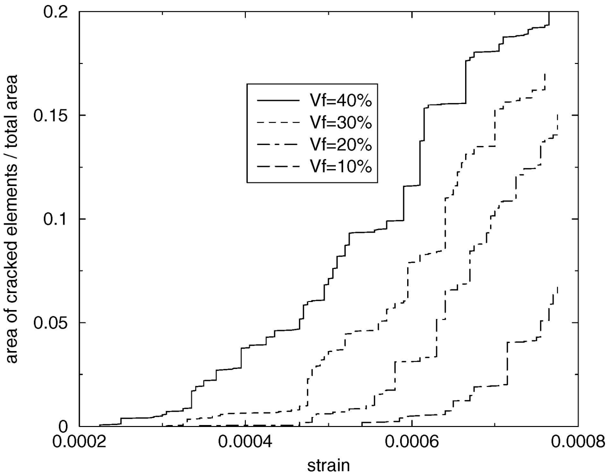


Figure 18 Damage evolution for different volume fractions of particulate phase.

4. Discussion and conclusions

In this paper, an approach for the investigation of fracture and damage in brittle materials has been presented. The damage evolution is simulated by a probabilistic failure criterion in conjunction with a microstructural based finite element code (OOF). One practical consequence of this approach is that the finite element model can be constructed from microstructures, i.e., a digitized micrograph, so that arbitrary inclusion patterns, shapes and sizes of heterogeneities as obtained from actual images are readily modeled. Adaptive schemes and mesh refinement strategies are available in order to capture microstructural details. Microcrack formation and propagation due to increasing applied load is investigated in arbitrary microstructures of complex materials, such as polycrystals and composites. The microstructure is converted into a finite element mesh and, for the prescribed loading condition, the microstructural stresses are calculated by the FEM solver. A Monte Carlo failure criterion based on Weibull statistics is implemented, and fracture is modeled by a reduction of stiffness of the broken element perpendicular to the crack plane and a stress redistribution among neighboring elements. In this way, it is possible to model continuously changing element topology due to progressive material failure and crack paths can be analyzed. The results show that distribution of damage is strongly affected by local failures probabilities (i.e., the value of the Weibull modulus m) as well as by stress concentrations. This means that both the particular microstructure and the loading conditions play a key role in the evolution of damage accumulation.

In particular, polycrystals were investigated in order to assess the effect of grain properties on the accumulation of microcrack damage. The fracture mechanism is ruled by the interplay between stress concentrations and local failure probabilities.

As regards particulate composites microstructures, it was found that particle size plays the most critical role in the cracking process. In fact, larger particles tend to fracture at a lower deformation level than smaller ones and therefore act as nucleation sites for damage initiation [2]. Moreover, the volume fraction of particles plays a significant role. Thus, it can be concluded that an RVE model that is homogeneous over a region of a particulate composite should depend on local values of particle size, inclusion volume fraction as well as materials properties.

However, it should be noted that this approach has implicit assumptions that are subject to verification. The Weibull assumption (the weakest link hypothesis) presumes that the whole sample fails when the critical condition is reached. In this paper, the Weibull criterion was applied through a Monte Carlo process for each single element. Other failure models may prove to be more appropriate.

Moreover it is assumed that is physically plausible for macroscopic reliability laws to provide parameters which can be applied discretely to small elements within a microstructure. As mentioned previously, this means that the finite element discretization is coarse enough to average over a distribution of pre-existing flaws which are very small compared to the characteristic element size. Since a particular system may have some variability, the Monte Carlo method will generate a statistical basis to understand the nature of the variability and its relation to microstructure. It is worth noting that other authors adopted a similar approach based on the Weibull law to characterize the strength of fibers in composites [41].

The present model is two-dimensional and therefore situations where three-dimensions are required for numerical prediction, such as crack propagation in a real composites, are only qualitatively represented by means of a two-dimensional model. Other authors emphasized the importance of 3D microstructural modeling [10, 11], showing that the predicted damage was more considerable in 3D compared to 2D approaches. Nevertheless, 2D models are often assumed when describing the mechanical and fracture behavior of heterogeneous materials (see for example [29]), and only a few studies consider 3-D effects [10, 11]. The general agreement between these two-dimensional numerical results and the experimental ones (e.g., two-dimensional micrographs of damaged composites) indicates that this model fulfills the role of developing engineering intuition on the effect of microstructure on reliability. The 2D modeling approach is not seen as a serious limitation as a design tool; however, three-dimensional models would be more predictive. Other future developments could include the analysis of the interfaces and surfaces of complex and heterogenous materials, for example the development of damage by decohesion at the particle/matrix interface. Other microstructures such as functionally graded materials (FGMs) have been analyzed by a similar method and will appear elsewhere. An experimental validation of the present model would be desirable; the combined use of experimental investigations and of numerical simulations is essential to gain meaningful indications on the material properties.

Moreover, it would be interesting to compare this model with some formal methods of damage mechanics, e.g., the analytical work of Kachanov [42, 43], Ladeveze [44–46], Nemat-Nasser and Hori [47].

The results of this work provide a basic insight into the influence of the microstructure on the mechanical properties, with particular regard to failure mechanisms. This can help the design of the final material microstructure, with the aim of optimizing the microstructure itself. Tailored properties could be produced by clever processing techniques if the role of microstructural features is understood.

Moreover, the versatility of the OOF code allows the analysis of real materials microstructures. Therefore the study of the mechanical and fracture behavior of heterogenous materials is not limited to the RVE, but the actual microstructure with all its complex features (e.g., shapes, dimensions, positions and volume fraction of the second phase) may be throughly investigated. The methods illustrated in this paper also provide the means to derive homogeneous properties that could be used in conjunction with the RVE techniques.

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