BRIDGING THE SCALES WITH STATISTICAL DAMAGE MECHANICS

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ABSTRACT

Statistical damage mechanics establishes the connection between the disordered microstructure and the macroscopic properties of a damaged material. During the damage process the specimen changes from random homogeneous, when the micro-cracks develop by nucleation at the weak spots of microstructure, to heterogeneous, when the micro-cracks density enlarges. The macro-parameters of the quasi-brittle specimen in both the hardening and softening phases are algebraic expressions of the damage function $\overline{D}(\bar{\varepsilon}, L)$. The microstructure of the damaged specimen, during the process, was modeled as a two-dimensional Voronoi-Delaunay lattice. The Family-Vicsek scaling relation is applied to the simulation data to scale the function $\overline{D}(\bar{\varepsilon}, L)$.

1. INTRODUCTION

Many engineering solid materials, such as polycrystal ceramics, metals, and alloys, have random homogeneous microstructure. In structural applications micro-cracks nucleate, propagate and cluster, which leads to heterogeneous microstructure and structural failure. Krajcinovic and Rinaldi (K&R) [1] consider the homogeneous to heterogeneous phase transition, including the failure, using the tools of statistical mechanics and fractal geometry. A lattice model is used to reproduce the damage process in quasi-brittle material up to the threshold of failure.

2. LATTICE MODEL AND SIMULATION RESULTS

On the microscale and in two-dimensional space a polycrystal is similar to a spring network of random Voronoi polygon / Delaunay simplicial graph in Figure 1a. In the perfect triangular lattice, all polyhedrons are honeycombs and the simplicial Delaunay graphs are triangular. Voronoi and Delaunay graphs are dual. Voronoi polygon represents a grain of polycrystal and a bond of the Delaunay lattice is representative of a grain boundary. In this paper all grains are distorted hexagons whose edges have different lengths (normally distributed). Since the distributions of structural imperfections are random in a real microstructure, the distribution of fracture toughness of the grain boundary, γ_{gb}, must be random as well. A micro-crack forms when one spring breaks due to the applied load. The micro-cracks smaller than the grain boundary are introduced through the link strength distribution. The growth of these micro-cracks from their initial length to the length of the grain boundary is assumed to be instantaneous. This lattice model accounts for inter-granular micro-cracks only, which is appropriate when the grain-boundary fracture toughness γ_{gb} is less than the cleavage energy. The dual Voronoi tessellation is necessary to assess micro-cracks adjacency and coalescence, as shown in Figure 1b.

K&R [1] use the lattice model to simulate uniaxial tensile tests for four lattice size $N = \{24, 48, 96, 192\}$ (10 replicates per size), where N is the number of grains per side. Each

simulation is carried on incrementally by applying small displacement steps up to the threshold of failure and by computing the equilibrium (compatible) configuration at each step, where only the springs loaded under their critical strength are retained in the lattice.

The effective macro-stress $\bar{\sigma}$ and the damage parameter $\bar{D}$ (defined later in CH 4) are collected in the simulations. The mean $\bar{\sigma}$ *vs.* $\bar{\varepsilon}$ and $\bar{D}$ *vs.* $\bar{\varepsilon}$ curves from simulations are shown in Figure 2 for all sizes *N*. The $\bar{\sigma}$ *vs.* $\bar{\varepsilon}$ curves provide the macroscopic constitutive relations of the effective Cauchy element at the macroscopic scale and highlight the size-effect in the softening response. The results explain why continuum models and micromechanics with representative volume element (RVE) should not be used in the softening regime. All four lattice sizes represent good RVEs before the peak of the $\bar{\sigma}$ *vs.* $\bar{\varepsilon}$ curve, when the microstructure is ergodic and statistical homogeneous.

3. PHASES AND PHASE TRANSITIONS

The mechanisms of the damage evolution change from nucleation to propagation and clustering of micro-cracks when the micro-cracks density grows. Such change corresponds to the transition from an ordered phase, the hardening, to a disordered phase, the softening. In the beginning of the hardening phase damage density develops by random nucleation of microcracks, whereas close to the end of this phase (at the peak of the $\bar{\sigma}$ *vs.* $\bar{\varepsilon}$ curves) the formation of grain-boundary micro-cracks is highly correlated and few clusters propagate and coalesce. The transition is revealed by the characteristic "saturation knee" (Hansen et al. [2]) in the $\bar{D}$ *vs.* $\bar{\varepsilon}$ curves. The disorder of the microstructure is responsible for the damage localization in the softening. A random change of the lattice texture does not influence the lattice behavior at small damage density but alters the locations of the hot spots, where ─due to the presence of micro-cracks─ the fluctuations of the microscopic stress field exceed significantly the average stress. At least one cluster has enough energy to span the specimen at the peak of the $\bar{\sigma}$ *vs.* $\bar{\varepsilon}$ curve. A material specimen is homogeneous at the beginning of the hardening but is random heterogeneous close to the peak and afterwards. At the threshold of failure a second phase transition occurs when the lattice goes from "connected" phase to a "disconnected" phase.

In statistical mechanics order-disorder phase transitions are described by order parameters, which distinguish an order from a disordered phase [3]. K&R [1] suggest the following definition

$$\langle \phi \rangle \equiv \langle 1 - \bar{D} \rangle \qquad (1)$$

of the order parameter $\langle \phi \rangle$ to describe the failure threshold for this problem. If the displacement is controlled, the damage growth is stable and a softening phase exists. Else, when the load is controlled, the phase transition at the peak coincides with the instantaneous specimen failure. In the parlance of statistical mechanics, the latter case corresponds to a first order transition (the order parameter goes discontinuously from a non-zero to a zero value) and the former to a second order transition (the order parameter goes continuously to zero at the failure).

4. DAMAGE PARAMETER AND SCALING

The definition of damage parameter for the lattice at small damage densities is

$$\bar{D} = \frac{n}{2e^{-1.6}L^2} \cong \frac{\bar{\varepsilon}}{0.00432} \qquad (2)$$

where n is the number of broken bonds and L the lattice size. K&R [1] introduce definition (2) based on the similarity with the parallel bar system (PBS – Ref [4]) and on the resemblance of random nucleation with a transient chaotic process (usually described by a fat fractal of integer fractal exponent = 2) up to the peak N_P. For the monotonic tensile test, the constitutive equation can be written in scalar form as

$$\bar{\sigma} = E_0 \left(1 - \bar{D}\right) \bar{\varepsilon} \tag{3}$$

where E_0 is the Young's modulus of the material in pristine conditions. At small damage density, by virtue of (2), one obtains $\bar{\sigma} = \bar{E}_o \left(1 - \bar{\varepsilon}/0.00432\right)\bar{\varepsilon}$, which shows very good agreement with simulation data over the hardening phase.

Close to the peak and in the softening regime the stress response and damage parameter depends on L. The constitutive relation (3) depends on the scaling function $\bar{D}(\bar{\varepsilon}, L)$. Scaling is based on the scale-invariance (fractality) of fractal objects and enables to infer the statistics of a process on any scale from the known statistics of the same process on one scale [4]. The concept of scaling is fundamental in statistical damage mechanics to bridge the scales and is applicable for the existence of fractal sets in both phases of the damage process. In the beginning of the softening phase the correlation length of the dominating clusters is a fractal and at the end is multifractal. The $\bar{D}$ vs. $\bar{\varepsilon}$ data for different lattice size should map into a single curve if scaled properly. In this paper, K&R propose a scaling procedure based on the repeated application of the Family-Vicsek scaling relation

$$\bar{D}(\bar{\varepsilon}, L) = L^{\alpha} f\left(\frac{\bar{\varepsilon}}{L^{\gamma}}\right) \tag{4}$$

in the both hardening and softening phases. The fractal exponents α and γ are the scaling exponents of $\bar{D}$ and $\bar{\varepsilon}$ of the power law to be determined numerically.

4.1. Scaling: hardening regime
In the beginning, the simulation data are close to a straight line but deviate progressively at the peak. By using (4), the data collapse on a single curve throughout the hardening regime, including the data at the peak, for $\gamma = \alpha = -0.035$. The scaling (4) is feasible here because the damage at the peak is a fractal quantity and has the role of the saturation threshold. A simple analytical formula for the damage parameter, such as

$$\bar{D} \cong a\bar{\varepsilon} + b\frac{\bar{\varepsilon}^2}{L^{\alpha}}, \tag{5}$$

captures the data simulation of the hardening phase and can be used in (3). The coefficients a and b are deduced from simulations ($a = 275$ and $b = -14862$ here). The scaling is correct because scaled $\bar{D}$ vs. $\bar{\varepsilon}$ curves in Figure3a collapse on a single curve for all sample averages and lattice sizes. The peak points collapse in the point $\left(\bar{\varepsilon}_p, \bar{D}_p\right) = \left(0.0021, \ 0.5\right)$ in Figure 3a.

4.2. Scaling: softening regime
After the peak, in the softening regime, the scaled $\bar{D}$ vs. $\bar{\varepsilon}$ curves in Figure 3a are still distinct and size dependent. The data of the softening regime can be separated from the hardening data in the new shifted frame of reference shown in Figure3a, centered in $\left(\bar{\varepsilon}_p, \bar{D}_p\right)$ and having coordinates

$\bar{\varepsilon}_s = (\bar{\varepsilon} - \bar{\varepsilon}_P)/L^\alpha$ and $\bar{D}_s = \bar{D}/L^\alpha - 0.5$. The scaling-relation (4) is applied again but only on the softening regime

$$\bar{D}_s(\bar{\varepsilon}_s, L) = L^z g\left(\frac{\bar{\varepsilon}_s}{L^z}\right).$$

(6)

The result of (6) is shown in Figure 3b when $z = -0.52$. The data collapse is evident. The non-linear analytical function

$$\bar{D} \cong L^\alpha \bar{D}_p + a_1 L^\alpha \bar{\varepsilon}_s + b_1 L^\alpha L^z \left(1 - e^{-c_1 \frac{\bar{\varepsilon}_s}{L^z}}\right)$$

(7)

provides a very good approximation of the damage parameter in the softening regime. The three parameters $a_1 = 15.80$, $b_1 = 2.2$ and $c_1 = 100$ are again determined from simulations but they are not independent of each other. As shown in Figure3b, the softening data maintain C^1 continuity with the hardening data after scaling (6), i.e. $a_1 + b_1 c_1 = \partial \bar{D}/\partial \bar{\varepsilon}\big|_{\bar{\varepsilon}_p}$. Also, close to failure, the

$\bar{D}$ vs. $\bar{\varepsilon}$ curves in the softening phase are straight lines of slope $a_1 = \partial \bar{D}/\partial \bar{\varepsilon}\big|_{failure}$. Hence, there is

only one degree of freedom left in (7) to be determinable via non-linear regression.

5. CONCLUSIONS

The statistical mechanics models, based on thermodynamics, fractal and multifractal geometry, can provide the foundation for the design from nano- to macro-structures. Statistical mechanics models, such this one, are suitable for the entire damage process, both when the material is statistical homogeneous and when it is heterogeneous, and can be used to estimate the failure threshold. Therefore, statistical models can predict damage tolerance and durability, which are necessary to structural design and to device acceptable maintenance and inspection programs. Statistical damage mechanics might offer an ideal framework to address the controversial issue of whether or not the softening phase is an intrinsic property of the material.
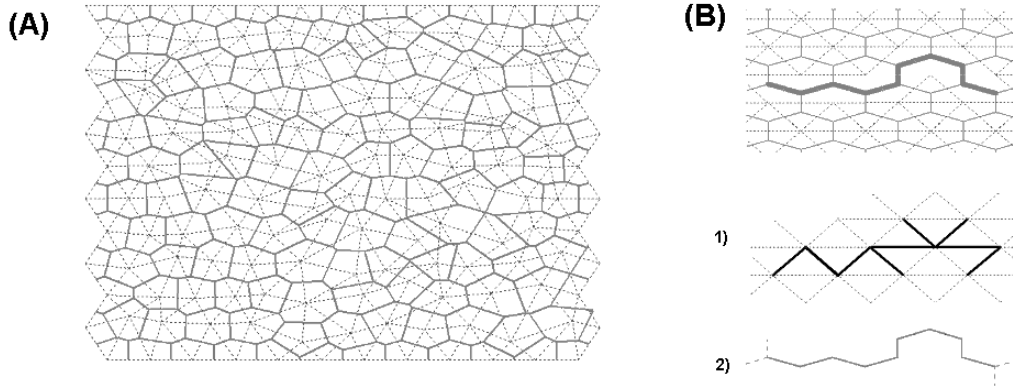

Figure1: Voronoi/Delaunay graphs of the microstructure(A). Adjacency assessment in Voronoi(B)
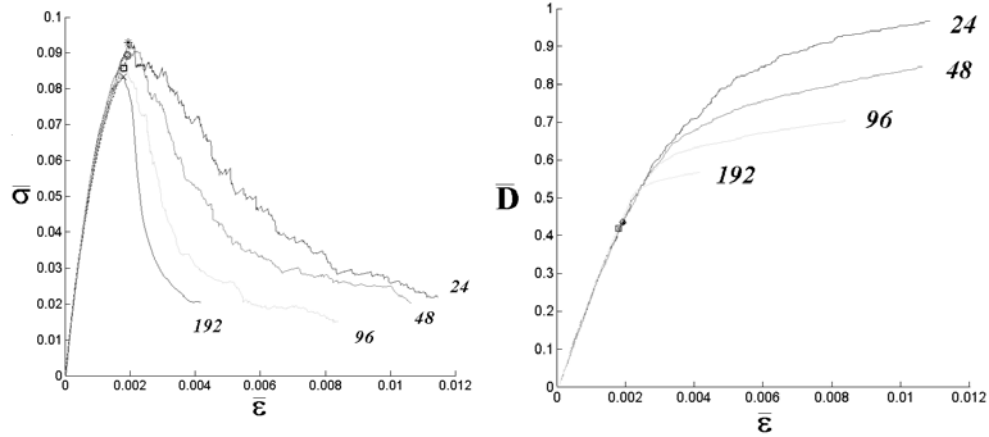
Figure 2: Mean curves $\bar{\sigma}$ *vs.* $\bar{\varepsilon}$ (A) and $\bar{D}$ *vs.* $\bar{\varepsilon}$ (B)
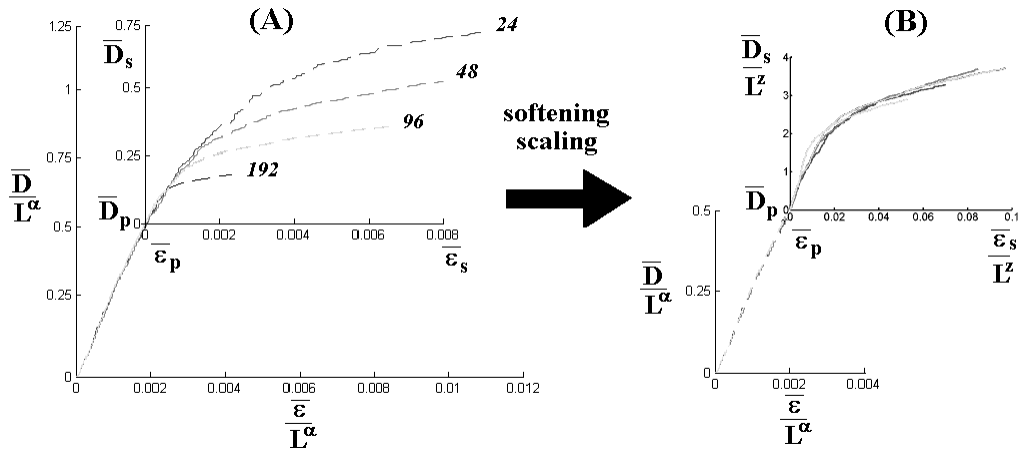

Figure 3: Scaling procedure of the data in hardening (A) and softening regime (B).

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