

ASYMPTOTIC INDEPENDENCE OF MATERIAL FAILURE AT DIFFERENT SCALES – THE ROLE OF SMALL-SCALE FLUCTUATIONS

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ABSTRACT

Most materials are heterogeneous and aperiodic at micro and nanoscales; the properties, interaction etc. of the heterogeneities are random functions of space and time. An adequately detailed probabilistic description of the material microstructure is required for modeling material behavior and failure at all scales of interest. While it is possible to observe surfaces of solids down to nanometer resolutions, it remains a challenge to observe internal microstructural evolution in situ at a comparable resolution, and indirect methods are required for modeling small-scale stochastic damage phenomena. It is important to include both the spatial and the temporal aspects of the small-scale fluctuations. This paper proposes a general model of how the random material microstructure, composed of a matrix and embedded defects, evolves in time and space as a specimen is subjected to external actions. Local stationarity, strong mixing and dispersed extremes are assumed and the limiting distributions of the local average and the local maximum response are elicited. The asymptotic independence of extremal processes and hence failure (defined as first passage of a space-time process) at widely different scales is demonstrated.

Keywords: damage, stochastic, point process, spatial, mixing, random field, scale dependent, extreme, failure, first passage

INTRODUCTION

Performance of materials plays a central role in the success and advancement, and sometimes in unexpected failures, of engineered systems. Failure of components – whether mechanical or electronic in nature and whether micro- or macroscopic in size – is often structural in origin. Material response to loading is affected by a range of parameters that include loading rate, boundary conditions, temperature, presence of electrical and magnetic fields and, importantly, composition at the nano- and microscales. While it is generally acceptable to take a continuum view on material behavior when dealing with scales larger than RVEs (representative volume elements), most materials are discrete, heterogeneous and aperiodic at smaller scales and undergo rearrangement reversibly or irreversibly (including creation of new surfaces) under external actions. Yet, a variety of available models of damage growth continue with the continuum assumption even when dealing with phenomena clearly below the RVE limit.

The chemical and mechanical properties, shape, size, orientation, interaction etc. of the nano- and microscale heterogeneities are random and sometimes discontinuous functions of space and

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time; hence, an adequately detailed probabilistic description of the random material microstructure is required. Indeed, much of the response and property variabilities at any given scale and application of engineering interest can be traced to fluctuations at smaller scales. Meaningful description and future prediction of material behavior and failure, whether for traditional or emerging materials, should take this small-scale randomness into account.

While it is possible to observe material *surfaces* down to nanometer resolutions, e.g. with scanning electron or atomic force microscopy, it remains a challenge to observe internal microstructural evolution in situ at a comparable resolution, and indirect methods involving imaging and analytical modeling are required. It is possible in principle to study every cell, grain, void, inclusion (including their interactions) etc. within a given material volume under a set of external actions and thus describe the entire region over an interval of time. However, even if this were analytically and computationally feasible, such an approach would produce a prohibitively large amount of information. Instead, it is more tractable to describe the region in probabilistic terms so that all relevant characteristics of the field are conveyed by adopting a probabilistic description that is sufficiently detailed for the purpose at hand.

It is important to note that small-scale fluctuations can occur both in space and time, and a model of stochastic damage growth should account for both aspects. It may be insufficient to deal solely with temporal fluctuations, or take snapshots of spatial fluctuations alone. The behavior of a process in the spatial dimension can be very different from that in the temporal dimension (Niu 1998). The coupling of spatial and temporal fluctuations in material damage accumulation has not been investigated adequately in the existing literature.

BACKGROUND

Local Averages and the RVE

Consider some variable property or response of a material volume that needs to be measured. If the time-variant nature of the property dominates, while its distribution in space is either not relevant or is averaged in some sense, the property (or its residual after removing the deterministic component) is described as a stochastic process indexed with time. Examples include fatigue crack growth rate (e.g., Lin and Yang 1983), the damage state variable based on continuum damage mechanics (CDM) (e.g., Bhattacharya and Ellingwood 1998) etc. CDM defines damage in an “average” volume-wide sense, and relates the effective macroscopic response with the state of the material microstructure. Consequently, spatial fluctuations in damage cannot be accounted for in CDM; this is acceptable as long as the focus is on the macro-scopic effect of damage, and “damage” is restricted to a slow volume-wide degradation of the micro-structure resulting in loss of stiffness (Bhattacharya and Ellingwood 1998; Krajcinovic 2000). In a more general case, a quantity may vary with time as well as in space, with the fluctuation being random in nature. Examples include earthquake excitation, stiffness of a material undergoing damage, etc. The quantity is then described as a space-time random process, $X(\underline{z}, t)$, indexed with up to four parameters (\underline{z} = coordinates of a point).

In attempting to measure any random property or response, some spatial or temporal averaging is frequently employed. Most engineering measurements, including such familiar quantities as wind speed, density, stiffness, temperature etc. are essentially such averages due to limitations of the measuring devices (inertia, finite size, response delay etc.) (Vanmarcke 1983). Since the integration or averaging is over finite intervals of space and time, the estimates differ when they are from different regions of space and time, and consequently, they are modeled as random variables or random processes (or fields). Local averages from different regions of space (or time) are correlated. In the absence of periodicity (or when periodicity is removed), the magnitude of

correlation decreases with increasing separation. Consider a random field $X(\underline{z})$ and its local average over a volume V , $X_V(\underline{z}) = (1/V) \iiint_V X(\underline{w}) d\underline{w}$. It is important to note that information only on the average process $X_V(\underline{z})$, rather than on $X(\underline{z})$, may be available. $X_V(\underline{z})$ is random (as mentioned above) and if the probability distribution of $X_V(\underline{z})$ (and hence its mean and variance) are independent of \underline{z} , and the correlation between $X_V(\underline{z}_1)$ and $X_V(\underline{z}_2)$ is a function only of $(\underline{z}_2 - \underline{z}_1)$, then $X_V(\underline{z})$ is statistically homogeneous (in the weak sense). This property, importantly, may hold only for sufficiently large V . Furthermore, if the correlation depends only on the scalar distance between the two points, X_V is said to be isotropic.

As stated before, most solids are microscopically heterogeneous, disordered and aperiodic. Traditionally in continuum mechanics, this problem has been tackled by assuming the existence of the RVE i.e., the representative volume element. As long as the resolution remains above the scale of the RVE (i.e., in the macroscale), the continuum assumption holds. Mathematically, the RVE is an infinite length scale limit relative to the microscale, or the length scale of a single heterogeneity, in which the material appears uniform (Ostoja-Starzewski 1998).

In the context of randomness, properties obtained by averaging over domains equal to or larger than the RVE are statistically homogeneous. It should be noted that a material may be statistically homogeneous for some but not all properties. Moreover, the size of the RVE is not necessarily constant for a given material: a finite domain in a heterogeneous material volume that has the RVE property may lose that property in the presence of material damage.

Three characteristic lengths may be used to define the scale of a problem (Krajcinovic and Vujosevic 1998): size of the material texture, L_m (e.g. grain size), the correlation length, ξ , and the specimen size, L . The correlation length is the largest distance over which two defects can directly affect each other's growth. The length of the RVE satisfies: $\max(L_m, \xi) < L_{RVE} < L$. At localization of damage, the correlation length, ξ , approaches the specimen length, L . There is no consensus about the actual size of an RVE. For example, on one hand, RVE size of 10 – 100 times the size of an inhomogeneity, and on the other, a small volume of the order of a few grains, have been reported in the literature (Ostoja-Starzewski 1998). Frantziskonis (1995) attempted to estimate the correlation length of the displacement field in rocklike materials using ultrasonic pulses and measuring the bulk attenuation averaged over a macroscopic volume.

The Need for Small-scale Modeling

The need to model material behavior below the RVE limit has long been felt (e.g. Beran 1968). Ostoja-Starzewski (1998) has shown that a locally isotropic, smooth but inhomogeneous elastic material does not exist below the scale of the RVE. Ostoja-Starzewski (2002) has also shown that a random field that is not ergodic cannot lead to a continuum model. Local averaging, and by extension the concept of RVE (assuming it exists), works when one is interested in aggregate (or effective) information. However, when one is interested in local peaks or extremes of a process, then averaging may be counter-productive – one needs to make sure that the extremes are not lost by an excessively long averaging window. Analytical models and instruments should possess sufficient resolution and sensitivity to capture these extremes.

Micro- or nanostructural fluctuations affect global behavior and failure of materials. For example, although fracture is a macroscopic phenomenon, it is very sensitive to details at the atomic scale, including crystal structure, and nonlinear features of atomic bonding (Marder 1999). At this scale, weak interatomic forces like Van der Waals forces, hydrogen bonds, electrical forces cannot be neglected. Moreover, these forces are highly sensitive to thermal forces (Huet 1997). A fundamental study of statistical fracture mechanics should therefore account for randomness at this scale. Processes such as fatigue crack growth which progress over small increments of time and

space are also affected by these fluctuations and show marked variability both in trajectories and growth rates. Virkler et al. (1979) performed constant amplitude (load-controlled, room-temperature) fatigue tests on aluminum specimens and observed sudden increases and decreases in crack growth rates as if “the crack was passing through a different material possessing different properties”. For the same reason, small and short crack growth is more random than that of long cracks.

Small-scale structural fluctuations affect non-mechanical systems as well. For example, the fabrication and performance of micro-electronic devices are affected by the distribution of stresses and strains at the nanoscale (Freund 2000). A uniform elastic strain imposed on a doped semiconductor (with a periodic crystal lattice) affects the electrical transport through the device. The distribution of electron or hole current per unit area of conduction cross section at sub-micron scales has been found to vary spatially even under nominally uniform strains; a possible explanation for the breakdown of this continuum assumption is the non-uniform strain field created by the small heterostructures (conduction barrier formed by bimaterial interfaces).

PROPOSED DAMAGE GROWTH MODEL

Spatial Distribution and Time Evolution of Defects

Consider a deformable body Ω bounded by the surface $\partial\Omega$. For simplicity, assume Ω to consist of a two-phase material – i.e., matrix (phase 1) and defects (phase 2) embedded in the matrix. The defects are distributed randomly in the matrix according to a spatial point process, Π . The spatial distribution of these defects is not too dense such that almost surely no more than one defect is present in a small neighborhood around any given point, \underline{z} . Also, the number of defects in any bounded region $A \subset \Omega$ is finite. Depending on the process in which the material is manufactured or assembled, the spatial density of the defects may not be uniform across the volume of the material; in other words, this point process is not necessarily homogeneous.

In the special case when the numbers of defects in non-overlapping regions are independent, the process Π can be modeled as a spatial Poisson process in state space \mathbb{R}^3 with mean measure, $\mu(B) = \int_B \lambda(\underline{z}) d\underline{z}$, where B is a bounded set in \mathbb{R}^3 and $\lambda(\underline{z})$ is the intensity of the process. The Poisson assumption is clearly violated, however, when factors such as finite size of defects, coalescence of several defects into one defect, or the disintegration of one defect into several etc. are considered (see, e.g., Sobczyk and Kirkner 2001).

At the initial time t_0 the domain Ω and every region within it are in thermodynamic equilibrium, i.e., unless acted on by external agents, the domain Ω , its subsets, including the set of defects, do not evolve in time.

Now consider the properties of the defects. A defect at location \underline{z} may be characterized at time t by a set of properties (i.e., marks), $\Theta(\underline{z}, t)$, that include its volume, surface area, density, orientation, elastic modulus, damage state, nearest-neighbor distance, etc. In general, $\Theta(\underline{z}, t)$ is random in nature. Even if at the initial time t_0 the field $\Theta(\underline{z}, t_0)$ is homogeneous, due to the effect of the external actions, at later times $\Theta(\underline{z}, t)$ becomes non-stationary in time as well as in space. At any fixed \underline{z} , the evolution of Θ may be modeled as Markovian in time. It is likely that the elements of $\Theta(\underline{z}, t)$ at any given \underline{z}, t are dependent on each other.

We now have a marked process $M(t) = \{\underline{z}(t), \Theta(\underline{z}, t)\}$ with state space,

$$S(t) = \mathbb{R}^3 \times X \quad (1)$$

where X is the range of the random variables, $\underline{\Theta}$. Eq (1) emphasizes that $S(t)$, the state space of $M(t)$, may evolve with time owing to some external action $E(t)$, for example, when Ω is subjected to loading. Hence there is a function $g(E(t))$ that maps $S(t_1)$ into $S(t_2)$, $t_2 > t_1$. For example, the location of a defect may change owing to migration, the shape of the defect may change causing its surface area and volume to change, and so on.

Again, in the special case, when (i) $\Pi(t)$ is Poisson, (ii) $\underline{\Theta}(\underline{z}, t)$ is independent of $\Pi(t)$, (iii) $\underline{\Theta}(\underline{z}_1, t)$ and $\underline{\Theta}(\underline{z}_2, t)$ are independent for two distinct points $\underline{z}_1 \neq \underline{z}_2$ at all t , and (iv) the mapping g does not produce an atom, i.e., it does not pile distinct points of $S(t_1)$ on a single point of $S(t_2)$, then $M(t)$ is a Poisson process (Kingman 1993).

Independence between marks at two different locations and between the marks and the point process, as stated in the preceding paragraph, is too restrictive since, in general, $\underline{\Theta}(\underline{z}, t)$ is influenced by past and present values of the marks throughout Ω . It is more reasonable to suppose that the influence decreases with increasing separation in space and time. Specifically, it may be assumed that only the *current* (in time) knowledge of *near-by* (in space) points is sufficient to describe the evolution of $\underline{\Theta}(\underline{z}, t)$. This dependence structure may be formalized with a suitable mixing condition: For an arbitrary fixed t and any constituent θ of $\underline{\Theta}$, denote by \mathfrak{A} the σ -field generated by the random variables $\{\theta(\underline{w}, t), \underline{w} \in \Omega\}$. Denote the set of near-by points for a given location \underline{z} by $C(\underline{z}; t)$ and a set of distant points by $C'(\underline{z}; t)$, with a suitably defined distance $d(C, C'; \underline{z}, t)$ between them. Corresponding to C and C' , let \mathfrak{B} and \mathfrak{B}' be, respectively, the two sub σ -fields of \mathfrak{A} . Then one of several possible mixing coefficients may be defined to measure the dependence between \mathfrak{B} and \mathfrak{B}' (Doukhan 1994); for example, the strong mixing coefficient is,

$$\alpha(\mathfrak{B}, \mathfrak{B}') = \sup\{|P(U \cap V) - P(U)P(V)|; U \in \mathfrak{B}, V \in \mathfrak{B}'\} \quad (2)$$

The field θ is called strongly mixing if $\theta(C)$ and $\theta(C')$ become asymptotically independent (i.e., $\alpha(\mathfrak{B}, \mathfrak{B}') \rightarrow 0$) as $d(C, C'; \underline{z}, t)$ increases regardless of the cardinalities of C and C' (Rosenblatt 1985). Weaker mixing conditions, such as distributional mixing, may also be assumed (see, e.g., Leadbetter et al 1983). Note that these dependence structures are different from a Markov assumption for the discrete field $\underline{\Theta}(\underline{z}, t)$.

Statistics of Material Response

Consider some important property or response, $R(\underline{z}, t)$, of Ω . For simplicity, assume that R is a scalar. It may be convenient to denote by R some energy of the system since, in thermo-mechanics, energy is the only quantity that has the same meaning at all scales (Li 1999). R is either a constituent of $\underline{\Theta}$, or a function of $\underline{\Theta}$. Its observed value at location \underline{z} and time t is usually an average over some volume ΔV around \underline{z} and time interval ΔT around t :

$$R_{\text{ave}}^{\Delta V, \Delta T}(\underline{z}, t) = \frac{1}{\Delta V} \frac{1}{\Delta T} \int_{\Delta V(\underline{z})} \int_{\Delta T(t)} R(\underline{w}, \tau) d\underline{w} d\tau \quad (3)$$

Due to physical or technical limitations as stated above, there exist lower bounds, $|\Delta V_0|$ and ΔT_0 , to the elemental volume and time interval over which R can be measured. For given t , if the distribution of $R_{\text{ave}}^{\Delta V, \Delta T}(\underline{z}, t)$ is the same for any $\underline{z} \in \Omega$ as long as the size of the averaging volume $|\Delta V| > |\Delta V_M|$, then $|\Delta V_M|$ is the size of the RVE at time t for the response R . It should be noted

that $|\Delta V_M|$ may be different for other responses or at other times.

Quite different from the local average above, the maximum value of the response R in the volume ΔV around \underline{z} and the time interval ΔT around t is:

$$R_{\max}^{\Delta V, \Delta T}(\underline{z}, t) = \max [R(\underline{w}, \tau); \underline{w} \in \Delta V(\underline{z}), \tau \in \Delta T(t)] \quad (4)$$

$R_{\max}^{\Delta V, \Delta T}(\underline{z}, t)$ may not always be directly observable, in which case it needs to be estimated analytically.

Now suppose that randomness in R arises only from the defect phase (phase 2) of the material and that the contribution of the matrix is deterministic. Without loss of generality, let R be centered at the mean field. The observed response (Eq (3)) therefore becomes:

$$R_{\text{ave}}^{\Delta V, \Delta T}(\underline{z}, t) = \frac{1}{N(\Delta V(\underline{z}))} \frac{1}{\Delta T} \int_{\Delta T(t)} \sum_{i=1}^{N(\Delta V(\underline{z}))} R_i(\tau) d\tau = \frac{1}{\Delta T} \int_{\Delta T(t)} \bar{R}(\tau; \Delta V(\underline{z})) d\tau \quad (5)$$

where R_i is the response of the i th defect located at \underline{z}_i , $N(\Delta V(\underline{z}))$ is the number of points of the process $\Pi(t)$ in the volume ΔV around \underline{z} , and \bar{R} is the instantaneous average over the volume ΔV . The maximum response (Eq (4)) on the other hand becomes:

$$R_{\max}^{\Delta V, \Delta T}(\underline{z}, t) = \max [R_i(\tau); 0 \leq i \leq N(\Delta V(\underline{z})), \tau \in \Delta T(t)] = \max_{\tau \in \Delta T(t)} R_m(\tau; \Delta V(\underline{z})) \quad (6)$$

where $R_m(\tau; \Delta V)$ is the instantaneous maximum in the volume ΔV around \underline{z} . In the trivial (but unrealistic) case when (i) the responses are all equal, and (ii) ΔT is small enough so that R does not appreciably change during the time interval, then the average response and the maximum response are identical.

Note, however, that R is a non-stationary field on Ω at any given time. Let us now investigate the asymptotic nature of the normalized partial sum, $\bar{R}(\tau; \Delta V(\underline{z}))$, and the local extreme, $R_m(\tau; \Delta V(\underline{z}))$, of the non-stationary field R . In the following assume that at any arbitrary time t , (i) R has finite variance and $E[|R_i|^{2+\delta}] < \infty$, for some $\delta > 0$, (ii) the variance of \bar{R} is $\sigma^2/N(V(\underline{z}))$ with $\sigma^2 = \sum_{\underline{w} \in \Delta V} E(R(\underline{z})R(\underline{w})) > 0$ (iii) R is a strongly mixing field with respect to σ -fields generated by the random variables $\{R(\underline{w}, t), \underline{w} \in \Delta V(\underline{z})\}$, and (iv) ΔV is small enough (but larger than $|\Delta V_0|$ above) so that the field R within it may be considered stationary.

First, we consider the nature of \bar{R} . Let \bar{R} be computed from a sequence of finite subsets of ΔV such that the subsets do not increase only in one spatial direction. Further, the strong mixing coefficient, $\alpha(k)$, k being the distance between sets C and C' of ΔV , is of the order of k^{-d} ($d > 1$ is the dimension of the Euclidean space), and is such that $\sum_{k=0}^{\infty} k^{d-1} \alpha^{\delta/(2+\delta)}(k) < \infty$ for $|C| \leq 1, |C'| \leq 1$ and $\sum_{k=0}^{\infty} k^{d-1} \alpha^{\delta/(2+\delta)}(k) < \infty$ for $|C| + |C'| \leq 4$. Then, by the Central Limit Theorem, $\bar{R}(\tau; \Delta V(\underline{z}))$, approaches the Gaussian distribution (Doukhan 1994). It should be mentioned that, the stationarity of R is not critical to the asymptotic normality here, $\bar{R}(\tau; \Delta V(\underline{z}))$ approaches the Gaussian subject to a further set of restrictions (Doukhan 1994).

Now, we consider the nature of R_m . As long as the field R is strongly mixing (as assumed above), it satisfies ‘‘condition D’’ (Leadbetter et al. 1983) which is a type of distributional mixing.

Condition D weakens the strong mixing condition by replacing events U and V in Eq (2) by $\{R(\underline{w}_i; t) \leq u, \underline{w}_i \in C(\underline{z}; t)\}$ and $\{R(\underline{w}_i; t) \leq u, \underline{w}_i \in C'(\underline{z}; t)\}$, respectively. Assume further that high values of R do not cluster around any point in ΔV , i.e., “condition D’” (Leadbetter et al. 1983) is also satisfied by R . Under these conditions, R_m , suitably normalized, converges to one of the classical extreme value distribution. It should be mentioned here that, if R cannot be considered stationary within ΔV , R_m still has a limiting distribution $H(x)$ (for which $x_0(H) = \sup\{x : H(x) < 1\}$ and $x_1(H) = \inf\{x : H(x) > 0\}$ satisfying (i) $\ln H(x)$ is concave, or (ii) $x_0(H) < \infty$ and $\ln H(x_0(H) - e^{-x})$ is concave for $x > 0$, or (iii) $x_1(H)$ is finite and $\ln H(x_1(H) + e^{-x})$ is concave for $x > 0$) under a further set of conditions (Husler 1986).

Asymptotic Independence of Failure at Different Scales

A large class of material failure is covered by the criterion that failure occurs when a relevant material response exceeds its critical value for the first time in (t_0, t) and anywhere in Ω (e.g., der Kiureghian and Zhang 1999). The critical response R^* for a given mode of failure, however, may differ depending on the scale of interest, as shown in the following for local (small-scale) and global (macroscale) failures:

$$F_L = \{\max R(\underline{z}, \tau) > R_{local}^*; \underline{z} \in \Omega, \tau \in (t_0, t)\} = \left\{ \max_{0 \leq \tau \leq t} \max_{\Omega} R_m(\tau; \Delta V) > R_{local}^* \right\} \quad (7)$$

$$F_G = \{\max R_{ave}(\underline{z}, \tau) > R_{global}^*; \underline{z} \in \Omega, \tau \in (t_0, t)\} = \left\{ \max_{0 \leq \tau \leq t} \max_{\Omega} \bar{R}(\tau; \Delta V) > R_{global}^* \right\} \quad (8)$$

The asymptotic distributions of $\bar{R}(\tau; \Delta V)$, and $R_m(\tau; \Delta V)$ have been described above. Now recall from the previous section that, within ΔV , (i) R constitutes a zero-mean stationary field with finite variance, (ii) R is strong mixing, and (iii) R satisfies condition D’. Hence, it can be shown that $\bar{R}(\tau; \Delta V)$, and $R_m(\tau; \Delta V)$, suitably normalized, are asymptotically independent (Anderson and Turkman 1991; Hsing 1995). Consequently, $\max R(\underline{z}, \tau)$ and $\max R_{ave}(\underline{z}, \tau)$ in Eqs (7) and (8), respectively, are asymptotically independent for any $\underline{z} \in \Omega$ and $\tau \in (t_0, t)$. Hence the limit states F_L and F_G , referring to the same mode of failure, are independent. It is thus incorrect to take a macroscopic approach to failure or to apply continuum-based models when a first-passage criterion concerning small-scale phenomena is involved.

CONCLUSION

A model of stochastic damage evolution based on defects occurring in a matrix according to an inhomogeneous point process is presented. The points, and their marks, evolve in time due to external actions. This evolution is Markovian in the time dimension. At any given time, a mark constitutes a discrete and inhomogeneous random field. This field is assumed strongly mixing and locally homogeneous satisfying the dispersed extreme property (condition D’). Under appropriate conditions, it is shown that local averages are asymptotically normal, local extremes approach one of the extreme value distributions, and the two are asymptotically independent. These results can be generalized to more than one mark and more than one type of defects.

The important conclusion is that the maximum of the local averages and that of the local extremes are independent, hence, first passage type failures are independent phenomena at different scales, even when nominally referring to the same failure mode. Thus it is incorrect to take a macroscopic approach to failure or to apply continuum-based models when a first-passage criterion

concerning small-scale phenomena is involved. This may also explain why some bulk strength properties are weakly correlated with local ones.

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