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Scaling strength distributions in quasi-brittle materials from micro- to macro-scales: A computational approach to modeling Nature-inspired structural ceramics

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ABSTRACT

This paper presents an approach to predict the strength distribution of quasi-brittle materials across multiple length-scales, with emphasis on Nature-inspired ceramic structures. It permits the computation of the failure probability of any structure under any mechanical load, solely based on considerations of the microstructure and its failure properties by naturally incorporating the statistical and size-dependent aspects of failure. We overcome the intrinsic limitations of single periodic unit-based approaches by computing the successive failures of the material components and associated stress redistributions on arbitrary numbers of periodic units. For large size samples, the microscopic cells are replaced by a homogenized continuum with equivalent stochastic and damaged constitutive behavior. After establishing the predictive capabilities of the method, and illustrating its potential relevance to several engineering problems, we employ it in the study of the shape and scaling of strength distributions across differing length-scales for a particular quasi-brittle system. We find that the strength distributions display a Weibull form for samples of size approaching the periodic unit; however, these distributions become closer to normal with further increase in sample size before finally reverting to a Weibull form for macroscopic sized samples. In terms of scaling, we find that the weakest link scaling applies only to microscopic, and not macroscopic scale, samples. These findings are discussed in relation to failure patterns computed at different size-scales.

1. Background and significance

Many materials exhibit a quasi-brittle behavior, *i.e.*, their ultimate failure is triggered by a significant number of local events (in contrast to the purely brittle behavior of many ceramics and glasses), yet it is not preceded by highly dissipative processes associated with large inelastic deformations and strain hardening (as with ductile materials like metals). Such behavior is found in geological (*e.g.*, rocks), biological (*e.g.*, bone) and engineering/constructional (*e.g.*, ceramic composites, concrete) materials (Bažant, 1999, 2004). In this paper, we are particularly interested in cellular ceramic structures, which have recently found potential high-impact applications in tissue engineering (Deville et al., 2006) and high-performance composites (Munch et al., 2008).

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One issue with the engineering use of quasi-brittle materials is associated with the statistical and size-dependence of their failure properties, which can make reliable prediction a difficult challenge. Experimental analyses are often of little help as they cannot reach the target failure probabilities required for certification; for example, a prescribed failure probability of 10^{-6} would require 10^{6} repeated experiments. Moreover, the standard procedures of fracture mechanics, consisting of studying smaller scale samples and then extrapolating the results to larger, more realistically scaled samples, are limited by the lack of methods which are effectively able to "bridge the length-scales". Thus, for material design and failure prediction of quasi-brittle materials for engineering applications, experimental studies must be augmented by theoretical tools based on mechanical modeling. However, failure can be a complex phenomenon to model, as it involves both local and global phenomena, *i.e.*, small defects induce localized cracks and stress redistribution at nano- to micro-scales coupled with the fact that the macro-scale size of a structure can statistically dictate the probability of activating the worse-case defects.

Many authors have studied the failure of quasi-brittle materials, from such multiple viewpoints. Our objective here is not to draw an exhaustive portrait of the field, but to note several pertinent studies to better position our own approach. A critical analysis is undoubtedly the Weibull theory which describes the failure of brittle (in-series) systems, based on a specific strength (*i.e.*, Weibull) distribution and a power law for the volumetric scaling (Weibull, 1939, 1951; Hild, 2001), together with that of Daniels who established that the corresponding strength distribution of large in-parallel systems must tend toward a Gaussian distribution (Daniels, 1945). These analyses are essential for the understanding of the statistical failure of quasi-brittle materials. They have been extended by many authors to account for, *e.g.*, multiaxial fracture in Weibull theory (Evans, 1978; Guillaumat and Lamon, 1996), or different load sharing mechanisms in Daniels theory (Phoenix, 1974, 1978; Calard and Lamon, 2004). They are, however, limited in their application to realistic systems, as for example with Daniels theory which fails to describe the transition from Weibull to Gaussian behavior, and to predict the distribution's tail (which cannot be Gaussian) (Bažant, 2004; Bažant and Pang, 2007).

With respect to cellular ceramics, Gibson and Ashby (1997) derived the structure-stiffness relationships for many porous structures simply using beam and plate theories, although their approach cannot directly treat the statistical and size-dependent aspects of failure.

Similar micromechanical approaches have been proposed for many biological and synthetic quasi-brittle materials, *e.g.*, Ji and Gao (2004) and Begley et al. (2012), but again the key stochastic and size-dependent aspects of quasi-brittle failure were not directly considered. (These analyses are invariably based on a single representative volume element, where Cox's, 1952 shear lag principle is used to estimate the redistribution of stresses around cracks.)

There are also the purely macroscopic approaches, *e.g.*, De Borst et al. (1995), Desmorat et al. (2007), and Genet et al. (2013b); but as these analyses are based on continuum damage mechanics (Lemaître and Desmorat, 2005; Lemaître et al., 2009), they cannot explicitly model microstructure or microscopic damage processes, but only their indirect effect on the macroscopic mechanical properties. They are, however, extremely efficient at dealing with specific structures and loads, but require a large amount experimental data for calibration, and are not suitable to derive true structure-properties relationships.

An intermediate approach is that of Bažant et al. (Bažant et al., 1991; Bažant and Xi, 1991; Bažant, 1999, 2004). Based on energetic principles, these authors were able to derive scaling laws for the strength of various quasi-brittle materials, although this method does not permit the scaling of the distributions themselves (Bažant, 2004). More recently, they introduced a hierarchical model of chains and bundles of representative volume elements (RVEs), starting from the atomic scale, to derive some fundamental conclusions on the theoretical scaling of strength in quasi-brittle systems (Bažant and Pang, 2007; Bažant et al., 2009; Le et al., 2011; Le and Bažant, 2011). Most importantly, they were able to predict the transition from Gaussian to Weibull of the strength distributions of structures of increasing sizes (Bažant and Pang, 2007).

In a recent article, we presented our first approach to bridge the scales, with a model based on Sanchez–Palencia's theory of periodic homogenization and Weibull's theory of statistical failure (Genet et al., 2013a), with application to robocast scaffolds (Houmard et al., 2013). Material structure is introduced at microscopic scales, while the sample size is naturally handled on the macroscopic level, the two dimensions being linked through homogenization; statistical failure is then predicted through the computation of a Weibull-like integral at both size-scales. This approach not only has significant predictive capabilities but also has limitations; as the successive failure of the material's constituents is not explicitly represented, a virtual, *ad hoc*, "macroscopic" crack population is introduced, which must be identified experimentally on the macroscopic scale.

In the present paper, we propose a computational method to directly link the strength distributions of the constituents of quasi-brittle materials and macroscopic samples made from these constituents. The idea is to overcome the intrinsic limitations of approaches based on a single RVE, which are really only suitable to deal with homogeneous phenomena (on the scale of the structure), but not strictly with localized events such as those triggering failure. We achieve this by modeling as many RVEs as necessary to produce reliable predictions. Since the number of RVEs that can be modeled at a microscopic level of description is rapidly limited by computational capabilities, we introduce a multi-level numerical method which permits the computation of samples of virtually any size, with essentially no loss of information compared to a direct microscopic computation but with a drastically reduced computational cost. Micro-cells, where physical mechanisms are finely described, are replaced by mechanically and statistically equivalent "macro-cells" containing only a very few degrees of freedom. As a consequence, structural-level computations can be run at a very reduced cost, and a large number of stochastic cases can be explored in a reasonable time.