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The impact of stochastic microstructures on the macroscopic fracture properties of brick and mortar composites

J. William Pro [a], Rone Kwei Lim [b], Linda R. Petzold [c,d], Marcel Utz [e], Matthew R. Begley [f,g,*]

[a] *Department of Mechanical Engineering, 2235C Engineering II Building, University of California, Santa Barbara, CA 93106, USA*

[b] *Department of Computer Science, 5110 Harold Frank Hall, University of California, Santa Barbara, CA 93106, USA*

[c] *Department of Mechanical Engineering, 5107 Harold Frank Hall, University of California, Santa Barbara, CA 93106, USA*

[d] *Department of Computer Science, 5107 Harold Frank Hall, University of California, Santa Barbara, CA 93106, USA*

[e] *School of Chemistry, University of Southampton, SO17 1BJ, UK*

[f] *Materials Department, 2361A Engineering II Building, University of California, Santa Barbara, CA 93106, USA*

[g] *Department of Mechanical Engineering, 2361A Engineering II Building, University of California, Santa Barbara, CA 93106, USA*

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ABSTRACT

This paper examines the effect of non-uniform microstructures on the macroscopic fracture properties of idealized brick and mortar composites, which consist of rigid bricks bonded with elastic–plastic mortar that ruptures at finite strain. A simulation tool that harnesses the parallel processing power of graphics processing units (GPUs) was used to simulate fracture in virtual specimens, whose microstructures were generated by sampling a probability distribution of brick sizes. In the simulations, crack advance is a natural outcome of local ruptures in the cohesive zones bonding the bricks: the macroscopic initiation toughness for small-scale yielding is inferred by correlating the critical load needed to advance a pre-defined crack with an associated far-field energy release rate. Quantitative connections between the statistical parameters defining heterogeneous brick distributions and the statistics of initiation toughness are presented. The nature of crack tip damage and stresses ahead of the crack tip are illustrated as a function of brick size variability. The results offer quantitative insights that can be used to identify microstructural targets for process development, notably specific brick size distributions that still provide macroscopic toughening.

1. Introduction

The ability to connect local microstructural features with macroscopic mechanical properties is a central challenge in materials development, as such connections effectively define 'processing targets' associated with acceptable levels of heterogeneity. This challenge is particularly acute for quasi-brittle composites that exploit ordering of microstructural features, as local disruptions to ordering can serve as defects that limit global performance [1–4]. Bio-inspired 'brick and mortar' composites are an excellent example of this [5–7,4,8,9]; the ideal microstructure will have perfectly aligned stiff features and achieve toughness through perfectly overlapping features that spread damage (or equivalently, provide bridging over large length scales).

However, the physical reality is that most high throughput processing routes invariably introduce heterogeneous distributions of brick size and therefore overlap distances, which limit the effectiveness of the microstructure. As

* Correspondence to: 2361B Engineering II, Santa Barbara, CA 93106, USA. Fax: +1 805 893 8486.

E-mail address: begley@engineering.ucsb.edu (M.R. Begley).

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such, the macroscopic performance of these composites is less than optimal, as real materials (both natural and synthetic) exhibit imperfections at different length scales, including large defects/pores [10–17], distributions in brick sizes and shape [18–20], and distributions in mortar properties (e.g. strength) from interface to interface. These features not only reduce the effective macroscopic mechanical properties of the material (broadly defined), but they can also lead to substantial variability in properties from one test specimen to the next [21–24,5,6].

The stress–strain response of brick and mortar composites has been modeled extensively in a deterministic sense via analytical models as well as conventional finite element simulations [25–29,22,30–32]. However, even for uniform brick arrangements, direct links between microstructure and the resulting *fracture toughness* (arguably their most desirable property) are limited [6,33,34,29]. It should be noted that while the work-to-failure during uniform deformation is related to toughness, the presence of non-uniform deformation at the tip of a crack leads to important differences [33]. To our knowledge, the impact of *non-uniform* and statistically-defined brick arrangements on macroscopic fracture toughness has not been analyzed. As a result, there is a significant need for a quantitative understanding of the link between statistical distributions in microstructure (e.g., brick sizes, shape, mortar properties) and the resulting statistics of fracture properties.

Previous analyses of the impact of heterogeneous brick arrangements on *uni-axial* behavior have provided insights that are relevant to the present explicit study of fracture toughness. These works defined representative volume elements (RVEs) of brick arrangements within finite element models with embedded cohesive zones [18,35]. For example, Barthelat et al. studied the effect of statistical size and shape distributions in the microstructure using a large RVE containing several hundreds of tablets generated via Voronoi tiling. Their results indicated important differences in composite stress–strain response of a microstructure with statistical variations when compared to that of a 'perfect' microstructure, and they are in excellent agreement with experiment [18]. In the work of Bekah et al., the authors also implemented statistics within the microstructure by introducing a random variation in tablet length and offset [35]; the results indicated a reduction in both strength and work to failure as a result of the variation. Moreover recently, statistical strength predictions in scaffolded ceramic structures (analogous to natural nacre) have begun to emerge [30]; these calculations have enabled predictions of strength probability distributions in periodic materials, and can be generalized for arbitrary geometry and loading.

The objective of this work is to elucidate the statistical characteristics of macroscopic fracture properties that result from statistical variations in local microstructural features, using as a reference the 'perfect' material (e.g., one with no variation in microstructure). The current models exploit the highly efficient GPU-based computational approaches developed by Pro et al. and Lim et al. [33,34] to conduct a broad number of virtual fracture tests. The results confirm some of the trends suggested by previous works, yet provide more complete statistical links between parameters describing microstructural heterogeneity and macroscopic fracture properties. The simulations utilize virtual specimens comprising several hundreds of thousands of bricks, with sizes determined via sampling from a statistical distribution. The approach explicitly tracks individual motions of each brick (all of different sizes) and predicts crack evolution through the rupture of cohesive zones bonding the bricks. The efficiency of the numerical method allows a large number of virtual tests, such that the statistics of the response can be well quantified.

The results offer new insight into the design of synthetics, illustrating the role of statistics in the microstructure on both the average and standard deviation in initiation fracture toughness, as well as the resulting damage and stress distributions ahead of a dominant pre-crack. The simulation results give key insight into the sensitivity of the composite to local variations in brick size, in terms of the computed average and variance from a statistically significant subset of virtual fracture tests.

2. Modeling approach

2.1. Microstructural idealizations

As illustrated in Fig. 1, the material is modeled using an idealized microstructure consisting of an overlapping grid of comparatively stiff bricks bonded together by thin, compliant mortar sections. For many synthetic composites the bricks can be modeled as rigid bodies with only rotational and translational degrees of freedom, as described in detail in Pro et al. [33]. The mortar, presumed to be present in low volume fraction, is idealized with a piece-wise cohesive zone law (shown schematically in Fig. 2) inserted between all brick faces, and is characterized by a finite stiffness (k_n), strength (σ_0), and work to failure (Γ_i). Note that this cohesive zone law may be alternatively expressed in terms of the critical and full rupture displacements (Δ_Y and Δ_R, respectively, as shown in Fig. 2) of the interface, as follows: $\Delta_Y = \sigma_0/k_n$ and $\Delta_R = \Gamma_i/\sigma_0$. Naturally, this gives rise to a *dimensionless interface ductility*, defined as Δ_R/Δ_Y (or alternatively as the ratio $k_n\Gamma_i/\sigma_0^2$), which was shown in [33] to directly scale the resolution and size of the plastic zone (in bricks). To limit the scope of the study, it is assumed that the bricks all have the same height (h), and that the mortar (interface) properties are constant from interface to interface; the impact of different brick heights and statistical mortar behaviors is left for future work.

Heterogeneity within the microstructure is introduced by assigning a random width (defined via the aspect ratio $\overline{w}_i = w_i/h$) to each brick in the system (dictated by sampling a skew-normal brick size distribution using computer-generated pseudo-random numbers [36]), and subsequently stacking them in an arrangement of space-filling rectangles as shown in Fig. 1(d). The distribution in brick widths is defined in terms of its population mean $\langle\overline{w}\rangle$ (i.e. average brick size), standard deviation in brick size