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Stochastic failure of isotropic, brittle materials with uniform porosity

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Abstract

Porous materials present serious technological constraints on all applications, such as battery electrodes, solid oxide fuel cells, synthetic bone grafts, filters, pharmaceutical powder compacts and feed pellets. Despite the significance of reliability in brittle materials, current literature is limited in pore–pore interaction effects on fracture statistics of brittle porous materials (BPMs). In this paper, a two-dimensional finite element (FE) simulation-based approach was developed to assess the pore–pore interactions and their impact on fracture statistics of isotropic microstructures. The classical fracture mechanics approach was combined with FE simulations that account for the interactions to predict the decrease in the fracture stress with increasing porosity. Rules were directly compared against experimental data for porous polycrystalline alumina, hydroxyapatite, and all the other data combined in Fig. 6. The maximum reliability of BPMs was shown to be limited by the underlying pore–pore interactions. Weibull modulus decreased more than threefold for a change in porosity from 1 to 2 vol.%. The Weibull moduli were between 7 and 18 in the range of 2–31 vol.% porosity. Even the microstructures with the same porosity level and size of pores showed substantial differences in fracture strength.
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Keywords: Porosity; Weibull modulus; Ceramics; Alumina; Hydroxyapatite

1. Introduction

Improving technology demands material properties that are optimized not only for high strength but also for improved toughness, transport properties and long-term reliability that are often achieved through porosity. Consequently, an understanding of the failure behavior of brittle porous materials (BPMs) is vital in developing materials for various applications. Brittle fracture is initiated by pre-existing flaws, such as pores, surface scratches, inclusions or other types of inhomogeneities [1]. The effect of grain size on brittle fracture has also become apparent [2,3]. Accordingly, crack size and failure stress have been related through fracture mechanics, which is based on the stress fields in front of the crack [4]. However, if the crack tip stress field is enhanced or shielded by microstructural inhomogeneities, the fracture strength, σ_f, also changes. Therefore, in spite of great progress [5–10], the effects of large pore densities and the effects of pore–pore stress field interactions on fracture behavior of BPMs are still unclear. In addition, few studies have investigated the effect of porosity on Weibull statistics [11–14] because a large number of specimens are needed with various porosity levels.

Porous materials present serious technological constraints on all applications, ranging from pharmaceutical powder compacts and feed pellets [15] to solid oxide fuel cells (SOFCs) [16–19]. For example, porous hydroxyapatite (HA) used as a synthetic bone graft has to withstand mechanical stresses while containing a minimum pore size of 150 μm for tissue ingrowth [20]. In general, traditional materials such as sintered ceramics exhibit some level of porosity that can initiate fracture [1]. Other materials in which porosity is utilized and causes failure include, but are not limited to, dental ceramics [21], bone cements [22,23], catalyst pellets [24], porous silicon carbide [25] and battery electrodes [26].

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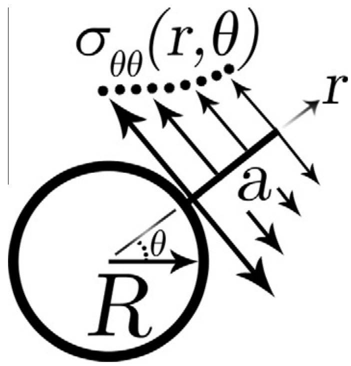

Fig. 1. Schematic picture of a pore–crack arrangement in which the crack is assumed to be present at the highest geometric factor position, R is the radius of the pore, a is the crack length and $\sigma_{\theta\theta}(r,\theta)$ is the cubic polynomial fitted to the $\sigma_{\theta\theta}$ distribution near the pore [72].

Fundamentally, the strength of a material is expected to decrease with the introduction of a mechanical discontinuity, which acts as a stress concentrator [27]. Accordingly, experimental studies on alumina [7,28–30], zirconia [28,29], thoria [31], chromium carbide [31], lead zirconate titanate (PZT) [32], niobium-doped lead zirconate titanate (PNZT) [9], HA [33] and glass [5,6] have shown that there is a decrease in strength with increasing pore volume fraction, V_p. The trends in σ_f decrease were fitted by a power function [34] and exponential functions [28,35]. However, a connection between microstructure and failure stress must be established to provide a quantitative explanation for BPM fracture. Vardar et al. [32] proposed the use of Weibull statistics based on the analytical stress field solutions around spherical pores assuming no stress interaction. In Vardar's model, however, the effect of pore size on failure stress is absent, which contradicts the experimental observations of Wallace [7]. Evans et al. [8] combined fracture mechanics and statistics to predict porous glass fracture [6], assuming that a combined pore–crack geometry (Fig. 1) is responsible for the failure. Although Evans approach captures the pore size effects, it does not contain pore–pore interactions limiting its use to low porosity levels. Schneider et al. [36] used Weibull statistics (assuming constant parameters) and stress distribution in a porous microstructure calculated by the finite element method (FEM) to explain the failure of porous aerated autoclaved concrete. However, Weibull theory assumes non-interacting cracks [37–39]. As a result, the Weibull parameters are not constant for microstructures with interacting cracks and mechanical inhomogeneities [40]. Nonetheless, any fracture data is fitted by the flexible two-parameter Weibull distribution function [37,38]

$$F(\sigma,V) = 1 - \exp\left[-\frac{V}{V_0}\left(\frac{\sigma}{\sigma_0}\right)^m\right] \tag{1}$$

where the failure probability, F, is a function of the uniaxial homogeneous tensile stress, σ, and the volume of the specimen, V. The Weibull modulus, m, also known as the shape parameter, represents the level of fracture stress scattering. A high m means little scattering; a low m means more scattering. The scale parameter, σ_0, is the characteristic strength and V_0 is a normalizing volume. The Weibull theory relates the higher end tail of the crack size distribution to fracture stress scattering [41–43]. However, the scattering also depends on interaction effects [40,44,45].

Historically, pore–pore interactions have been suggested to be minimal for porosity of less than 10% [8,10]. Here, we demonstrated that interaction effects in two-dimensional (2-D) space are crucial even for $V_p \leqslant 0.02$. As a result, surface porosity becomes a determining factor in fracture behavior. In this context, the effect of pore and inclusion clustering on plastic deformation [46,47], damage evolution in fiber composites [48] and other physical properties [49] has been investigated. Plastic flow studies show that there is a softening effect due to strain concentration in the pore clusters [46,47]. However, the focus in plasticity studies is on the bulk response of the material rather than the local intensified stresses, which are vital for brittle fracture. Babuška et al. [48] investigated the stress distribution in a 2-D fiber composite. They show that the change in effective elastic properties with the spatial distribution of fibers is small compared to maximal stresses at the fiber–matrix interface. Chen and Papathanasiou [50] showed that the inter-fiber distance has the greatest effect on peak stresses in a 2-D composite structure. The stress dependence on fiber spacing was also discussed by Pyrz [51] and Pyrz and Bochenek [52], who found a correlation using nearest-neighbor statistics. Sevostianov and Kushch [53] showed that an explicit relation exists between maximum stresses and nearest neighbors in a porous microstructure. The peak stresses were described by the Gumbel distribution [54], which is based on extreme value statistics.

A decreasing Weibull modulus with increasing porosity has been reported for niobium-and tantalum-doped zirconia [12], titania [13], alumina [14] and HA [11,55–60]. Also, the Weibull modulus did not show a significant change with increasing porosity for NiO–YSZ (yttria-stabilized zirconia) [19], $MgAl_2O_4$ [16] and NiO–TZ3Y (yttrium partially stabilized tetragonal zirconia) with other additions [18]. Fan et al. [11] described three regions for Weibull modulus and porosity relationship based on their extensive experiments on HA, together with data from 16 different research groups and eight different materials, a first-time collection of more than 1500 fractured specimens. Accordingly, Fan et al. [11] showed that the values of the Weibull moduli form a "U" shape in which m is higher in regions I ($V_p < 0.1$) and III ($V_p > 0.55$) than in region II ($0.1 < V_p < 0.55$), with m values between 4 and 11 [11].

Despite the importance of reliability in brittle materials [61–64], there is no systematic work on pore–pore interaction effects on fracture statistics of BPMs. To the best of the authors' knowledge, only one numerical study that shows the effect of co-linear crack stress field interactions on Weibull modulus is available [65]. The lack of microstructural control in addition to the inherent scatter of brittle fracture strength hinders the use of a deterministic