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Deviations from Weibull statistics in brittle porous materials

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Abstract

Brittle porous materials (BPMs) are used for battery, fuel cell, catalyst, membrane, filter, bone graft and pharmaceutical applications due to the multifunctionality of their underlying porosity. However, in spite of its technological benefits the effects of porosity on BPM fracture strength and Weibull statistics are not fully understood, limiting the wider use of these materials. By combining two-dimensional finite-element simulations and classical fracture mechanics we found that BPM fracture strength decreases at a faster rate under biaxial loading than under uniaxial loading. Three different types of deviation from classic Weibull behavior can be identified: P-type corresponding to a positive lower tail deviation, N-type corresponding to a negative lower tail deviation, and S-type corresponding to both positive upper and lower tail deviations. Pore–pore interactions result in either P-type or N-type deviation in the limit of low porosity, whereas S-type behavior occurs when low and high fracture strengths coexist in a set of fracture data.

Keywords: Weibull modulus; Biaxial fracture; SOFC fracture; Porous alumina; Porous hydroxyapatite

1. Introduction

Porous materials are ubiquitous in nature. For example, bone [1], exoskeleton [2], tooth [3] and wood [4] use connected porosity to transport nutrients and decrease weight without impairing structural reliability. Modern industry also uses porous materials that serve more than one purpose [5]. Specifically, brittle porous materials (BPMs) are used in applications such as rechargeable batteries [6], solid-oxide fuel cells [7–10], synthetic bone grafts [11], catalysts [12], membranes [5], thermal insulators and filters [13]. A wider use of BPMs demands a deeper understanding of their fracture behavior and fracture strength scattering.

The relationship between porosity, P, and fracture strength, σ_f, is unclear despite the large number of experimental studies on the mechanical behavior of BPMs that have been reported [14–24,21,25,7–10,26,27]. Classically, the decrease in strength with increasing porosity is a result of stress concentration and area reduction, and demands a sharp decrease in failure stress with the introduction of a single pore. Such a situation contradicts the experimental observation of a slight decrease in failure stress for up to ~3% porosity [15,14,28,18,16,27] compared to the expected 50% decrease due to a single spherical pore. The concept of area reduction predicts a linear decrease in failure stress. However, the decrease in failure stress follows a non-linear change, especially for a porosity range of more than 10% [15,14,28,18,29,16,27]. Historically, the change in σ_f with porosity has been fitted to power [30] and exponential functions [29,31]. A function that captures realistically the effects of the pore–pore stress field interactions and pore size is absent from the literature.

Microstructure-based approaches such as effective flaw size [18], fracture statistics based on interacting pore–crack geometries [17], and Weibull statistics combined with analytical stress solutions [28] and finite-element calculations [32] have been used to predict the effect of porosity on BPM fracture [33]. The effective flaw size [18] and fracture statistics approaches of interacting pore–crack systems do

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not account for pore–pore interactions [17]; however, the observed decrease in σ_f with increasing pore size is captured. Modified Weibull statistics that include concentrated stress fields around spherical pores can predict the failure behavior of porous lead zirconate-titanate [28], but the effect of pore size is not present. In finite-element method (FEM) simulations that include the pore–pore interactions [32], Weibull statistics become stress and volume dependent for porous and hence constant parameters cannot be used [34].

The effect of porosity on the Weibull statistics of BPMs is not well understood. The Weibull modulus is reported to decrease with increasing porosity for tantalum-doped zirconia [20], titania [21], alumina [22] and hydroxyapatite (HA) [26,24,23,35–38]. The Weibull modulus is also reported to remain statistically indifferent with increasing porosity for NiO–YSZ (yttria-stabilized zirconia) [10], $MgAl_2O_4$ [7] and NiO–TZ3Y (yttrium partially stabilized tetragonal zirconia) with other additions [9]. Fan and coworkers defined a U-shaped behavior of m in the 0–65% porosity range based on their comprehensive experiments on HA and other literature data—a total of more than 1500 fracture specimens. Fan et al. described three regions in which m shows distinct behaviors. The Weibull modulus decreases in Region I ($P \leq 10\%$), remains statistically indifferent in Region II ($10\% < P \leq 55\%$), and increases in Region III ($P > 55\%$) [26].

Overall, it has been demonstrated that the Weibull modulus is affected by pore–pore stress-field interactions [39]. The Weibull moduli of idealized porous microstructures sharply decrease up to 2% porosity and stabilize between 6 and 18 in the 2–31% porosity range [39]. FEM simulations of 840 unique microstructures with non-overlapping circular pores under uniaxial loading, which resulted in 21 different m values, show similar dependence on porosity compared to literature data—83 m values of 14 different BPMs [39]. Afferrante et al. also showed that interactions between collinear cracks affect the value of m through numerical simulations [40]. A decrease in the crack–crack distance results in strong stress interactions that break the non-interacting flaw assumption in the Weibull theory.

The Weibull moduli of brittle, bulk materials are related to the type of the crack size distribution [41–43]. In a Weibull plot, an inverse power-law distribution of crack sizes results in a linear arrangement of fracture stresses [41]. However, any bimodal or multimodal distribution of flaw sizes deviates from the Weibullian behavior [44]. Similarly, the failure behavior of BPMs shows positive [23] and negative [24,21] deviations from the well-known linear behavior. Additionally, the fracture stresses of BPMs form S-shaped curves in a Weibull plot [45,21]. Also, an analogy between mechanical and dielectric strengths is suggested [46] and similar shapes of dielectric breakdown are observed in a Weibull plot [46,21]. In spite of the great progress, the availability of a rationale that explains the deviations from classical Weibull statistics remains unavailable.

In this paper, pore–pore interaction effects on Weibull statistics are investigated by a combined finite-element and fracture mechanics approach. Results are directly compared to alumina [16] and hydroxyapatite experiments [26]. The effects of stress state change from uniaxial to equibiaxial tensile on fracture statistics are examined. Three different deviations from Weibull statistics—positive, negative and S-shaped—can be identified and correlated with the underlying microstructural interactions.

2. Theoretical framework

Fracture strength scattering was quantified by the two-parameter Weibull distribution function [47,48]:

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

where the failure probability, F, is a function of the uniaxial homogeneous tensile stress, σ, and the volume of the specimen, V. V_0 is a normalizing volume, σ_0 is the characteristic strength, and m is the Weibull modulus. Large values of m correspond to a narrow scattering distribution, small values of m correspond to a broad scattering distribution.

In contrast, the classical fracture mechanics approach to calculate the fracture strength, σ_f, is:

$$\sigma_f = \frac{K_{Ic}}{Y\sqrt{\pi a}} \tag{2}$$

where K_{Ic} is the fracture toughness, a is the crack size, and Y is the geometric factor that embodies the amplified stress field acting on the crack surfaces obtained from the analytical stress field solutions around a pore. However, Y does not contain the pore–pore stress field interactions. Here, we used FEM to calculate the geometric factor for each microstructure—the main difference with the existing approaches to understanding BPM fracture. In the present study, the geometric factor contains pore–pore and pore–crack interactions. Pore–pore interactions are included by combining FEM simulations and the formalism of Shah [49], the details of the Y calculation are summarized in a recent publication, [39].

Figs. 1 and 2 demonstrate the stress distributions calculated for a microstructure with 4.4% porosity. The random spatial distribution of pores always produces an inhomogeneous stress distribution even for isotropic materials. As a result, one maximum stress point in the microstructure will trigger catastrophic failure.

3. System abstraction and numerical setup

The mechanical response of linear-elastic and isotropic 2-D microstructures with non-overlapping circular pores under plane-stress conditions were simulated in the object-oriented finite-element program, OOF2 [50]. The details of the simulation procedure can be found in Ref. [39]. In a departure from earlier work [39]; simulations