Modeling Failure in Brittle Porous Ceramics

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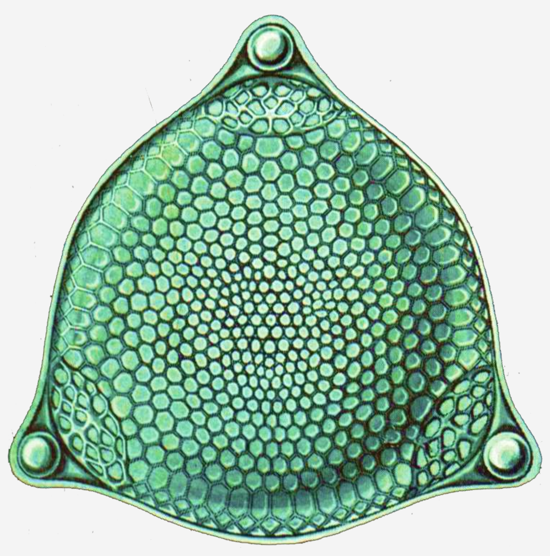
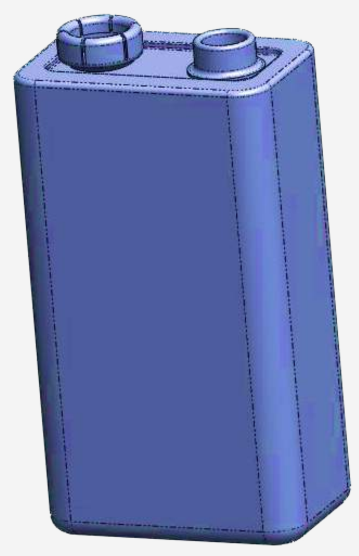
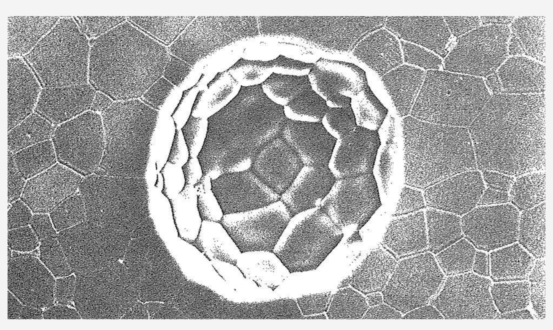
Abstract: The effect of porosity on brittle fracture is unclear. Here, the classic fracture mechanics approach is combined with finite element simulations to understand effects of pore-pore and pore-crack stress interactions on fracture behavior of brittle porous materials.



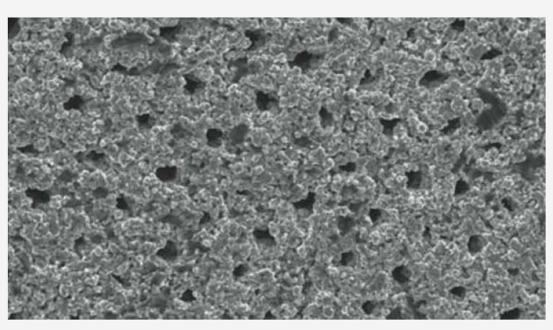
Algae , diatom, pore size ≈2 μm [1].



Battery, 9V [2].



Porous alumina, pore size ≈50 μm [3].

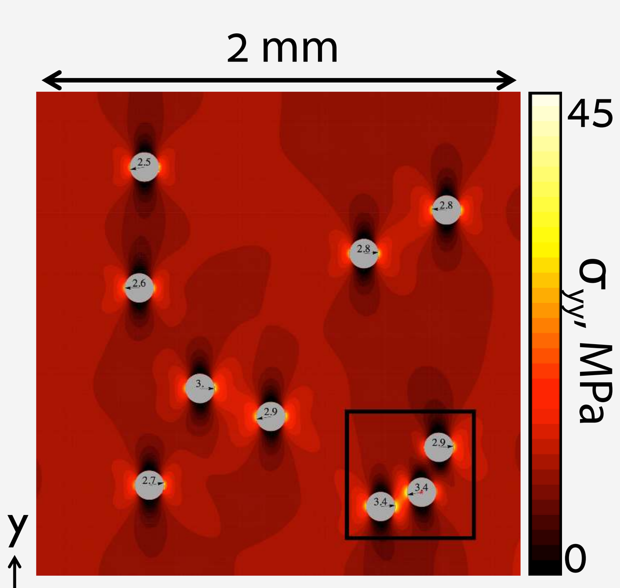


Cathode, $LiCoO_2$, pore size ≈6 μm [4].

Simulation approach:

1. Generate microstructures:

Forty different microstructures with fixed number and size of non-overlapping circular pores were generated for each porosity level-a total of 840 unique microstructures.



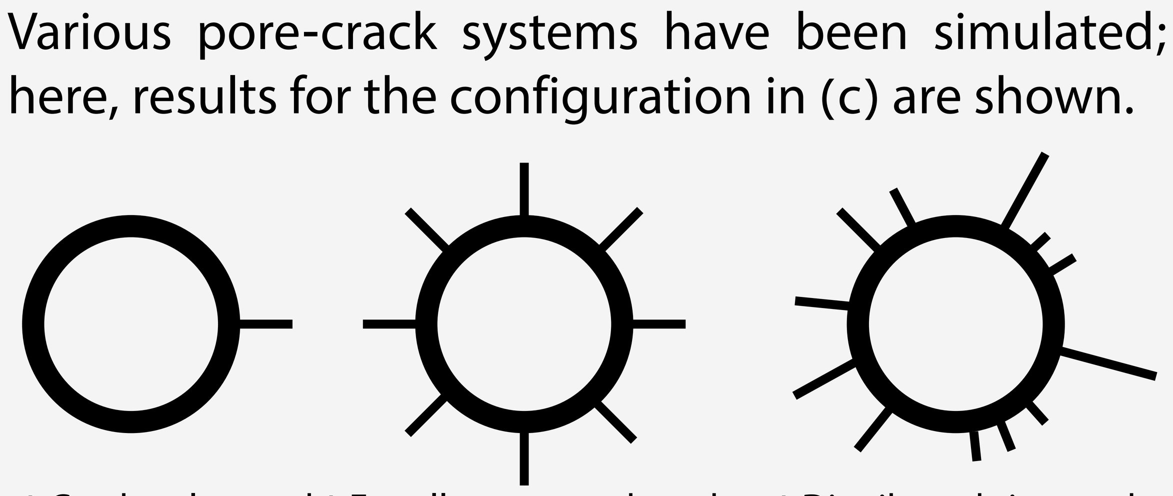
σ_{yy} distribution under uniaxial (vertical) loading

2. FEM simulations:

Finite element simulations were performed to obtain stress distributions under uniaxial and biaxial loading using OOF2 [5].

3. Pore-crack system:

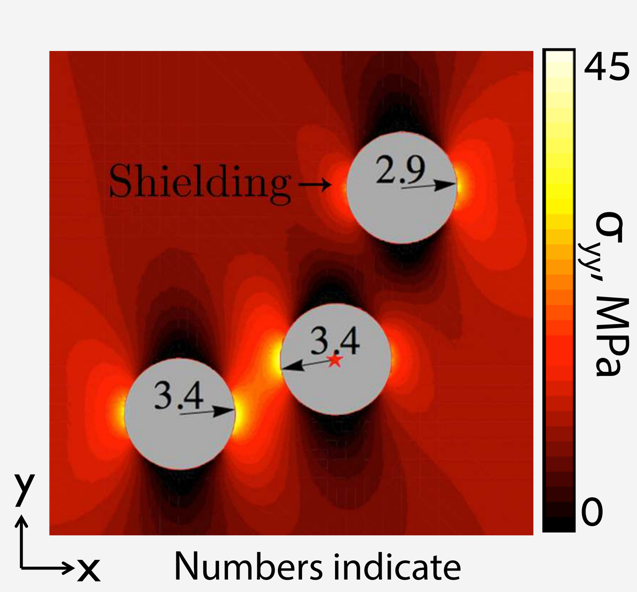
Various pore-crack systems have been simulated; here, results for the configuration in (c) are shown.



a) Crack only at maximum stress b) Equally separated cracks at random orientations c) Distributed size cracks at random orientations

4. Geometric factor:

Tangential stresses were used to calculate geometric factors (Y) for a given crack size.

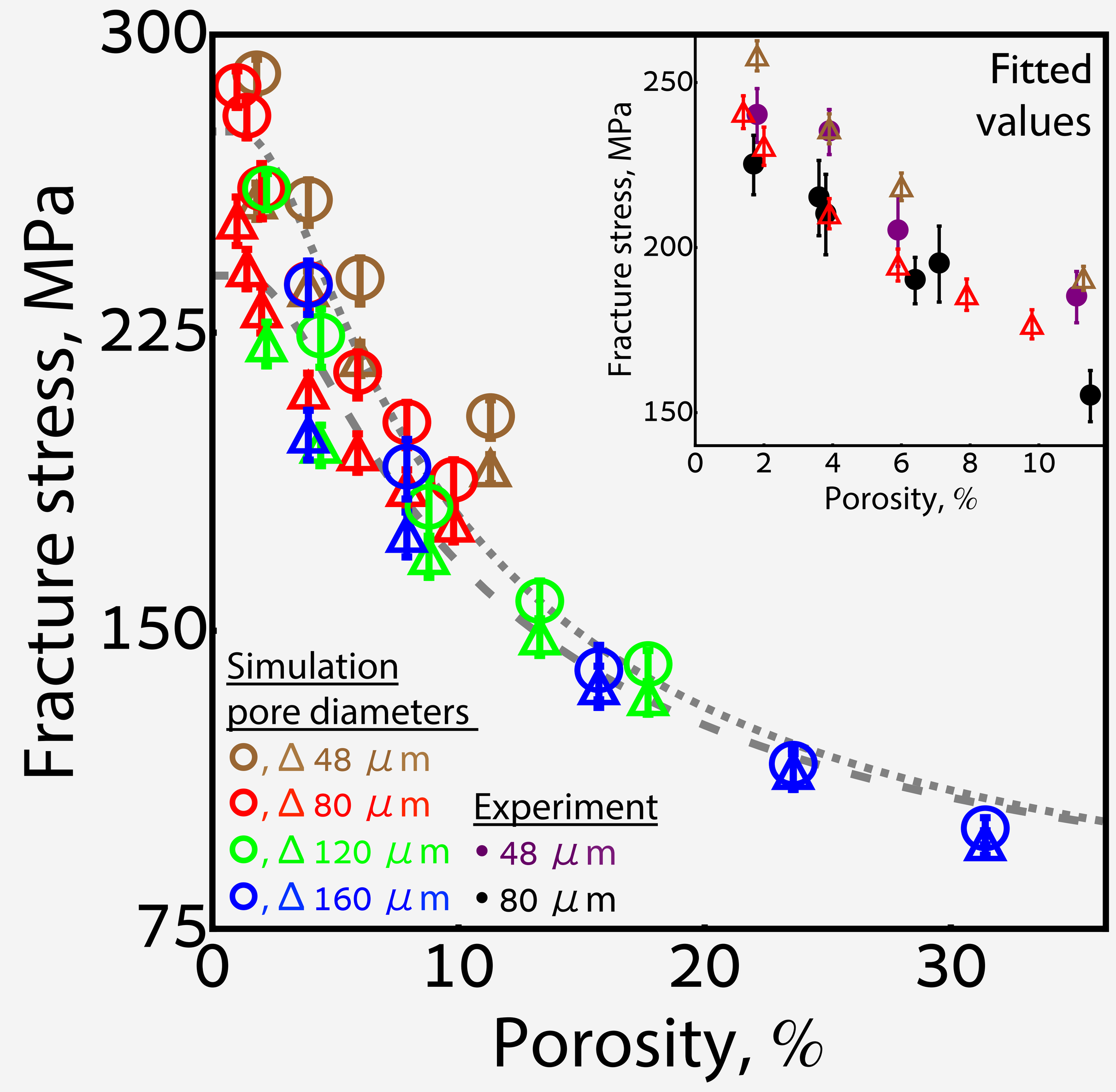


Numbers indicate maximum Y for each pore.

5. Fracture toughness fit:

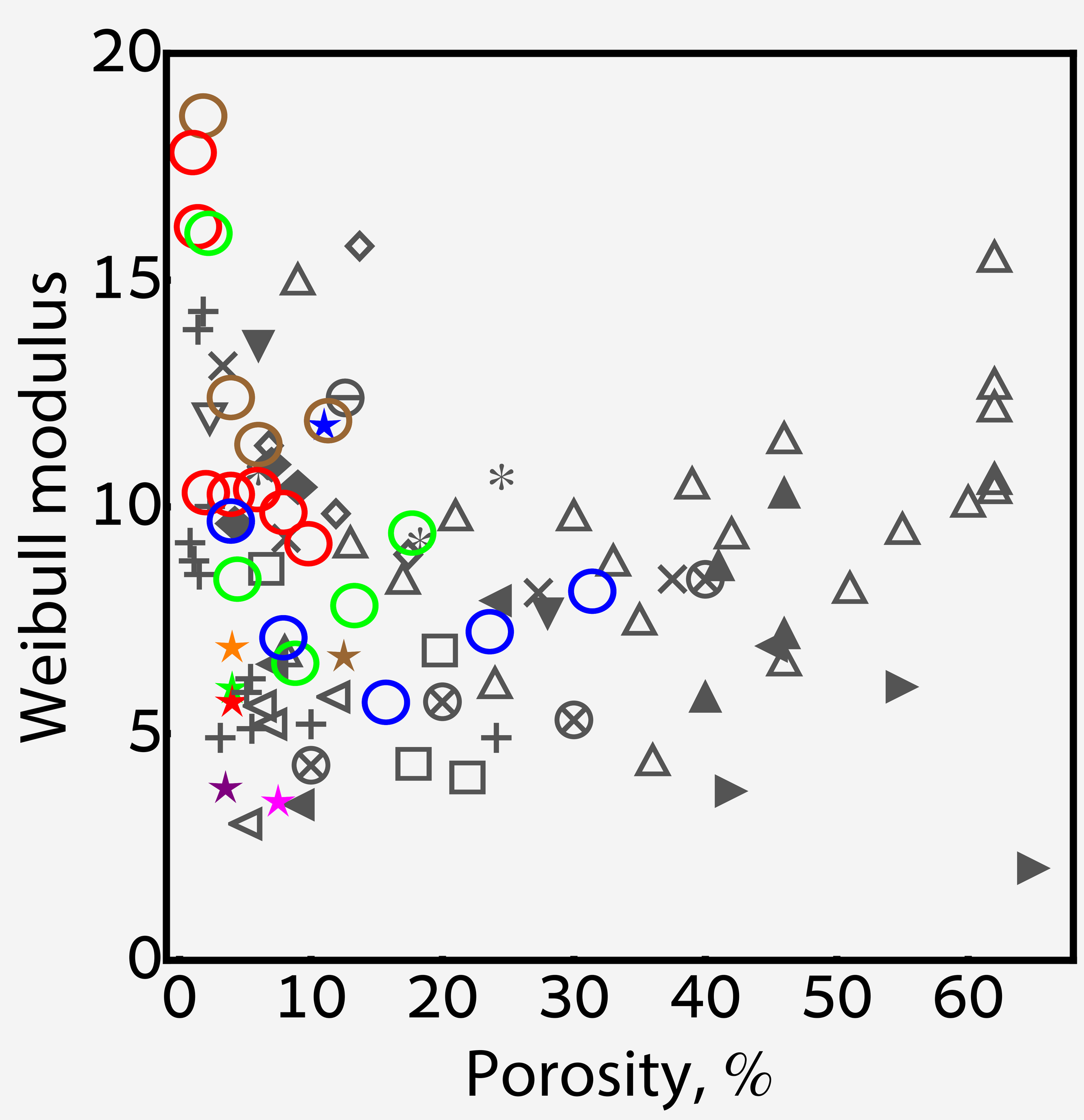
Calculated geometric factor and crack size values are used to fit porous alumina fracture strengths to obtain a fracture toughness, K_{Ic}=3.0 MPa√m is found for the pore-crack system shown in 3c.

Effect of porosity on fracture strength:



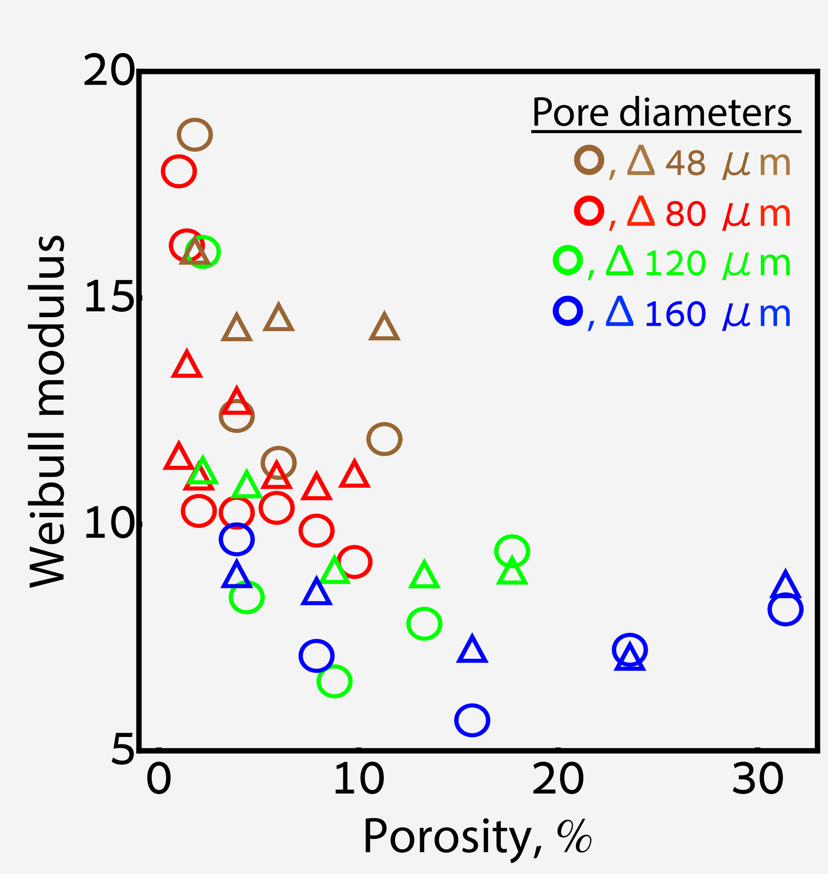
Change in fracture stress with porosity under uniaxial=Δ and biaxial=**O** loading, described by a new function: $\sigma_f = \sigma_{max} - \sigma_{dec}\exp(-d/P)$, where *P* is porosity, adapted from [3, 6, 7].

Effect of porosity on Weibull modulus:



Change in Weibull modulus with porosity under biaxial loading, simulation results are **O**=48, **O**=80, **O**=120, and **O**=160 μm diameter pores. Triangles correspond to hydroxyapatite, ★ and ◆ to fuel cell materials, x to alumina, and + to zirconia, adapted from [6, 7].

Effect of loading on Weibull modulus:

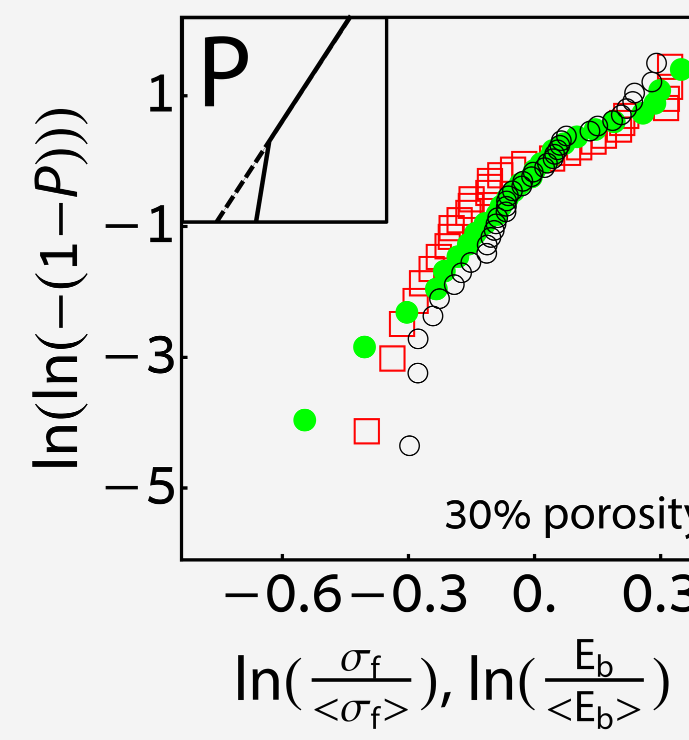


Change in Weibull modulus with porosity under uniaxial=Δ and biaxial=**O** loading, adapted from [7].

Deviations from Weibull statistics:

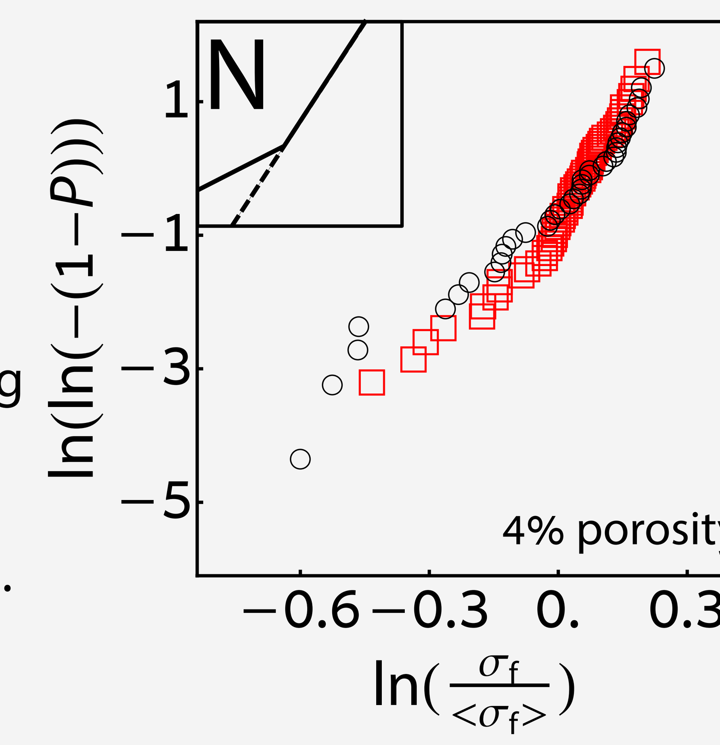
1. P-type deviation:

Lower tail deviates towards to mean σ_f due to strong pore-pore interactions. Weibull plot showing normalized σ_f for titania=□, dielectric strength=•, and simulation σ_f=**O** [7].



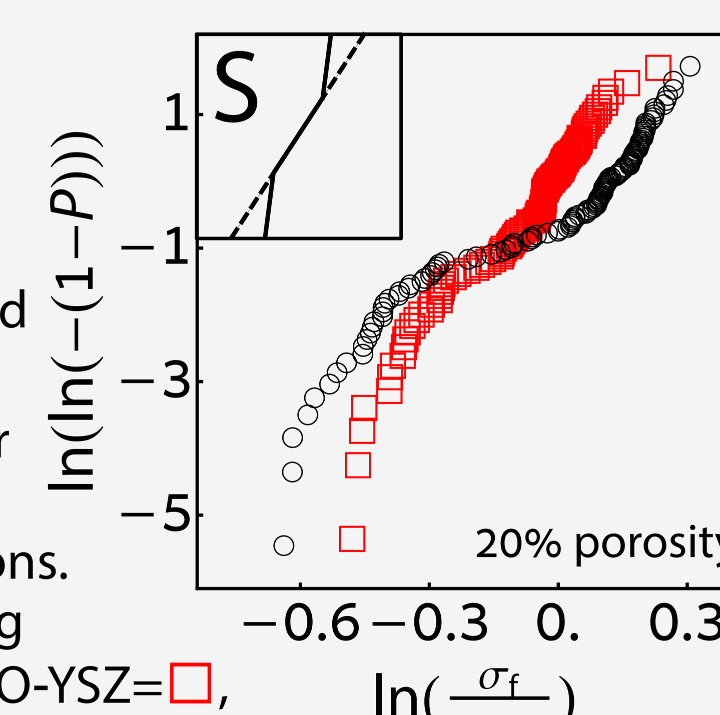
2. N-type deviation:

Lower tail deviates away from mean σ_f due to strong pore-pore interactions. Weibull plot showing normalized σ_f for NiO-YSZ=□, and simulation σ_f=**O** [7].



3. S-type deviation:

Lower tail deviates towards to mean σ_f due to strong pore-pore interactions and upper tail deviates due to large number of microstructures with weak interactions. Weibull plot showing normalized σ_f for NiO-YSZ=□, and simulation σ_f=**O** [7].



Conclusions:

- Random spatial distribution of pores limits Weibull modulus.
- Weibull modulus is lower under biaxial loading than under uniaxial loading.
- Three different types of deviations, P-type, N-type, and S-type, from Weibull statistics are identified.
- Pore-pore stress interactions are the main reason behind the decrease in fracture stress with increasing porosity in brittle porous materials.
- The formula: $\sigma_f = \sigma_{max} - \sigma_{dec}\exp(-d/P)$ describes the fracture strength vs. porosity relationship more accurately because it captures experimentally observed plateaus for P<3% and P>20%.
- Biaxial loading results in a steeper decrease in fracture strength compared to uniaxial loading.

References:

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