

## MICROSTRUCTURE OPTIMIZATION OF POROUS CERAMICS: A DISCRETE ELEMENT APPROACH

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Porous ceramics have numerous applications such as catalysis, filtering, membranes, thermal insulation, electrodes or bone scaffolds. Such ceramics are useful in applications where pores must be interconnected to provide a flow pathway for gases or liquids into the material. Another typical functional requirement is to maximize the free surface to enhance chemical reactions at interfaces. Porosity ranges from 20% to 50% to fulfill the appropriate conditions in these applications. Residual porosity is obtained either by partial sintering; by deliberately introducing pore formers into the initial powder or by freeze-casting a suspension. In any case, pores weaken an already brittle material. Thus, there is an inherent contradiction between the requirement of a large amount of porosity and the need for some strength and toughness. In that context, microstructural optimization based on numerical simulations offers a powerful tool, providing it operates at the pertinent length scale.

Porous ceramics are processed by sintering a powder. Because the sintering stage is only partial to keep some porosity, the final microstructure keeps a particulate signature with individual particles still being observable after sintering. Particles have bonded together through solid necks, giving its strength to the material. In this work, we take advantage of the discrete nature of partially sintered porous ceramics to model the material as a 3D assembly of bonded spherical particles [1-3]. The model is enriched with a physically based fracture criterion at the local scale of each bond [4].

Realistic 3D microstructures are generated numerically by numerically sintering random packings of particles. The obtained numerical samples are tested in tension and in compression. Some of them are equipped with an initial crack to measure  $K_{Ic}$  toughness. Using LEFM, strength and toughness are evaluated and compared favorably to experimental results. The simulation results are used to derive useful scaling laws relating the effective Young's modulus  $E$  to strength and toughness and to microstructural parameters (particle size, average bond size and number of bonds per particle). We demonstrate that introducing some heterogeneity in the microstructure (such as pore formers or aggregates) improves the displacement-limited design performance index  $K_{Ic}/E$  (Fig. 1).

We apply the same methodology to real microstructures, which have been voxelized by 3D nanotomography (Fig. 2). These microstructures have been obtained by freeze-casting and exhibit a strong anisotropy. Quantitative comparison is carried out with real crushing tests on actual microstructures.

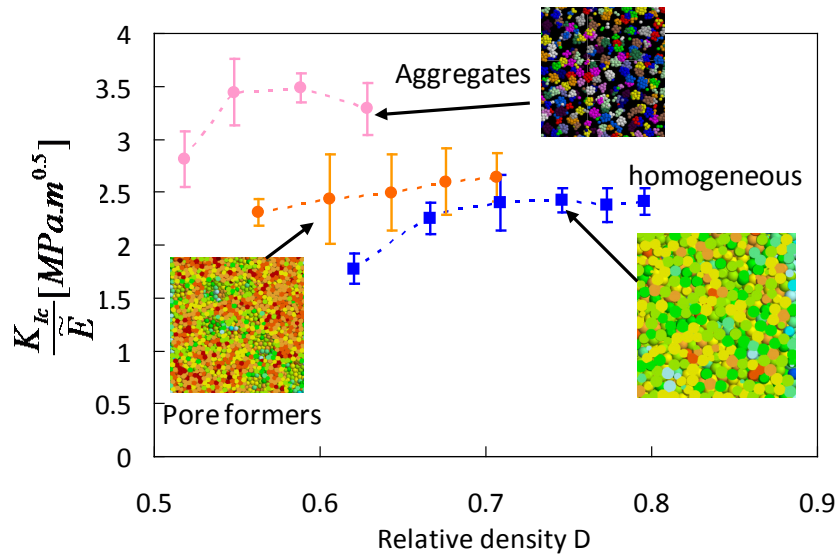


Fig.1: Evolution of the performance index  $K_{Ic}/E$  for imposed displacement conditions. For a given relative density (or residual porosity), microstructures obtained from aggregated powders exhibit a larger index of performance.

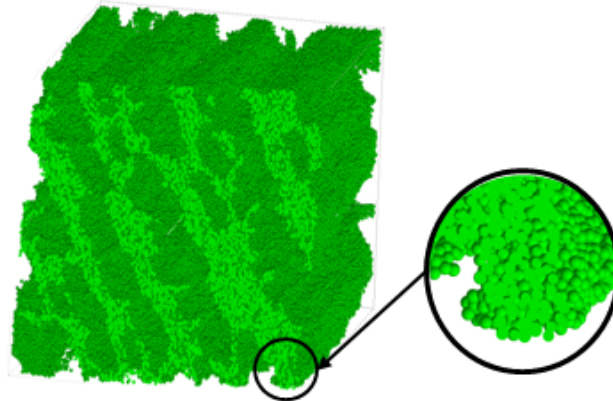


Fig.2: Ceramic microstructure obtained by freeze-casting, characterized by 3D nanotomography and discretized with discrete elements representing individual particles. The numerical microstructure is then crushed uniaxially.

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