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Elasticity and strength of partially sintered ceramics

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ABSTRACT

A discrete element model for the elastic and fracture behavior of partially sintered ceramics is presented. It accounts for the granular character of the material when a large amount of porosity (typically $>0.2-0.4$) is left after sintering. The model uses elastic force-displacement laws to represent the bond formed between particles during sintering. Bond fracture in tension and shearing is accounted for in the model. Realistic numerical microstructures are generated using a sintering model on random particle packings. In particular, packings with fugitive pore formers are used to create partially sintered microstructures with large pores. The effective elastic response and the strength of these microstructures are calculated in tension and compression. The link between important microstructural features such as bond size or coordination number and macroscopic behavior is investigated. In particular, it is shown that porosity alone is not sufficient to account for the mechanical properties of a partially sintered material.

1. Introduction

Porous ceramics are widely used as thermal isolators, filters, matrices for fiber reinforced composites, electrodes for SOFC or SOEC (Solid Oxide Fuel or Electrolyser Cells), membranes or bone scaffolds. Porosity typically ranges from 20% to 50% in such applications. While keeping high temperature properties and chemical erosion resistance, porous ceramics take advantage of their large surface area to enhance transport properties. This functionality of the material comes at the expense of a degradation of mechanical properties characterized by a decrease in both elastic modulus and fracture strength. Due to their ionic or covalent structure, ceramics tend to fracture with very limited plastic deformation, which results in poor toughness. For porous ceramics, the pores act as stress concentrators, further decreasing the toughness (Flinn et al., 2000). Thus, the mechanical properties of porous ceramics and their stability under operating conditions are generally viewed as the main limiting factor for their use in practical applications. Fundamentally, there is an inherent contradiction between the optimal microstructure for functional performance (high pore volume and surface area) and durable thermomechanical performance (low pore volume and surface area). It is therefore critical to gain a more thorough understanding of the mechanical behavior, and in particular of the fracture behavior of porous ceramics. Linking pertinent microstructural features to macroscopic behavior in order to reach predictive capabilities for quantitative models is paramount for reaching this goal. Relevant characteristics of porous ceramics include naturally the pore volume fraction but also the pore shape and size as well as the size and type of the contacts between solid grains.

For non-porous or very low porosity ceramics a large amount of modeling work (mostly two dimensional) has been undertaken in the last decade to include realistic microstructural features in the fracture process (see for example Warner

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and Molinari, 2006; Paliwal and Ramesh, 2008). For porous ceramics, there exists much less work attempting to link mechanical properties to microstructure. Most investigations have concentrated on phenomenological models linking the pore volume fraction to the mechanical properties (Boccaccini and Fan, 1997; Mukhopadhyay and Phani, 1998; Munro, 2001) and are limited to the elastic properties (Roberts and Garboczi, 2000; Jefferson et al., 2002; Raether and Iuga, 2006). More recently Pecqueux et al. (2010) have decoupled the effect of microporosities and macroporosities in bioceramics to phenomenologically model the compressive strength of porous ceramics with very large macropores.

Because porous ceramics are processed by partially sintering an assembly of particles, the discrete character of the ceramic material needs to be taken into account. When the porosity is large enough (typically >0.2), this has actually been recognized in some models by representing a partially sintered ceramic as a set of overlapping solid spheres that have formed bonds together. The elastic properties may then be calculated by the Finite Element Method (Roberts and Garboczi, 2000; Raether and Iuga, 2006) or by the Discrete Element Method (DEM) (Jefferson et al., 2002). However these models have limited their scope to elasticity and do not consider fracture. To our best knowledge, the only attempt to use DEM for simulating the fracture of porous ceramics was described by Fujita et al. (2004) on complex mullite/alumina mixtures for use as matrices for porous matrix ceramic composites. These authors enriched the model developed by Jefferson et al. (2002) to incorporate a fracture criterion at the length scale of the bonds between sintered particles. They demonstrated that the macroscopic toughness of the porous ceramics scales with the square of the bond size.

The model presented in this paper aims at calculating both elastic and fracture properties of partially sintered ceramics by the Discrete Element Method. It accounts properly for the local elastic and fracture behavior of the solid bonds formed between the discrete particles that have sintered together. Additionally, the microstructure that mimics the porous ceramic is obtained from a numerical procedure based on the same Discrete Element Method with appropriate sintering contact laws. The paper is organized as follows: In Section 2, we summarize the main components of the contact model between sintered particles. Section 3 describes the numerical sintering procedure that provides realistic porous samples. Tensile and compressive tests that are used for characterizing these samples are qualitatively described in Section 4. Quantitative results on the elasticity and on the strength are discussed in Sections 5 and 6, respectively. Finally, Section 7 is devoted to the effect of introducing artificial pores that are larger than the natural pores between particles, thus showing the importance of microstructure beyond the simple pore volume fraction parameter. Whenever possible, we attempt to compare our results with experimental data from the literature.

2. Model description

Particles that constitute the partially sintered material are modeled as truncated spheres overlapping geometrically neighboring particles (Fig. 1). The contact laws define the interaction between two particles that are bonded together by a solid elastic bridge which has formed during prior sintering processing at high temperature. The sintering process itself will be briefly explained in the next section when describing the generation of samples.

For two particles of radii R_1 and R_2, we define the equivalent radius R^*:

$$R^* = \frac{R_1 R_2}{R_1 + R_2}, \tag{1}$$

while the solid bridge size is given by its radius a_b (Fig. 1). Note that Eq. (1) is used both to define the contact geometry between two particles and between a particle and a plane ($R_2 \to \infty$). We distinguish two types of contacts: (i) contacts between two bonded particles that have formed a solid bridge, and (ii) contacts between two particles whose bond has broken and that are back into contact. The normal and tangential forces between bonded particles are derived from a simplified version of the model of Jefferson et al. (2002). For two particles with elastic constants E and ν, which have accumulated a normal displacement u_N (as compared to the initial stage of the bond with overlap h_b, Fig. (1), the normal

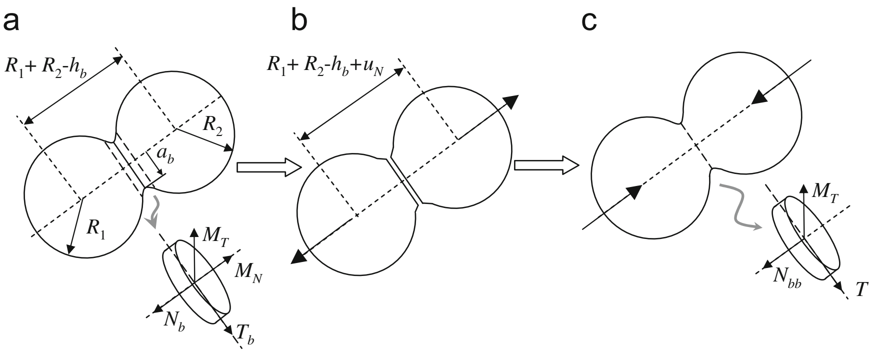

Fig. 1. The three possible stages of a solid bridge forming a bond between two particles. (a) Initial status (unbroken). (b) Broken bond. (c) Contact after bond fracture.