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Tensile strength and toughness of partially sintered ceramics using discrete element simulations

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ABSTRACT

The fracture behavior of highly porous ceramics is simulated using the discrete element method. Spherical particles model the powder used to obtain the partially sintered ceramic material. Three-dimensional representative volume elements of porous microstructures made of several tens of thousands of particles were first generated by numerical sintering. Elastic force–displacement laws model the solid bonds formed between particles during sintering. A realistic fracture criterion, based on the local stress intensity factor associated with the bond between two particles, is also introduced. The simulation of tensile tests allows the assessment of the effective strength of these microstructures as a function of the residual porosity. Furthermore, the introduction of a pre-crack in a sample subjected to a remote tensile stress allows the critical stress intensity factor to be calculated. Porous electrodes for electrochemical applications represent an important application field for these ceramics. Those discrete element simulations should be an effective tool for optimizing their microstructure at the micron length scale.

1. Introduction

Porous ceramics obtained by partial sintering of powders are used for a wide range of applications including filtering, thermal insulation, bone scaffolds, or electrodes for SOFC/SOEC (Solid Oxide Fuel Cells/Solid Oxide Electrolyser Cells).

The microstructures of these materials are often designed to enhance transport properties by increasing the pore volume fraction (typically from 20% to 50%) and the surface area. However increasing the porosity drastically reduces their strength leading to failure and durability issues. For example, in the case of electrochemical cells, localized cracking may not always lead to the full loss of the cell but can certainly decrease its electrochemical performances by breaking up the ionic and electronic conduction paths. It is thus critical to gain a better understanding of the fracture behavior of those porous ceramics in order to relate relevant microstructural parameters to the strength and the toughness of the material. In that respect, it is worth recalling that because those porous ceramics are made via powder sintering, their final microstructure retains a particulate architecture where initial particles are still observable.

Extensive work has been carried out to model the influence of the porosity on the elastic modulus of ceramic materials [1–5], including Discrete Element Method (DEM) approaches [4,5]. The fracture strength of porous ceramics has also been addressed using analytical approaches (e.g. [6]), homogenisation approach [7] or simulations [5,8,9], but modeling of the toughness is more scarce [6,10–12].

DEM is a well fitted modeling tool to represent the complex microstructure of partially sintered porous ceramics. This is because in DEM, each particle is modeled as a distinct entity with specific mechanical interactions with its neighbors.

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Nomenclature

a	half-crack size
a^*	relative bond radius
a_b	bond radius
a_c	critical defect size
c_0	equivalent size of the initial flaw
E	particle Young's modulus
h	initial overlap between particles
K_{I0}	crack tip toughness
K_I	stress intensity factor
K_{Ic}	critical stress intensity factor
u_N	normal displacement
u_T	accumulated tangential displacement
M_N	normal resisting moment
M_T	tangential resisting moment
N_b	normal force
P	porosity
P_0	green porosity
T_b	tangential force
f_N	normal correction function
f_T	tangential correction function
r	distance to the crack tip along the crack axis
R	particle radius
W	half-width of the periodic array of collinear cracks
Y	geometric factor
α	critical bond stress adjustable parameter
ε_{zz}	axial strain
$\bar{\psi}$	adjustable parameter of the normal contact law
θ_N	accumulated normal rotation
θ_T	accumulated tangential rotation
γ_s	surface energy
Γ	bond toughness
ν	particle Poisson's ratio
σ	remote stress
σ_c	bond fracture stress
σ_f	macroscopic fracture stress
σ_{zz}	axial stress

Realistic microstructures can thus be generated by "numerical sintering" and then strained to characterize their mechanical behavior [5].

The aim of this study is to demonstrate the capability of DEM to obtain quantitative data on strength and toughness of partially sintered ceramics which should be of great interest for the microstructure optimization of this class of materials. In a first part, the strength is determined via the introduction of a bond fracture criterion in the model, and compared to experimental data on porous alumina. In a second part, it is shown that a fracture mechanic approach can be advantageously used to avoid the use of an adjustable parameter in the bond fracture criterion. The toughness of a given porous microstructure is obtained by applying Linear Elastic Fracture Mechanics (LEFM) to the tensile test simulation of a sample containing a pre-crack and strained up to failure.

2. Model description

Only a brief description of the DEM principles and of the contact model is provided here. More details may be found in previous publications [5,13–15]. The DEM is based on the representation of material particles by discrete spheres that interact mechanically with each other through their contacts (Fig. 1). The first stage of the simulation consists in generating a 3D aggregate of overlapping spheres of radius R that represents a partially sintered porous body. In order to obtain a realistic microstructure the sintering step is modeled using a DEM approach [13,15]. The DEM sintering simulation provides the position of the particles after shrinkage and rearrangement according to a set of parameters relevant for alumina [13]. Then the radius a_b of the circular necks or bonds formed between the particles during the sintering is deduced using Coble's model [16]: