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Finite element simulations of the deformation of fused-cast refractories based on X-ray computed tomography

Kamel Madi [a,*], Samuel Forest [a], Michel Boussuge [a], Sylvain Gailliègue [a], Emilie Lataste [b], Jean-Yves Buffière [b], Dominique Bernard [c], Dominique Jeulin [a]

[a] Ecole des Mines de Paris, CNRS, Centre des Matériaux, UMR 7633, BP 87, 91003 Evry, France
[b] GEMPPM, INSA Lyon, Bat. St Exupéry, 20 Av. Albert Einstein F-69621, Villeurbanne Cedex, France
[c] Institut de Chimie de la Matière Condensée de Bordeaux, ICMCB/UPR CNRS 9048/87, Av. du Dr Albert Schweitzer, 33608 Pessac Cedex, France

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Abstract

This work consists in building a 3D numerical model of the microstructure of a fused-cast refractory (two-phase material). Creep tests at temperatures as high as 1400 °C reveal a major influence of the morphology of the phases on the material behavior. A possible 3D connectivity of the zirconia grains, related to the fabrication process, may explain the observed high creep resistance. In order to have a realistic representation of the microstructure, 3D pictures have been obtained using X-ray microtomography at the European Synchrotron Radiation Facility in Grenoble (ESRF). Volumetric tetrahedral grids are generated from the exploitation of these pictures using available meshing techniques. Finite elements calculations are performed to study the influence of the glassy phase content on the stiffness of the material. Simulations are compared with experiments. In particular the notions of geometrical and mechanical percolation are investigated numerically. High elastic stiffness is predicted, even for large amorphous phase contents. A percolation threshold is observed for the geometry of the hard phase (zirconia phase) but not for the Young's modulus.

Keywords: Zirconia; Amorphous phase; Tomography; Fused-cast refractories; Percolation; Finite element

1. Introduction

This work focuses on the study of a zirconia-rich fused-cast refractory used for building glass furnaces. The manufacturing process of fused-cast refractories is similar to that used in metallurgical foundry, that is melting of raw materials at very high temperature, casting into molds and then controlled cooling. The stage of cooling is a critical step in the fabrication process, that strongly influences the quality of the final product. Numerous experimental techniques (tension, compression and bending tests, creep experiments, ultrasonic measurements, etc.) were performed to investigate the material behavior [1,2]. Our work aims at reaching a better understanding and the simulation of the phenomena occurring during the cooling stage, from the properties of the constituents and from a realistic numerical modeling of the microstructure topology. This work focuses on the original 3D morphology of the investigated material, induced by the fabrication process. The connectivity of the hard phase is shown to play a significant role on the macroscopic mechanical behavior of the material. This first contribution concentrates on the elastic behavior of the material. The role played by the constituents on the stiffness of the material is discussed.

2. Microstructure of the material

2.1. 2D representation

The investigated material, called HZ for high zirconia content, is a zirconia-rich material (88 vol.% zirconia).

* Corresponding author.
E-mail address: kamel.madi@ensmp.fr (K. Madi).

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2D optical microscopy (see Fig. 1(a)) revealed that zirconia (the hard phase) is surrounded by a darker thin-layer of amorphous phase (12 vol.%) (the weak phase) with a glass transition temperature of about 780 °C. At higher temperatures, the amorphous phase behaves inside the material like a Newtonian fluid with a decreasing viscosity with increasing temperature. Creep tests were performed on this material at temperatures as high as 1400 °C. Surprisingly, they revealed that this material exhibits a high creep resistance up to temperatures 600 °C higher than the glass transition temperature of the amorphous phase. Moreover, this observation remains true for another fused-cast material of the alumina–zirconia–silica system containing 28 vol.% of the same amorphous phase [3]. This kind of behavior is very different from the mechanical response of conventional sintered ceramics at high temperature, that strongly depends on the volume fraction and on the viscosity of the intergranular amorphous phase [4,5]. Preliminary 2D simulations of creep in the HZ material (see Fig. 1(b)) have been performed with a mesh representative of most sintered ceramics (individual grains surrounded by a continuous intergranular phase) [6]. Even when the behavior of zirconia is assumed to be purely elastic, considering the decrease in viscosity of the amorphous phase leads to a strong overestimation of the creep rate when compared to experiments. A Norton creep law with a stress exponent equal to 1 was considered for the glassy phase. This suggests that the 3D topology of the microstructure could have a great influence on the observed properties and should be investigated.

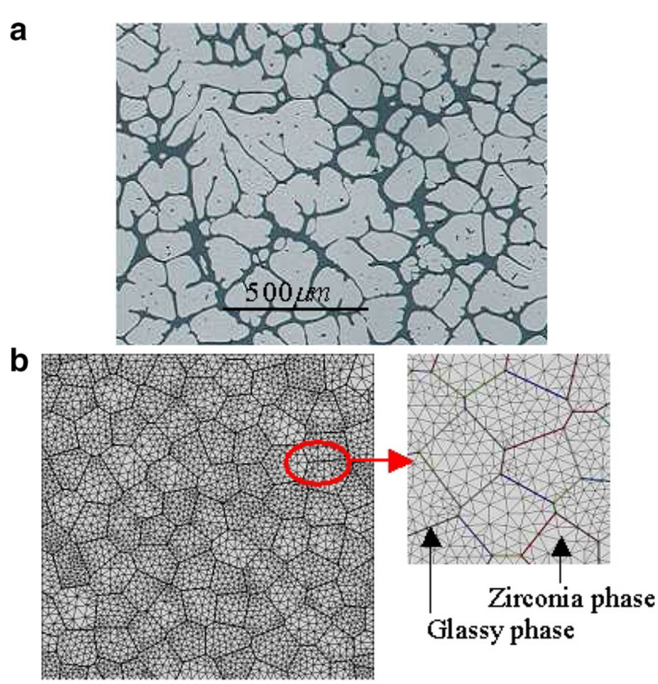

Fig. 1. (a) Microstructure of the HZ material (optical micrograph: amorphous phase in dark, crystal zirconia phase in bright), (b) simulated microstructure with meshed grains boundaries (100 grains).

2.2. 3D morphology

2.2.1. X-ray tomography

To get a 3D representation of the material, high energy X-ray tomography at the European Synchrotron Radiation Facility (ESRF, Grenoble, France) has been used. This technique basically consists in recording several radiographs of a sample at different angular positions and in reconstructing a 3D map of the X-ray attenuation coefficient within the material using adequate algorithm and software [7]. This technique can reveal all the microstructural features (inclusions, cracks, pores, constituting phases, etc.) that induce a change in attenuation along the path of the X-ray beam. From this point of view, there is a high contrast between the high X-ray attenuation of zirconia compared to that of the amorphous phase. Fig. 2 illustrates a 3D image of the microstructure of the HZ material obtained with the highest resolution (1.4 µm) available on the ID19 beamline (X-ray energy: 40 keV) that has been used at ESRF.

2.2.2. 3D connectivity of the phases

In order to study the 3D connectivity of the phases in the material, the concept of geometrical percolation has been used. This notion has been introduced by Kanit [8,9] to study the possible percolation of a phase in a heterogeneous material. Using image analysis tools and a mathematical morphology algorithm based on the 3D geodesic reconstruction, two important concepts are defined: (i) the image of the interconnected phase is defined as the set of all points in a given phase that can be connected to two opposite sides of the image following paths entirely contained in the same phase; (ii) the percolation ratio is defined as the ratio between the volume fraction of the interconnected phase to the whole volume fraction in the microstructure of this phase. It is always lower than or

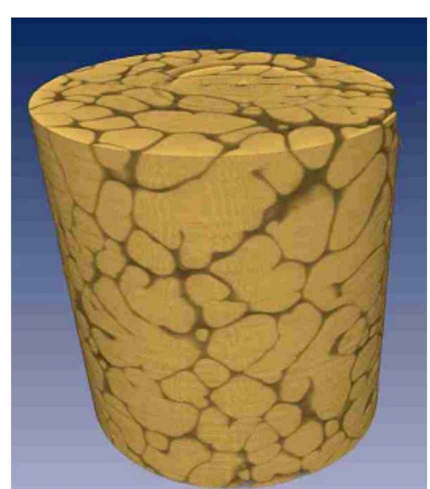

Fig. 2. 3D representation of the phases obtained by X-ray tomography (zirconia in bright, amorphous phase in dark). Diameter of the specimen: 500 µm, height: 1400 µm.