Available online at www.sciencedirect.com

ScienceDirect

Acta Materialia 70 (2014) 30–44

Acta MATERIALIA

www.elsevier.com/locate/actamat

Modeling microstructural damage of silicate-based ceramics and its influence on macroscopic fracture strength

F.A. Gilabert [a,*], V. Cantavella [a], M. Dal Bó [b], E. Sánchez [a]

[a] Instituto de Tecnología Cerámica-Asociación de Investigación de las Industrias Cerámicas (ITC-AICE), Universitat Jaume I, Campus Riu Sec, 12006 Castellón, Spain

[b] Graduate Program in Materials Science and Engineering (PGMAT), Department of Mechanical Engineering, Federal University of Santa Catarina (UFSC), 88040-900 Florianópolis, SC, Brazil

Received 20 December 2012; received in revised form 7 January 2014; accepted 15 January 2014
Available online 13 March 2014

Abstract

The aim of this work is to clarify the influence of quartz inclusions added to a vitreous matrix on the macroscopic fracture toughness (K_{IC}). We use numerical simulations to model a silicate-based ceramic material as a heterogeneous region composed of an isotropic brittle matrix and a distribution of embedded quartz inclusions. Using the material point method (MPM), we present a two-dimensional study, that albeit an approximation, sheds light on the role of the material composition in the fracture behavior observed in these ceramic materials. The value of K_{IC} is calculated from the maximum strength obtained via computational analysis of a single-edge-notch tension specimen. The model test allows us to study in detail the effects occurring in a region close to the main notch. Additionally, to validate and understand our numerical findings, we fabricated and characterized experimentally a representative set of specimens with the same features as the numerical ones. We focus our attention on the effect of both the size and volume fraction of the dispersed phase, as well as the initial state of microcracking of the material and its influence on the macroscopic mechanical performance. The simulations have shown the decisive role played simultaneously by the volume fraction and typical size of the inclusions that are cracked during the cooling process.

Keywords: Micromechanical modeling; Ceramic composites; Fracture toughness; Crack growth; Microcrack toughening

1. Introduction

The classical mechanism for obtaining a reinforced glass matrix in ceramic compositions involves a mismatch between the thermal expansion coefficients of the vitreous matrix and the dispersed inclusions [1,2]. This mismatch creates stresses in the matrix which may deflect cracks [3,4]. However, when the expansion coefficients of the matrix and the inclusions match, this reinforcement mechanism does not occur. In this case, other theories about glass matrix reinforcement in ceramic compositions have proposed that, at room temperature, the dominant strength-controlling factors are the volume fraction of the dispersed phases [5] and the elastic properties of each constituent phase [6]. On the other hand, it has also been pointed out that at high volume fractions of the dispersed phase, the strength is also dependent on the particle size of this phase [7]. Another important factor is the inclusion shape of the dispersed phase [8,9].

Despite all these factors apparently affecting the mechanical strength of high-performance ceramic tiles, the fracture toughness varies within quite a narrow range of 1–2 MPa $m^{1/2}$ [10]. In fact, recent studies carried out

* Corresponding author. Tel.: +34 964342424; fax: +34 964342425.
E-mail address: fran.gilabert@gmail.com (F.A. Gilabert).

http://dx.doi.org/10.1016/j.actamat.2014.01.026
1359-6454/

at ITC (forthcoming) have revealed that adding 20 vol.% of inclusions of quartz, alumina or zircon does not result in reinforcement of a glass matrix made of sodium feldspar. Therefore, the influence of the nature and the amount of the dispersed phase on the mechanical performance of the final solid is not yet well understood.

The present paper addresses part of the above experimental study. In particular, it reports on a numerical simulation to analyze the effect of the quartz particles, since quartz is the most abundant crystalline phase in porcelainware compositions, and many studies have emphasized its role in defining the mechanical properties of the final product [11–15].

We use a computational procedure based on the particle-in-cell technique [16], which is a combination of the finite-element method (FEM) [17] and particle dynamics simulations [18]. This procedure, also referred to as the material point method (MPM), was initially formulated by Sulsky et al. [19] in the framework of solid mechanics, and, up to now, has been successfully applied to a wide variety of problems [20–23]. As all the material properties are transported by the points, a static structured mesh is used as a background "scratchpad" for computations. This feature, which depicts such procedure as a meshless method, has facilitated the explicit incorporation of cracks [24], e.g. to simulate the transverse fracture process in wood [25] or more recently the microcracking in ceramic materials during the cooling process [26].

This paper is organized as follows. In Section 2 we briefly describe the experimental procedure used to obtain and characterize the material types that will be modeled; the simulation method is introduced in Section 3. Section 4 is devoted to the important issue of the procedure to create the material model, as well as to define the micromechanical features of the initial state. Section 5 presents and validates the numerical single-edge-notch-tension test (SENT) used to determine the macroscopic fracture toughness of the compositions numerically simulated. In Section 6 we show the simulated setup used to calculate the mechanical strength. In Section 7 we present the results of the simulation model, and some particularly interesting features obtained from the model are discussed in comparison with simple numerical tests and experimental measurements that we made from the actual specimens. Finally, we conclude by remarking on the main features as well as providing some general hints on possible improvements of future materials compositions using quartz as the dispersed phase.

2. Experimental

In this work we prepared and characterized four types of compositions that differ from each other in the amount and size of the inclusions, i.e. the volume fraction and the particle size distribution. Each sample consists of a glassy dense matrix to which a specific amount of quartz particle was added. A brief schematic description of the preparation process is provided.

2.1. Specimen preparation

The initial size of the natural feldspar powder particles was reduced in water by planetary milling for 30 min with alumina balls for high-energy milling. Once the feldspar was dried, quartz particles were added and the mixture was granulated as a 8 wt.% aqueous solution with 5 wt.% polyvinylalcohol. From this mixture of feldspar with quartz, 10 rectangular specimens were pressed at 35 MPa, resulting in specimens whose final dimensions were $70 \times 17 \times 5.9$ mm.

Sintering was done using an electric furnace (Pirometrol R-series), with an initial heating rate of 3.5 °C/s between 25 and 500 °C, followed by a heating rate of 0.4 °C/s up to 1200 °C. This temperature was held for 6 min, followed by a quenching process. This cooling consisted of a rapid extraction of the specimens from the furnace and forced ventilation using compressed air at 1 bar. Using two pyrometers, the top and bottom surface temperatures of the specimen were recorded. This rapid cooling gives rise to macroscopic mechanical stresses [10]. As a control test, we prepared an additional set of specimens but under slow cooling. This slow cooling consisted of keeping the specimens inside the furnace after it was switched off. Specimens were then extracted once the interior of the furnace reached room temperature. This type of cooling took about 2 h. In this way, we prevented the occurrence of macroscopic residual stresses in these control specimens. On the other hand, the average measured water absorption in all our specimens was lower than 0.5%.

We used two types of quartz powders to prepare our compositions: SE-100 and SE-8 (Sibelco). These raw quartz powders are commonly used industrially to produce porcelain tiles, which are a class of high-performance tile. Two volumetric fractions of quartz particles were used: 20% and 40%. For ease of specimen identification, we establish the following notation: letter "F", standing for fine, corresponds to compositions with SE-100 granulometry, whereas letter "C" stands for coarse and refers to compositions with SE-8 granulometry. This composition denomination, as well as the corresponding average inclusion diameters, are summarized in Table 1. The size distributions of these quartz inclusions are shown in Fig. 1. We used scanning electron microscopy (SEM; Philips XL30 CP) to observe the resultant microstructures at room temperature. Fig. 2a and b show the typical microstructural features of compositions F20 and C20, respectively. Of particular interest are the intragranular microcracks appearing in the reinforcing quartz grains. After inspecting different

Table 1
Nomenclature of the four compositions used.

Quartz type	Volume fraction		Diameters	
	20%	40%	D_{50} (μm)	D_{90} (μm)
SE-100	F20	F40	13.4	32.1
SE-8	C20	C40	31.4	98.5