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Original Research Article

Anisotropy of thermal expansion of 3Y-TZP, α-Al_2O_3 and composites from 3Y-TZP/α-Al_2O_3 system

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ABSTRACT

The work deals with determining of lattice parameters (not present in the literature till now) in the temperature range of 295–1473 K for tetragonal zirconia polycrystals, stabilized with 3 mol.% of yttria and for corundum (α-Al_2O_3). Basing on lattice parameters changes with temperature, thermal expansion coefficients for 3Y-TZP and α-Al_2O_3 monocrystals along *a* and *c* crystallographic axis were determined. The calculated values of axial coefficients of thermal expansion were used for creation of a micromechanical model for simulation of thermal expansion of materials, constituting the real microstructures of composites from 3Y-TZP/α-Al_2O_3. The results of simulations were compared with thermals expansion coefficients, determined by dilatometric measurements and performed for real composites.

1. Introduction

1.1. Motivation

Composites in the corundum/tetragonal zirconia system, due to their very good mechanical and tribological properties, excellent chemical resistance and confirmed biocompatibility, are readily used in many technical and biomedical applications [1,2]. The mentioned composites are widely used for cutting tool manufacturing, bearings components, bushings, valve seats, pump components or orthopaedics and dental prosthetics [3–8].

The weakest point of structural ceramics application is constituted by their relatively (when compared to metals) fracture toughness. Nevertheless, zirconia ceramics show the presence of a few mechanisms, distinctly increasing the fracture energy value and consequently increasing the K_{IC} parameter value. The most effective are martensitic phase transformation and the presence of residual stresses [9,10]. In the literature concerning TZP ceramics and composites of TZP/alumina system one can find many analytical [10–14] or numerical [7,15–19] models, searching for better understanding of the mentioned phenomena and leading to the improvement of zirconia and composite sintered products.

One of the most important thermomechanical property of zirconia, conditioning the value of thermal residual stresses and influencing the tetragonal to the monoclinic phase transformation, is their thermal expansion. Despite the long-lasting and intensive interest in zirconia materials

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properties there is a lack of experimental results, describing changes of axial coefficients of thermal expansion (CTE) of the tetragonal zirconia phase in a wide range of temperature changes. The mentioned above models can be considered a standard use for calculations of the mean values of CTE which must affect the accuracy of calculations results, especially close to the room temperature, where the temperature dependence of CTE is nonlinear.

In the presented paper the axial thermal expansion coefficients values for 3Y-ZrO_2 and α-Al_2O_3 were measured in the temperature range of 295–1473 K.

1.2. Literature review

Since the tetragonal zirconia phase (t-ZrO_2), whose presence determines high fracture toughness, is thermodynamically stable above the martensitic transformation temperature (1443 K [10]), technical applications use stabilized zirconia. The most often used chemical composition is a solid solution containing about 3 mol.% of yttria in zirconia. Such a composition assures a fully tetragonal sintered material at the room temperature.

Depending on the type of used stabilizing ion and its molar content, mechanical and thermal properties of the material are changing. With the increase of Y_2O_3 content thermal expansion of polycrystalline zirconia decreases [20,21], due to the changes of *a* and *c* lattice parameters of t-ZrO_2 [22].

Experimental data available in the literature describing changes of axial CTE's, depending on temperature changes for t-ZrO_2, concern mainly a pure oxide in the temperature range above the temperature of martensitic transformation [23–25]. Sparse data include also lower temperatures (to 773 K) for which axial CTE's were determined for a metastable tetragonal phase of ZrO_2 [26–28].

The data concerning axial CTE's changes of stabilized ZrO_2 are very rare. The information published by Schubert [29] concern 3Y-TZP but they describe only the mean values of CTE in the relatively wide range of temperatures (873 K – RT and 1073 K – RT). Practically, only Ochrombel et al. [30] showed detailed data concerning *a* and *c* lattice parameter changes in the temperature range of 333–1173 K. Due to this it is possible to calculate axial CTE's for t-ZrO_2 (stabilized with 3.3 mol.% of Y_2O_3).

Such a small amount of available experimental data for stabilized zirconia, which is an important structural material, and practically the lack of axial values of CTE's for the room temperature, confirms the necessity of investigations in this area. The results of these investigations could be applied for better understanding of materials based on zirconia and improve designing of engineering ceramics.

The second compound of the investigated composites is α-Al_2O_3. (Corundum). This phase belongs to the best characterized ceramic phases. In the literature one can find a lot of data concerning the dependence of lattice parameters [31–33] or axial CTE's [31,34,35] as the function of temperature. For this reason corundum is often used as a reference material in dilatometry [36,37]. In the presented work the reference values of lattice parameters and axial CTE's were used for the control of correctness and verification of results achieved for α-Al_2O_3 and, indirectly, for t-ZrO_2.

2. Experimental

2.1. Sample preparation

Composites investigated in this work were prepared applying commercially available powders of 3Y-TZP (TOSOH, TZ-3Y) and α-Al_2O_3 (TAIMEI Chemicals, TM-DAR). The same powders were used for lattice parameters measurement of monocrystalline phases. Composite powders were made by mechanical mixing of zirconia and alumina powders in the atrittor mill. Zirconia grinding media and ethyl alcohol environment were applied during mixing. Disc-shaped (18 mm in diameter and 1.5 mm high) samples were formed by uniaxial pressing at 50 MPa and then isostatically re-pressed at 300 MPa. The sintering process was conducted at 1773 K with 2 h soaking time at the maximum temperature. Composite samples were composed to assure different types of microstructure – isolated grains of the second phase dispersed in the matrix and duplex microstructure, containing two interpenetrating phases. Finally, five composite materials were manufactured. Their composition and names are given in Table 1.

2.2. XRD measurements of lattice parameters

Structural measurements were carried out in the range of 10–110° using CuKα radiation on Panalytical Empyrean diffractometer, equipped with PIXcel3D detector. For high temperature studies, Anton Paar HTK 1200N oven-chamber was used. Data collection was performed at 295, 323, 373, 473, 673, 1073 and 1473 K with ca. 55 min scans. Before the measurement, the sample (α-Al_2O_3 and 3Y-TZP powders) was equilibrated at a particular temperature for 5 min. Additionally, XRD measurements were also performed for 3Y-TZP powders pre-heated at 1273 K for 1 h.

2.3. Simulations of thermal expansion

2.3.1. Geometry of the RVE

Simulations of thermal expansion were conducted using the finite elements method (FEM), using the concept of the two-dimensional representative volume element (RVE) [38–40]. Geometry of RVE was prepared on the basis of numeric micrographs of microstructure of 3Y-TZP, α-Al_2O_3 and composites (Fig. 1), made with SEM microscope (NovaNano SEM

Table 1 – Chemical composition and marks for materials investigated in the work.

Sample	Volume fractions [% vol.]	
	3Y-TZP	α-Al_2O_3
ZrO_2	100	0
ZA15	85	15
ZA35	65	35
AZ50	50	50
AZ35	35	65
AZ15	15	85
Al_2O_3	0	100