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Phase composition, structure and mechanical properties of PSZ (partially stabilized zirconia) crystals as a function of stabilizing impurity content

M.A. Borik [b], V.T. Bublik [a], A.V. Kulebyakin [b], E.E. Lomonova [b], F.O. Milovich [a,*], V.A. Myzina [b], V.V. Osiko [b], N.Y. Tabachkova [a]

[a] National University of Science and Technology "MISIS", Leninsky pr. 4, 119049 Moscow, Russia
[b] Prokhorov General Physics Institute, Russian Academy of Sciences, 119991 Moscow, Vavilov Str., 38, Russia

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ABSTRACT

The structure of PSZ crystals have been studied in relation to the content of the stabilizing impurity (Y_2O_3) by X-ray diffraction and transmission electron microscopy. The measurement of both hardness and fracture toughness by microindentation have been carried out. Studies have shown that crystals of PSZ obtained by directional solidification of the melt consist of two tetragonal phases (*t* and *t'*), with varying degrees of tetragonality. The yttrium-enriched phase *t'* is "untransformable" in contrast to the *t* phase, with a lower content of yttrium, which, under the influence of mechanical stress, undergoes a martensitic transition to the monoclinic form. Increasing the stabilizing impurity concentration leads to an increase in the volume fraction of the "untransformable" phase. Increasing the concentration of Y_2O_3 also affects the form and dispersion of the twin domains. The character of the twinned structure changes depending on the concentration of the stabilizing impurity and the hierarchy of the twinning disappears above 3 mol.% Y_2O_3. In this work it is shown that the quantity of hardening (fracture toughness) is proportional to the content of the transformable *t* phase.

1. Introduction

Zirconia has several polymorphous modifications [1]. Due to the detrimental monoclinic-tetragonal phase transition, pure zirconia is used quite rarely. However, there are indications [2] that the effect of this phase transition can be eliminated by doping zirconia with an appropriate amount of MgO, CaO, Sc_2O_3, Y_2O_3 or rare-earth metal oxides to obtain a metastable cubic fluorite solid solution at room temperature.

The high melting points (2700–2800 °C), the chemical reactivity of the melt and the presence of polymorphic transitions have largely impeded the synthesis of zirconia based single crystals. For example, ZrO_2 single crystals have been grown using low temperature methods from melt solution, hydrothermal growth methods and from the gaseous phase [3]. These processes are quite time consuming, and the sizes of the resulting crystals were small. Using crucible-free melt growth methods (electric arc and zone melting) [4], ZrO_2 based solid solution single crystals have been obtained. However, the commercial synthesis of zirconia based single crystals has only become possible using direct RF melting in a cold crucible.

Of great interest are high strength and high toughness zirconia base materials. These include partially stabilized zirconia (PSZ) which is a solid solution of zirconia with small additions of yttrium oxide or oxides of other rare-earth or alkaline-earth metals. The mechanical and electric properties of these crystals make them suitable for a number of technical and industrial applications in electronics, materials processing and medicine. Such materials can be used to produce components for devices functioning under extreme conditions: at high mechanical loadings, in aggressive media, at elevated temperatures, without lubrication, etc. Such applications include bearings, support prisms, guide plates, and motor valves.

This material, with its high fracture toughness due to the inherent phase transition similar to martensitic transformations in steels, has received the name 'ceramic steel'. The transformation hardening mechanism has been described elsewhere [5]. These results have given a strong impetus to the development of the fundamental research of this zirconia based material, both its synthesis and applications. An advanced comprehensive review of the transformation hardening mechanism in structural ceramics has been reported [6] where the theoretical aspects of the transformation hardening mechanism have been analyzed and experimental results on the microstructure and mechanical parameters of zirconia base materials have been provided.

Zirconia based materials have a variety of unique physicochemical, electrical and mechanical properties including high strength, hardness, impact toughness, wear resistance, low coefficient of friction, high melting point, chemical inertness, low heat conductivity

* Corresponding author.
E-mail address: philippmilovich@gmail.com (F.O. Milovich).

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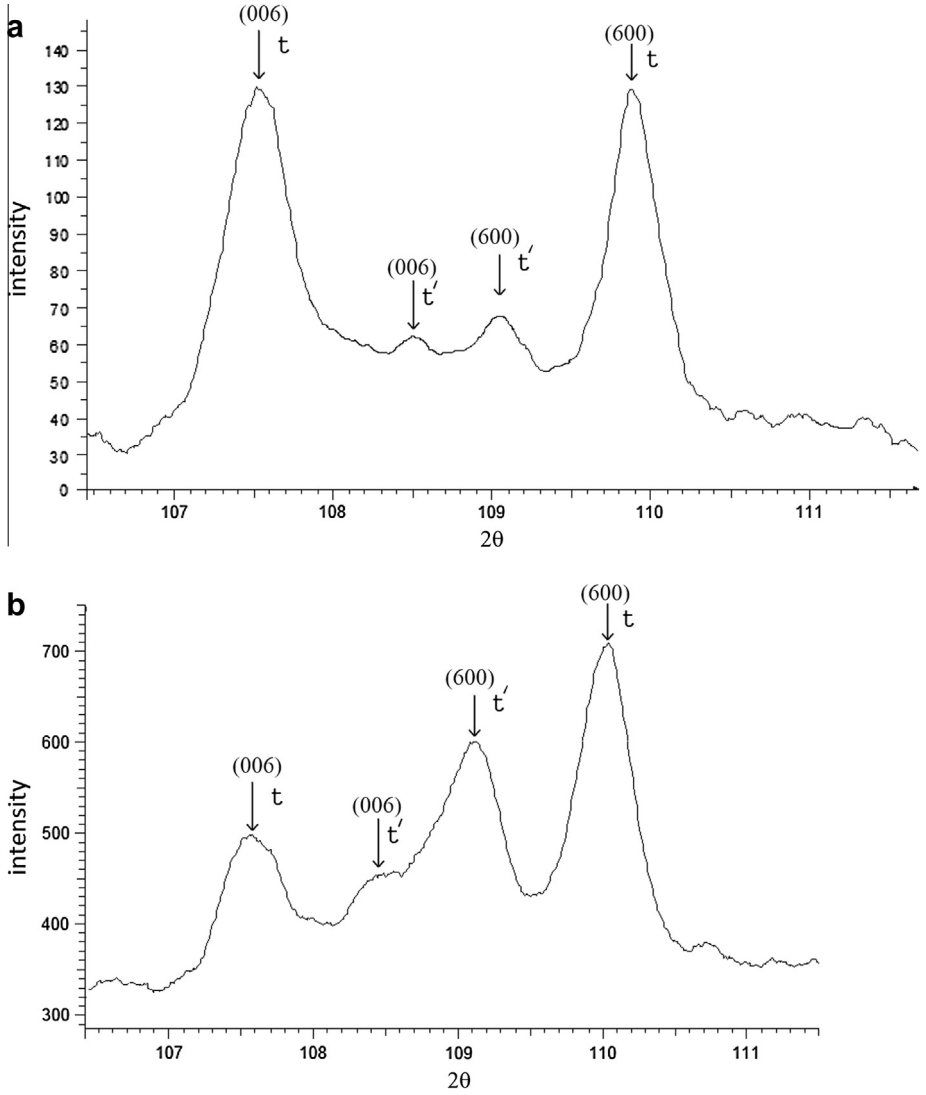

Fig. 1. (a) X-ray diffraction patterns of the YSZ 2.8 mol.% Y_2O_3, (b) X-ray diffraction patterns of the YSZ 4.0 mol.% Y_2O_3.

and biocompatibility. These properties account for the wide range of applications, from wear resistant ceramic bearings to medical and surgical instruments. Due to the existence of domain nanostructure in PSZ crystals and high mechanical strength of these crystals they may be used in the manufacture of instruments with very sharp cutting edges, for example, high-quality medical scalpels and instruments for precision machining of various materials (metal, wood, glass, crystals, etc.). The biological inertness of this material [7] enables its use in the manufacturing of implants for medicine.

Most studies of the properties of partially stabilized zirconia are based to research ceramics, also known as tetragonal zirconia polycrystals (TZP) [8–12].

Another method of obtaining PSZ is the synthesis of crystalline materials using melt crystallization methods. This approach facilitates the growing high density monolithic crystalline material with zero porosity and no grain structure.

The study of these crystalline materials provides a unique possibility of investigating the properties of the pure material not affected by grain boundaries, impurities, pores or other factors that contribute significantly to the physicochemical properties of these materials.

The aim of this work is to study the effect of the stabilizing impurity concentration on the phase composition, structure and properties of PSZ crystals grown by directional melt crystallization in a cold crucible.

2. Experimental

Yttrium oxide stabilized (concentration range 2.8–5.0 mol.%) PSZ crystals were grown using directional melt crystallization in a cold crucible at a 100 mm/h crystallization rate. The phase composition and structure of the PSZ were studied using X-ray diffraction on a Bruker D8 instrument and transmission electron microscopy on a JEM-2100 microscope at a 200 kV accelerating voltage. The specimens for the electron microscopy study were prepared as follows. Wafers were cut from the crystals so that the plane of the wafer was oriented either orthogonally to the ⟨1 0 0⟩ or the ⟨1 1 1⟩ crystal axes. The specimens were ground to a 200 μm thickness. 3 mm diameter discs were cut out of the source material by ultrasonic cutting, followed by the dimpling the center of the discs, and finally the specimens were thinned by ion beam etching. Hardness and fracture toughness were measured by microhardness indentation.

3. Results and discussion

In accordance with the ZrO_2–Y_2O_3 phase diagram [13], PSZ crystals growing during melt synthesis initially have a cubic structure, and a phase transformations occur during cooling in the solid state [14]. As the temperature decreases, the cubic phase becomes unstable and transforms to a tetragonal modification. The slight