

# Thermal conductivity of single crystals zirconia stabilized by scandium, yttrium, gadolinium, and ytterbium oxides

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## Abstract

The phase composition and heat conductivity of  $(\text{ZrO}_2)_{0.9}(\text{R}_2\text{O}_3)_{0.1}$  solid solution single crystals have been studied, where  $R = (\text{Gd}, \text{Yb}, \text{Sc}, \text{Y})$ ,  $(\text{ZrO}_2)_{0.9}(\text{Sc}_2\text{O}_3)_{0.09}(\text{Gd}_2\text{O}_3)_{0.01}$  and  $(\text{ZrO}_2)_{0.9}(\text{Sc}_2\text{O}_3)_{0.09}(\text{Yb}_2\text{O}_3)_{0.01}$ . Single crystals have been grown by directional melt crystallization in a cold skull. The phase composition of the crystals has been studied using X-ray diffraction and Raman spectroscopy. The heat conductivity of the crystals has been studied using the absolute steady-state technique of longitudinal heat flow in the 50–300 K range. We show that at a total stabilizing oxide concentration of 10 mol.% the phase composition of the crystals depends on the ionic radius of the stabilizing cation. The  $(\text{ZrO}_2)_{0.9}(\text{Sc}_2\text{O}_3)_{0.1}$  crystals have the lowest heat conductivity in the 50–300 K range while the  $(\text{ZrO}_2)_{0.9}(\text{Gd}_2\text{O}_3)_{0.1}$  solid solutions have the lowest heat conductivity at 300 K.

Analysis of the experimental data suggests that the heat conductivity of the crystals depends mainly on the phase composition and ionic radius of the stabilizing cation. Phonon scattering caused by the difference in the weight of the co-doping oxide cation has a smaller effect on the heat conductivity.

## Keywords

zirconia, crystal growth, heat conductivity, phase analysis.

## 1. Introduction

Zirconia based materials are widely used in engineering nowadays [1–3]. The combination of refractory properties, high thermal expansion coefficient, chemical inertness, ionic conductivity and good mechanical proper-

ties makes these materials attractive for a wide range of high-temperature and corrosive media applications. Due to their biological inertness and biocompatibility, high impact toughness and strength these materials are widely used in the fabrication of medical tools [4–5]. The optical properties of zirconia based single crystals and transpar-

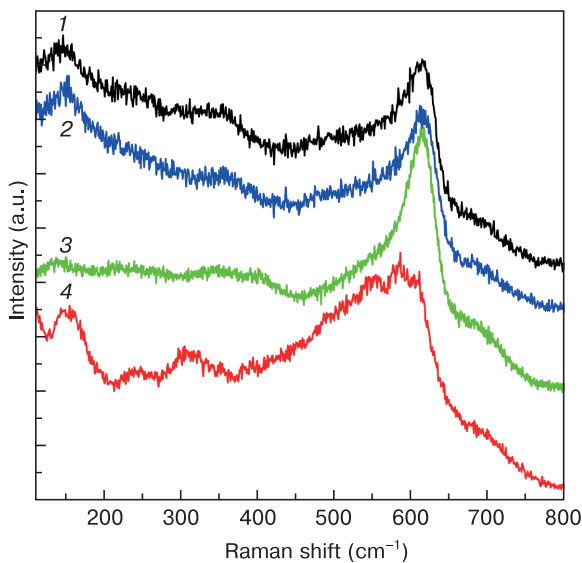
ent ceramics show good promise for photonics, micro- and nanoelectronics industries etc. [6].

At normal pressure zirconia have three polymorphic modifications: monoclinic, tetragonal and cubic which are stable in different temperature ranges. Stabilization of the high-temperature tetragonal and cubic phases at room temperature is usually achieved by doping with alkaline-earth and rare-earth elements, yttrium or scandium [7–9]. The composition, synthesis and heat treatment conditions of zirconia based solid solutions affect their phase composition, structure, thermal and electrophysical properties [10–12].

ZrO<sub>2</sub> based solid solutions are also widely used as heat-insulating protective coatings. These coatings can be operated at high temperatures and should have low heat conductivity and good mechanical properties for long-term operation [13–16].

Many types of crystals having a disordered structure including zirconia based solid solutions have low heat conductivity over a wide range of temperatures ( $0.1 < T < 300$  K) which is typical of amorphous materials [17]. This probably indicates a significant contribution of phonon scattering to the heat conductivity mechanism [18–22]. Heterovalent substitution of the Zr<sup>4+</sup> cations by stabilizing oxide R<sup>3+</sup> ones produces various types of defects (oxygen vacancies, R<sup>3+</sup> cations and defect complexes) [23–26]. The structural defects affect the intensity of phonon scattering intensity in the zirconia based solid solutions. Therefore the heat conductivity of these solid solutions can depend on the type and concentration of the stabilizing oxide.

Typically the thermophysical properties of the zirconia based materials are studied for ceramic specimens [10]. Single crystals in the study of the effect of the structure on the heat conductivity of the material provide data that are free from the effect of grain boundaries, pores and other features that are inherent to polycrystalline ceramics.



**Figure 1.** Raman spectra of crystals: (1) 10GdSZ, (2) 10YSZ, (3) 10YbSZ and (4) 10ScSZ

The heat conductivity of cubic and tetragonal single crystal solid solutions of ZrO<sub>2</sub>–Y<sub>2</sub>O<sub>3</sub> was studied earlier [27–28]. The temperature dependence of the heat conductivity was analyzed taking into account the phase composition, local structural features and electrophysical parameters of the single crystals. It was shown that the heat conductivity of the zirconia based solid solutions varies for different Y<sub>2</sub>O<sub>3</sub> concentrations and consequently different number of vacancies.

The aim of this work was to study the effect of the stabilizing cation (Gd, Yb, Sc, Y) on the heat conductivity of ZrO<sub>2</sub> based solid solution single crystals. The stabilizing oxide concentration in the test solid solutions was 10 mol.%.

## 2. Experimental

(ZrO<sub>2</sub>)<sub>0.9</sub>(R<sub>2</sub>O<sub>3</sub>)<sub>0.1</sub> solid solution crystals where R = (Gd, Yb, Sc, Y), (ZrO<sub>2</sub>)<sub>0.9</sub>(Sc<sub>2</sub>O<sub>3</sub>)<sub>0.09</sub>(Gd<sub>2</sub>O<sub>3</sub>)<sub>0.01</sub> and (ZrO<sub>2</sub>)<sub>0.9</sub>(Sc<sub>2</sub>O<sub>3</sub>)<sub>0.09</sub>(Yb<sub>2</sub>O<sub>3</sub>)<sub>0.01</sub> were grown using directional melt crystallization in a cold skull (130 mm diam.) at a 10 mm/h rate [29] on a Kristall-407 plant (frequency – 5.28 MHz, maximum output power 60 kW). The 6 kg charge was prepared from at least 99.99% purity ZrO<sub>2</sub>, Y<sub>2</sub>O<sub>3</sub>, Gd<sub>2</sub>O<sub>3</sub>, Yb<sub>2</sub>O<sub>3</sub> и Sc<sub>2</sub>O<sub>3</sub> powders.

The phase composition of the specimens was studied using X-ray diffraction on a Bruker D8 instrument and Raman scattering. The excitation source was a 633 nm laser.

The heat conductivity of the crystals was studied using the absolute steady-state technique of longitudinal heat flow in the 50–300 K range. The absolute heat conductivity determination error was within ± 6%. The 7×7×20 mm specimens were cut from the crystals along the growth axis and had an arbitrary crystallographic orientation.

## 3. Results and discussion

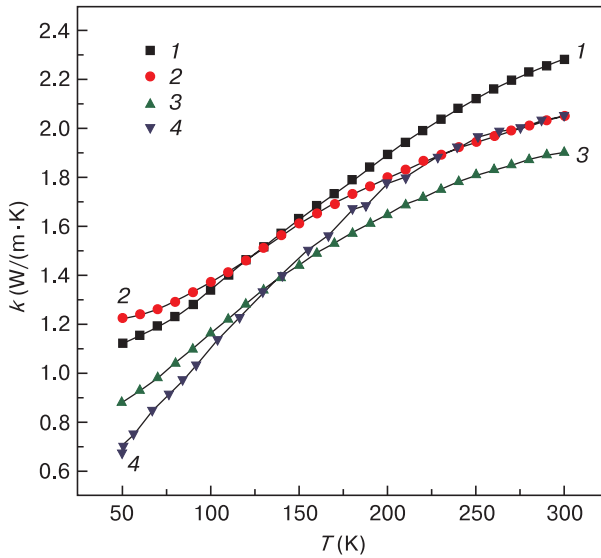
Two series of crystals were grown: ZrO<sub>2</sub> solid solutions stabilized with 10 mol.% Yb<sub>2</sub>O<sub>3</sub>, Y<sub>2</sub>O<sub>3</sub>, Gd<sub>2</sub>O<sub>3</sub> or Sc<sub>2</sub>O<sub>3</sub> hereinafter denoted as 10YbSZ, 10YSZ, 10GdSZ and 10ScSZ, respectively, and ZrO<sub>2</sub> solid solutions co-stabilized with 9 mol.% Sc<sub>2</sub>O<sub>3</sub> and 1 mol.% Gd<sub>2</sub>O<sub>3</sub> or 1 mol.% Yb<sub>2</sub>O<sub>3</sub> hereinafter denoted as 9Sc1GdSZ and 9Sc1YbSZ, respectively.

The 10ScSZ and 9Sc1GdSZ solid solution crystals were inhomogeneous and light-scattering but contained no pores. The other test specimens were homogeneous and transparent single crystals.

According to X-ray diffraction data the 10YbSZ, 10YSZ and 10GdSZ crystals had a cubic fluorite structure and were single-phase in the entire bulk. The 10ScSZ crystal was a mixture of two phases, i.e., the cubic and rhombohedral ZrO<sub>2</sub> modifications. Figure 1 shows the Raman spectra for the first series of the test single crystals. The spectra of the 10ScSZ crystals indicate the

presence of the rhombohedral phase while the Raman spectra of the 10YbSZ, 10YSZ and 10GdSZ crystals are typical of the cubic phase.

Figure 2 shows the temperature dependences of the heat conductivity  $k(T)$  for the  $ZrO_2$  single crystals stabilized with 10 mol.%  $Yb_2O_3$ ,  $Y_2O_3$ ,  $Gd_2O_3$  or  $Sc_2O_3$ .



**Figure 2.** Heat conductivity of crystals as a function of temperature: (1) 10YSZ, (2) 10YbSZ, (3) 10GdSZ and (4) 10ScSZ

As can be seen from the data in Fig. 2 the 10ScSZ crystal has the lowest heat conductivity in the 50 to 150 K range. The low heat conductivity of this single crystal originates from its phase composition, i.e., the presence of a mixture of the cubic and rhombohedral  $ZrO_2$  modifications. It should be noted that the  $ZrO_2$ – $Sc_2O_3$  system is more complex than the  $ZrO_2$ – $R_2O_3$  ( $R = Y, Yb, Gd$ ) systems from the viewpoint of phase composition and phase transitions. Unlike the  $ZrO_2$ – $R_2O_3$  ( $R = Y, Yb, Gd$ ) solid solutions having a cubic structure over a relatively wide range of concentrations the cubic solid solutions of the  $ZrO_2$ – $Sc_2O_3$  system exist in a narrow concentration range, from ~ 8 to 12 mol.%  $Sc_2O_3$  [30–32]. There are several variants of  $ZrO_2$ – $Sc_2O_3$  phase diagrams which show different phase boundaries. As shown in a number of earlier works [33–36] zirconia stabilization by oxides with different cation radii leads to the formation of different defect structures in the solid solution, both in the anion and in the cation sublattices. It was shown that in crystals with a large cation radius (e.g.  $Y^{3+}$ ,  $Gd^{3+}$ ) the oxygen vacancies occupy predominantly the first coordination shell of the  $Zr^{4+}$  ions and the second coordination shell of the big cations. In solid solutions with a small ionic radius close to that of the matrix cation (e.g.  $Sc^{3+}$ ,  $Yb^{3+}$ ) the oxygen vacancies may occupy the first and second coordination shells of the  $Zr^{4+}$  ions with the same probability, leading to a higher disorder of the solid solution structure. With an increase in the stabilizing oxide concentration the formation of defect complexes, ordering of the cation and anion sublattices and the formation

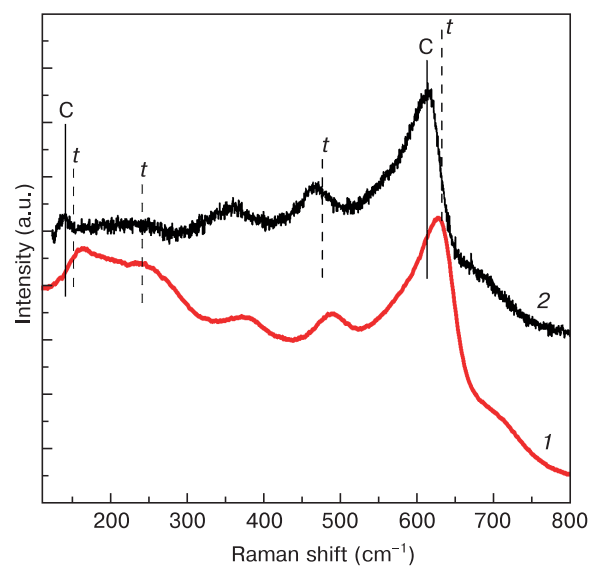
of new phases are controlled by the ionic radius of the stabilizing oxide cation [37].

Despite the difference in the low temperature heat conductivities (50–150 K) for the 10YbSZ and 10ScSZ crystals due to their different phase compositions, an increase in temperature makes their heat conductivities almost equal at 300 K. The small ionic radii of the  $Sc^{3+}$  and  $Yb^{3+}$  cations entail the variety of possible defect structures and a higher disordering of the cation and anion sublattices [37] and cause strong phonon scattering which remains intense with an increase in temperature. The difference in the weights of the  $Sc^{3+}$  and  $Yb^{3+}$  cations affects the heat conductivity of the crystals to a far less extent.

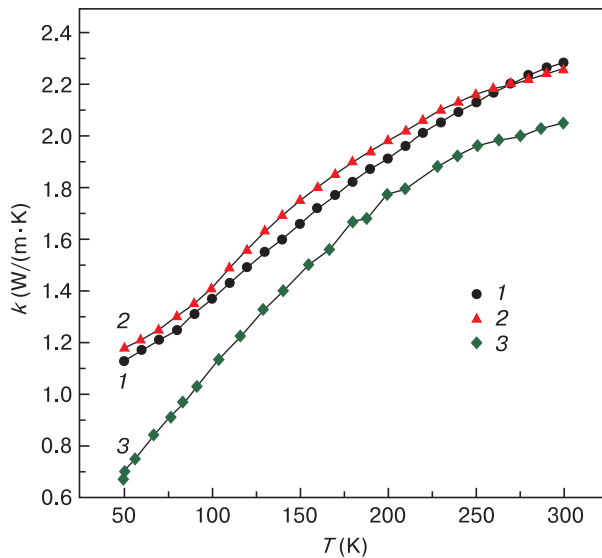
The low-temperature heat conductivities of the 10GdSZ crystals are higher than those of the 10ScSZ crystals. However in the 150–300 K range the heat conductivities of the 10GdSZ crystals are the lowest for this test series of specimens. The size of the  $Gd^{3+}$  cations is greater than those of  $Y^{3+}$ ,  $Yb^{3+}$  and  $Sc^{3+}$ , and this may cause greater stress and disorder in the anion sublattice and entail a lower heat conductivity of the 10GdSZ crystals as compared with those of other solid solutions at 300 K.

Zirconia is often stabilized with several oxides for the modification of the structure and physico-chemical properties of its solid solutions [13, 14, 20, 21]. We studied the heat conductivity of the material for gadolinium and ytterbium co-doping of the scandia-stabilized solid solutions. The heat conductivity of the 9Sc1GdSZ and 9Sc1YbSZ crystals was compared with that of the 10ScSZ crystals having the same stabilizing oxide concentration (10 mol.%) and hence the same number of oxygen vacancies produced by heterovalent substitution.

According to phase analysis the 9Sc1GdSZ crystals were a mixture of the tetragonal and cubic  $ZrO_2$  modifications. The 9Sc1YbSZ crystals had a cubic fluorite structure. Figure 3 shows the Raman spectra of the 9Sc1GdSZ and 9Sc1YbSZ crystals.



**Figure 3.** Raman spectra of crystals: (1) 9Sc1YbSZ and (2) 9Sc1GdSZ



**Figure 4.** Heat conductivity of crystals as a function of temperature  $k(T)$ : (1) 9Sc1GdSZ, (2) 9Sc1YbSZ and (3) 10ScSZ

Thus substitution of 1 mol.%  $\text{Sc}_2\text{O}_3$  in the 10ScSZ crystals for 1 mol.%  $\text{Gd}_2\text{O}_3$  or  $\text{Yb}_2\text{O}_3$  produces crystals with different phase compositions.

Figure 4 shows the temperature vs heat conductivity function  $k(T)$  for the 9Sc1GdSZ and 9Sc1YbSZ crystals. The temperature vs heat conductivity function for the 10ScSZ solid solution is shown for comparison.

The heat conductivities of the 9Sc1GdSZ and 9Sc1YbSZ crystals are close and higher than those of the 10ScSZ crystals in the entire experimental temperature range.

Thus zirconia co-doping with two types of stabilizing oxide may change the pattern of the  $k(T)$  function and the heat conductivity in comparison with that of the crystals stabilized by sole scandia. Zirconia co-doping with two stabilizing oxides while retaining the total stabilizing oxide concentration (10 mol.%) should change the defect structure of the cation sublattice. Co-doping with oxides one of which has a small ionic radius ( $R_{\text{Sc}^{3+}} = 0.87$ ) and the other one is a big cation ( $R_{\text{Gd}^{3+}} = 1.053$ ) changes the stress pattern in the crystal lattice. Furthermore this entails a change in the formation of defect complexes: a statistical distribution of oxygen vacancies relative to the

$\text{Zr}^{4+}$  and  $\text{Sc}^{3+}$  cations changes to a distribution for which the oxygen vacancies are predominantly located in the vicinity of the bigger stabilizing oxide cation  $\text{Gd}^{3+}$ . For co-doping with oxides both of which have small ionic radii ( $R_{\text{Sc}^{3+}} = 0.87$  and  $R_{\text{Yb}^{3+}} = 0.985$ ) these changes are far less intense. Furthermore the heat conductivity of the crystals also depends on its phase composition.

A change in the phase composition of the 9Sc1GdSZ and 9Sc1YbSZ crystals increases their heat conductivity in comparison with that of the 10ScSZ crystals. Phonon scattering caused by the difference in the radii and weights of the cations has a smaller effect on the heat conductivity.

## 4. Conclusion

$(\text{ZrO}_2)_{0.9}(\text{R}_2\text{O}_3)_{0.1}$  solid solution crystals where  $R = (\text{Gd}, \text{Yb}, \text{Sc}, \text{Y})$ ,  $(\text{ZrO}_2)_{0.9}(\text{Sc}_2\text{O}_3)_{0.09}(\text{Gd}_2\text{O}_3)_{0.01}$  and  $(\text{ZrO}_2)_{0.9}(\text{Sc}_2\text{O}_3)_{0.09}(\text{Yb}_2\text{O}_3)_{0.01}$  were grown using directional melt crystallization in a cold skull. The stabilizing oxide concentration in the test solid solutions was 10 mol.%.

The heat conductivity of the  $\text{ZrO}_2$  based solid solutions depends largely on the phase composition of the crystals. The presence of a mixture of the cubic and rhombohedral  $\text{ZrO}_2$  modifications in the  $(\text{ZrO}_2)_{0.9}(\text{Sc}_2\text{O}_3)_{0.1}$  crystals leads to the lowest heat conductivity of these crystals in the 50–100 K range compared with the other test crystal compositions. At 300 K the difference in the weights of the  $\text{Sc}^{3+}$  and  $\text{Yb}^{3+}$  cations has little if any effect on the heat conductivity. The ionic radius of the stabilizing cation has the greatest effect on the heat conductivity.

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