THERMAL EXPANSION, MECHANICAL AND OPTICAL PROPERTIES OF GALLIUM AND ALUMINUM SUBSTITUTED Zn_2TiO_4 SPINELS

Perfler, L.[1], Kahlenberg, V.[1], Jakopic, G.[2], Schaur, A.[3], Tribus, M.[1], Schmidmair, D.[1], Kaindl, R.[4]

[1]Institute of Mineralogy and Petrography, University of Innsbruck, Innrain 52f, 6020 Innsbruck, Austria
[2]MATERIALS – Institute for Surface Technologies and Photonics, JOANNEUM RESEARCH Forschungsgesellschaft mbH, Franz-Pichler-Straße 30, 8160 Weiz, Austria
[3]Institute for Structural Engineering and Material Sciences, Material Technology Innsbruck, University of Innsbruck, Technikerstr. 11/19a, 6020 Innsbruck, Austria
[4]MATERIALS – Institute for Surface Technologies and Photonics, JOANNEUM RESEARCH Forschungsgesellschaft mbH, Leobner Straße 94, 8712 Niklasdorf, Austria
Lukas.Perfler@uibk.ac.at

Polycrystalline samples of new $Zn_{1.75}Ti_{0.75}Ga_{0.5}O_4$, $Zn_{1.5}GaTi_{0.5}O_4$, and $Zn_{1.75}Ti_{0.75}Al_{0.5}O_4$ spinel were prepared by solid-state reactions in platinum crucibles and closed platinum capsules at 1523 K and 1623 K, respectively. The chemical composition of the colorless crystals was determined by wavelength-dispersive X-ray spectroscopy. Phase analysis and structural investigations were carried out by high-resolution powder X-ray diffraction and Raman spectroscopy. Crystal structure refinements of the inverse spinels $Zn_{1.75}Ti_{0.75}Al_{0.5}O_4$, $Zn_{1.5}GaTi_{0.5}O_4$, and $Zn_{1.75}Ti_{0.75}Ga_{0.5}O_4$ resulted in the following basic crystallographic data: cubic, *Fd*-3*m*, a = 8.37810(1) Å, V = 588.079(3) Å^3; a = 8.405473(8) Å, V = 593.863(2) Å^3 and a = 8.44015(1) Å, V = 601.244(2) Å^3, Z = 8. In addition, *in situ* high-temperature powder X-ray diffraction experiments enabled the investigation of the thermal expansion of the new spinel-type compounds. For sample preparation, required for further material analysis, the sintered tablets and fragments were embedded in epoxy resin and polished to a mirror-like surface finish. To determine the mechanical properties, nanoindentation experiments were performed with a Berkovich diamond indenter tip. Analyses of the load–displacement curves revealed a high hardness ranging from 10.2 ± 0.4 GPa to 11.8 ± 0.5 GPa and a reduced elastic modulus of 162 ± 5 GPa up to 178 ± 6 GPa. Furthermore, the optical properties of the spinel-type materials were studied by spectroscopic ellipsometry in the wavelength between 250 and 1000 nm. All materials exhibit a high refractive index ranging from n = 2.20 to n = 2.10 at 430.8 nm (Fraunhofer G line) with a similar low dispersion (0.09 to 0.07, n_G–n_B).