Thermodynamic Properties of the Crystalline Phosphate $Ni_{0.5}Zr_2(PO_4)_3$

V.I. Pet′kov[1,C], V.N. Loshkarev[2], M.V. Sukhanov[1], I.A. Schelokov[1], and E.A. Asabina[1,S]

[1]*Department of Chemistry, Nizhni Novgorod State University, Nizhniy Novgorod, Russia*
petkov@uic.nnov.ru

[2]*Russian Federal Nuclear Center - All-Russian Research Institute of Experimental Physics, Nizhni Novgorod, Sarov, Russia*

The phosphates having structural frameworks $[L_2(PO_4)_3]p-$ is already known for its flexibility with regard to ionic substitution and useful physico-chemical properties. Extremely wide variations of cation composition with the conservation of crystallographic characteristics permit to create new materials with stability to high temperatures, pressures and aggressive media, near-zero thermal expansion, low thermal conductivity, and catalytic activity. Phosphate $Ni_{0.5}Zr_2(PO_4)_3$ was synthesized by sol-gel method starting from aqueous solutions of $NiCl_2$, $ZrOCl_2$ and H_3PO_4. The compound belongs to the $Sc_2(WO_4)_3$ type family. Phase purity of the obtained compounds was checked by X-ray diffractometry and IR spectroscopy. Chemical compositions were determined by electron microprobe and chemical analysis. The heat capacity of the sample was measured using a low temperature adiabatic vacuum calorimeter (7-350 K) and differential scanning calorimeters (330-1000 K). The heat capacity of the phosphate increases monotonically over the entire temperature range studied. The main thermodynamic functions $H^0(T)-H^0(0)$, $S^0(T)$, $G^0(T)-H^0(0)$ in the range 0-1000 K were calculated, the standard entropy of its formation at 298.15 K was determined. The fractal dimension for the crystalline phosphate $Ni_{0.5}Zr_2(PO_4)_3$ between 20 K and 50 K was found to be 3, that corresponds to spatial (three-dimensional) structure of the compound. The thermal conduction behavior of $Ni_{0.5}Zr_2(PO_4)_3$ ceramic in the range 298-600 K was studied. The material exhibits lower values of thermal conductivity compared with partially stabilized zirconia, which is a leading thermal barrier material in use today and has thermal conductivities above 20 W/(m K).

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