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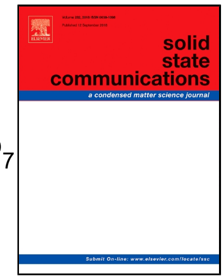

Phase transition and near-zero thermal expansion properties of $Zr_{0.5}Hf_{0.5}V_{2-x}P_xO_7$ (0≤x≤1.2)

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Phase transition and near-zero thermal expansion properties of $Zr_{0.5}Hf_{0.5}V_{2-x}P_xO_7$ (0≤x≤1.2)

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Abstract: In the study, $Zr_{0.5}Hf_{0.5}V_{2-x}P_xO_7$ (0≤x≤1.2) was prepared by solid state method and then the microstructure of synthesized samples was investigated. The microstructure, coefficient of thermal expansion (CTE) and phase transition of $Zr_{0.5}Hf_{0.5}V_{2-x}P_xO_7$ (0≤x≤1.2) were investigated with thermal dilatometry, x-ray diffraction (XRD) and Raman spectroscopy. The results showed that the samples were single cubic phase with the space group of $Pa\overline{3}$ in the crystal structure. When the substitution rate of P^{5+} was higher than 0.6, the 3×3×3 superstructure disappeared. The expansion coefficient of $Zr_{0.5}Hf_{0.5}V_{1.2}P_{0.8}O_7$ was calculated to be -0.53×10^{-6} K^{-1} under the linear thermal expansion in a very wide temperature range from 300 to 573 K. With the increase of P^{5+} content, the temperatures of positive-to-negative thermal expansion of $Zr_{0.5}Hf_{0.5}V_{2-x}P_xO_7$ firstly even decreased below room temperature and then increased. The synthesized $Zr_{0.5}Hf_{0.5}V_{2-x}P_xO_7$ exhibited near zero thermal expansion behavior in a wide temperature range around room temperature.

Keywords: phase transition, near-zero thermal expansion, $Zr_{0.5}Hf_{0.5}V_{2-x}P_xO_7$, X-ray diffraction (XRD), Raman spectrum

1. Introduction

The negative thermal expansion materials are characterized by abnormal heat shrinkage and cold expansion properties. The materials with negative thermal expansion (NTE), zero expansion, and arbitrary controllable expansion properties in the large temperature range are the basis for manufacturing high-precision equipment and show the wide application prospect in photoelectron, microelectronics, high-performance engines, and aerospace [1–14]. Since Sleight et al. found that cubic ZrW_2O_8 showed the large isotropic negative thermal expansion from 0.3 to 1050 K in 1996 [1], many negative thermal expansion materials had been developed. A wide variety of compounds had been identified as NTE compounds and a series of negative

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