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Development of Materials Based on Phosphates of NaZr2(PO4)3 with Low Thermal Expansion

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Abstract : NaZr2(PO4)3 (NZP) and their structural analogues are characterized by a peculiar behaviors on heating – they have different expansion and contraction along different crystallographic directions due to specific arrangements of crystal structure in these compounds. An important feature of such structures is the ability to incorporate into their structural analogues wide variety of metal cations having different size and oxidation states, with different combinations and concentrations. These cations are located in different crystallographic non-equivalent positions of octahedral tetrahedral crystal framework as well as in inter-framework cavities. Through, due to iso- and hetero-valent isomorphism of the cations (and the anions) in NZP, it becomes possible to tuning the compositions and to obtain the compounds with 'on a plan' properties. For the design of compounds with low and ultra-low thermal expansion including those with tailored thermal expansion properties, the following crystallochemical principles it seems are promising: 1) Insertion into crystal M1 position the cations having different sizes and, 2) the variation in the composition of compounds, providing different occupation of crystal M1 position. Following these principles we have designed and synthesized the next NZP-type phosphates series: a) where radii of the cations in the M1 crystal position was varied: Zr1/4Zr2(PO4)3 - Th1/4Zr2(PO4)3 (series I); R1/3Zr2(PO4)3 where R= Nd, Eu, Er (series II), b) where the occupation of M1 crystal position was varied: Zr1/4Zr2(PO4)3-Er1/3Zr2(PO4)3 (series III) and Zr1/4Zr2(PO4)3-Sr1/2Zr2(PO4)3 (series IV). The thermal expansion parameters were determined over the range of 25-800ºC. For each series the minimum axial coefficient of thermal expansion αa = αb, αc and their anisotropy Δα = Iαa - αcI, 10-6 K-1 was found as next: -1.51, 1.07, 2.58 for Th1/4Zr2(PO4)3 (series I); -0.72, 0.10, 0.81 for Nd1/3Zr2(PO4)3 (series II); -2.78, 1.35, 4.12 for Er1/6Zr1/8Zr2(PO4)3 (series III); 2.23, 1.32, 0.91 for Sr1/2Zr2(PO4)3 (series IV). The measured tendencies of the thermal expansion of crystals were in good agreement with predicted ones. For one of the members from the studied phosphates namely Th1/16Zr3/16Zr2(PO4)3 structural refinement have been carried out at 25, 200, 600, and 800°C. The dependencies of the structural parameters with the temperature have been determined.

Keywords : high-temperature crystallography, NaZr2(PO4)3, (NZP) analogs, structural-chemical principles, tuning thermal expansion
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