Application of the Crystal Chemical Approach to Predicting the Thermal Expansion of Compounds in the NZP Family

V.I. Pet'kov and E.A. Asabina[C,S]
Department of Chemistry, Nizhni Novgorod State University, Nizhni Novgorod, Russia
asea@uic.nnov.ru

B.I. Lazoryak
Department of Chemistry, Moscow State University, Moscow, Russia

The NZP ($NaZr_2(PO_4)_3$) structure predetermines many important properties of substances useful for modern and future technology. In particular, the thermal expansions of many of the NZP compounds are a relatively low (< 2• 10^{-6} K^{-1}) and their values vary from positive to negative. The observed axial thermal expansion and contraction behavior is explained on the basis of the crystal chemistry of the compounds. A system of empirical regularities of thermal expansions for the NZP compounds is proposed in the present work.

The thermal expansion of the Ti-containing materials with NZP-type structure was investigated by high-temperature X-ray powder diffractometry. The thermal expansion coefficients were determined between room temperature and 1273 K. It was shown for concrete situations that the combination of the effect of changing the cations in the framework, the effect of inserting ions into the interstitial positions of the NZP structures, and designing the solid solutions is an effective way to develop ceramics with predictable and controlled thermal expansions (sometimes with ultra low values) under anisotropy approaching zero.