21-Crystallography at Non-Ambient Temperatures and/or Pressures; Phase Transitions

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PS-27.01.12 ANISOTROPIC THERMAL EXPANSION CHARACTERISTICS OF SrZr2(PO4)6·2K2ZrF7(P2O7). SYSTEM CERAMIC MATERIALS BY X-RAY DIFFRACTION. By Chang-lin Kuo, Rong-fa Guo, Yue-hong Huang and Hui-ming Chen, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai, P.R. China.

Some of the compounds in strontium (potassium) zirconium phosphate silicate system are kinds of ceramic materials having ultra-low-thermal expansion and high-thermal shock-resistant properties (S. Y. Limaye, Patent, 1990: WO 90 12,766). These compounds normally crystallize in the hexagonal crystal system, and are characterized by only two principal thermal expansion coefficients, parallel and normal to the e or X axis.

An accurate value of the lattice parameter of the compounds in SrZr2(PO4)6·2K2ZrF7(P2O7) system have been determined at different temperatures, ranging from 293 to 1700 K, by X-ray powder diffraction. Unit-cell dimensions of seven compositions [K2Sr2Zr4(PO4)6, X = 0.6, 0.5, 0.4, 0.3, 0.2, 0.1, 0.0] at each temperature were obtained by the method of least-squares based on the measurement of 8-16 unambiguously indexed reflections recorded in the 2θ angle region 80 to 120° using a Rigaku-Denki high-temperature stage mounted on a 12 kW rotating anode X-ray generator with Cu Kα radiation (λ=1.54059 Å).

The lattice parameters were found to vary non-linearly with temperature and the dependence has been expressed by the third-order polynomial relations of the form:

$$a = a_0 + a_1 T + a_2 T^2 + a_3 T^3$$

(T in K)

Least-squares fit of the experimental data has led to the analytical expression results. For example, the lattice parameters of SrZr2(PO4)6 are as follows:

$$a = 8.6825 \times 10^{-2} - 1.0953 \times 10^{-2} T + 2.4105 \times 10^{-12} T^2$$

$$c = 23.4016 - 3.8332 \times 10^{-2} T + 1.0007 \times 10^{-12} T^2 - 3.0210 \times 10^{-17} T^3$$

The data have been used to evaluate the coefficients of thermal expansion at various temperatures. The temperature dependence of the coefficient of expansion can be represented by the equation

$$\alpha = 2.2703 \times 10^{-4} T - 2.5213 \times 10^{-17} T^2 + 8.3322 \times 10^{-17} T^3$$

$$\alpha_\text{e} = -1.639 \times 10^{-4} + 8.5536 \times 10^{-17} T^2 - 3.8734 \times 10^{-17} T^3$$

The relative percent thermal linear expansions are

$$\left[\frac{\Delta L}{L}\right]_T = 0.0679 \times 10^{-4} T - 1.261 \times 10^{-17} T^2 + 2.774 \times 10^{-17} T^3$$

$$\left[\frac{\Delta L}{L}\right]_e = 0.0145 \times 10^{-4} T + 4.277 \times 10^{-17} T^2 - 1.291 \times 10^{-17} T^3$$

The thermal expansion coefficients of all seven compositions were determined. Two principal thermal expansion coefficients of the compounds X ≤ 0.3 above room temperature are positive, but for X ≥ 0.8, they are negative. However, for compound K2Sr2Zr4(P2O7)(X = 0.6), one coefficient a0 is positive, and the other one a3 is negative. Therefore, the average thermal expansion of the bulk material of the compound X = 0.6 is lower than that of the other compositions. The measuring thermal expansion coefficients (ΔL/ΔT X°C) of different composition compounds by dilatometers method at temperature 700 K are:

- X = 0.2, a0 = 2.65; a3 = 1.74; X = 0.6, a0 = 0.16, a3 = 5.02. These results agree with the conclusion obtained from the X-ray diffraction method.

PS-21.01.13 THE EQUATION-OF-STATE OF Pd4, AT HIGH PRESSURE AND A HYDROSTATIC REGION IN THE DIAMOND ANVIL CELL

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ABSTRACT

The lattice constants of Pd4 were measured by X-ray diffraction in a diamond anvil cell up to average 111 GPa with peak pressure about 144 GPa. Results fitted to a Murnaghan equation for Pd4 yield values for the bulk modulus KB and its pressure dependence Kp of 198.5 GPa and 5.09, respectively. In addition, the R1, R2 splitting in the ruby fluorescence indicates the existence of a small hydrostatic region (about 1 micrometer) in the center of the culet surface of a diamond anvil.