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PS–21.01.12 ANISOTROPIC THERMAL EXPANSION CHARACTERISTICS OF $SrZr_4(PO_4)_6$--$KZr_2(PO_4)_3$ 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 ultralow-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 c or Z axis.

An accurate value of the lattice parameter of the compounds in $SrZr_4(PO_4)_6$--$KZr_2(PO_4)_3$ system have been determined at different temperatures, ranging from 293 to 1300 K, by X-ray powder diffraction. Unit-cell dimensions of seven compositions [$K_{2x}Sr_{1-x}Zr_4(PO_4)_6$, x=0,0.2,0.4,0.5,0.6,0.8,1.0] 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 K_a radiation (λ_{Ka1} = 1.540598Å).

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:

$$a_T = a_0 + a_1T + a_2T^2 + a_3T^3 \qquad (T \text{ in } K)$$

Least-squares fit of the experimental data has led to the analytical expression results. For example, the lattice parameters of $SrZr_4(PO_4)_6$ are as follows

$$a = 8.6825 + 1.9725 \times 10^{-5}T - 1.0953 \times 10^{-9}T^2 + 2.4105 \times 10^{-12}T^3$$
$$c = 23.4016 - 3.8332 \times 10^{-5}T + 1.0007 \times 10^{-7}T^2 - 3.0210 \times 10^{-11}T^3$$

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

$$\alpha_a = 2.2703 \times 10^{-6} - 2.5213 \times 10^{-10}T + 8.3232 \times 10^{-13}T^2$$
$$\alpha_c = -1.6382 \times 10^{-6} + 8.5536 \times 10^{-9}T - 3.8734 \times 10^{-12}T^2$$

The relative percent thermal linear expansions are

$$\left(\frac{\Delta L}{L_o}\right)_a = -0.0679 + 2.2703 \times 10^{-4}T - 1.261 \times 10^{-8}T^2 + 2.774 \times 10^{-11}T^3$$

$$\left(\frac{\Delta L}{L_o}\right)_c = 0.0145 - 1.6382 \times 10^{-4}T + 4.277 \times 10^{-7}T^2 - 1.291 \times 10^{-10}T^3$$

The thermal expansion coefficients of all seven compositions were determined. Two principal thermal expansion coefficients of the compounds $X \le 0.5$ above room temperature are positive, but for $X \ge 0.8$, they are negative. However, for compound $K_{1.2}Sr_{0.4}Zr_4(PO_4)_6$ (X=0.6), one coefficient α_a is positive, and the other one α_c 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 cofficients (all $\times 10^{-6}/°C$) of different composition compounds by dilatometers method at temperature 700 K are: X=0.2,α=2.65; X=0.4,α=1.74; X=0.6,α=-0.16; X=0.8, α=-5.02. These results agree with the conclusion obtained from the X-ray diffraction method.

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THE EQUATION-OF-STATE OF PdD_x AT HIGH PRESSURE AND A HYDROSTATIC REGION IN THE DIAMOND ANVIL CELL

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ABSTRACT

The lattice constants of PdD_x 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 PdD_x yield values for the bulk moduli K_o and its pressure dependence K_o' of 198.5 GPa and 5.09, respectively. In addition, the R_1-R_2 splitting in the ruby fluorescence indicates the existence of a small hydrostatic region (about 1 micr-meter) in the center of the culet surface of a diamond anvil.