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

PS-27.01.12 ANISOTROPIC THERMAL EXPANSION CHARACTERISTICS OF SrZr$_2$(PO$_4$)$_3$-KZr$_2$(PO$_4$)$_3$ SYSTEM. CERAMIC MATERIALS BY X-RAY DIFFRACTION. By Chang-lin Kuo*, Rong-fa Guo, Yue-he Huang and Hui-ming Chen, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghahi, 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$_2$(PO$_4$)$_3$-KZr$_2$(PO$_4$)$_3$ system have been determined at different temperatures, ranging from 293 to 1700 K, by X-ray powder diffraction. Unit-cell dimensions of seven compositions \[ K_xSr_{1-x}Zr_2(PO_4)_3 \] \( (x=0.0,0.2,0.4,0.5,0.6,0.8,1.0) \) 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$_\alpha$ radiation \((\lambda=1.540598\AA)\).

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:

\[
a_r = a_0 + a_1T + a_2T^2 + a_3T^3 \quad (T \text{ in K})
\]

Least-squares fit of the experimental data has led to the analytical expression results. For example, the lattice parameters of SrZr$_2$(PO$_4$)$_3$ are as follows:

\[
a = 8.6825 \times 10^{-2} - 1.0953 \times 10^{-2}T + 2.4105 \times 10^{-1}T^2 - 3.0210 \times 10^{-3}T^3
\]

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

\[
a_r = 2.2703 \times 10^{-4} - 5.2113 \times 10^{-1}T + 8.3232 \times 10^{-1}T^2 - 3.8734 \times 10^{-2}T^3 + 8.5536 \times 10^{-4}T^3
\]

The relative percent thermal linear expansions are

\[
\frac{\Delta L}{L_0} = -0.0679 \times 10^{-4}T + 1.261 \times 10^{-4}T^2 + 2.774 \times 10^{-3}T^3
\]

\[
\frac{\Delta L}{L_0} = -0.0145 \times 10^{-4}T + 4.277 \times 10^{-4}T^2 - 1.291 \times 10^{-3}T^3
\]

The thermal expansion coefficients of all seven compositions were determined. Two principal thermal expansion coefficients of the compounds \(X \leq 0.3 \) above room temperature are positive, but for \(X > 0.8\), they are negative. However, for compound K$_x$Sr$_{1-x}$Zr$_2$(PO$_4$)$_3 (X=0.6)$, one coefficient \(\alpha_1\) is positive, and the other one \(\alpha_2\) 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 \((\Delta L \times 10^{-5}/°C)\) of different composition compounds by dilatometers method at temperature 700 K are: \(X=0.2, \alpha_1=2.65; \alpha_2=-0.16; X=0.8, \alpha_1=5.02\). These results agree with the conclusion obtained from the X-ray diffraction method.

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PS-27.01.13 THE EQUATION-OF-STATE OF PdD$_4$ AT HIGH PRESSURE AND A HYDROSTATIC REGION IN THE DIAMOND ANVIL CELL.

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ABSTRACT

The lattice constants of PdD$_4$ 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$_4$ yield values for the bulk modulus \(K_0\) and its pressure dependence \(K'_0\) 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 micron-meter) in the center of the culet surface of a diamond anvil.

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