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Panguite, $(Ti^{4+},Sc,Al,Mg,Zr,Ca)_{1.8}O_3$, a new ultra-refractory titania mineral from the Allende meteorite: Synchrotron micro-diffraction and EBSD

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Abstract

Panguite (IMA 2010-057), $(Ti^{4+},Sc,Al,Mg,Zr,Ca)_{1.8}O_3$, is a new titania, occurring as fine-grained crystals with Ti-rich davisite in an ultra-refractory inclusion within an amoeboid olivine inclusion from the Allende CV3 carbonaceous chondrite. The phase was characterized by SEM, EBSD, synchrotron micro-diffraction, micro-Raman spectroscopy, and EPMA. The mean chemical composition of the type panguite is (wt%) TiO_2 47.97, ZrO_2 14.61, Sc_2O_3 10.67, Al_2O_3 7.58, MgO 5.54, Y_2O_3 5.38, CaO 3.34, SiO_2 1.89, FeO 1.81, V_2O_3 0.95, Cr_2O_3 0.54, HfO_2 0.28, sum 100.56 with a corresponding empirical formula calculated on the basis of 3 O atoms of $[(Ti_{0.79}Zr_{0.16}Si_{0.04})^{4+}_{\Sigma 0.99}(Sc_{0.20}Al_{0.20}Y_{0.06}V_{0.02}Cr_{0.01})^{3+}_{\Sigma 0.49}(Mg_{0.18}Ca_{0.08}Fe_{0.03})^{2+}_{\Sigma 0.29}]_{\Sigma 1.77}O_3$. Synchrotron micro-Laue diffraction (i.e., an energy scan by a high-flux X-ray monochromatic beam and white beam diffraction) on one type domain at sub-micrometer resolution revealed that panguite is an orthorhombic mineral in space group *Pbca*. The structure is a subgroup of the *Ia*3 bixbyite-type. The cell parameters are $a = 9.781(1)$, $b = 9.778(2)$, and $c = 9.815(1)$ Å, yielding $V = 938.7(1)$ Å^3, $Z = 16$, and a calculated density of 3.746 g/cm^3. Panguite is not only a new mineral, but also a new titania material, likely formed by condensation. It is one of the oldest minerals in the solar system.

Keywords: Panguite, $(Ti^{4+},Sc,Al,Mg,Zr,Ca)_{1.8}O_3$, new ultra-refractory mineral, new titania, Allende meteorite, CV3 carbonaceous chondrite, synchrotron micro-diffraction, EBSD