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A new mineral from the Bellerberg, Eifel, Germany, intermediate between mullite and sillimanite

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Abstract

A mineral intermediate between sillimanite and mullite, tentatively designated as "sillimullite," was studied by electron microprobe analyses and single-crystal X-ray diffraction methods. The chemical compositions derived from the microprobe results and the crystal-structure refinement are $Al_{7.84}Fe_{0.18}Ti_{0.03}Mg_{0.03}Si_{3.92}O_{19.96}$ and $Al_{8.28}Fe_{0.20}Si_{3.52}O_{19.76}$ (Fe is Fe^{3+}) corresponding to *x*-values of 0.02 and 0.12, respectively, in the solid-solution series $Al_{8+4x}Si_{4-4x}O_{20-2x}$ assigning Fe^{3+}, Ti, and Mg to the Al site. The composition derived from microprobe analysis is very close to a stoichiometric sillimanite (with Fe^{3+},Ti, and Mg assigned to Al sites), while the composition derived from diffraction data is midway between sillimanite and Si-rich mullites. The discrepancy is assumed to be caused by the occurrence of amorphous nano-sized SiO_2 inclusions in the aluminosilicate phase not affecting the diffraction data but detected in the microprobe analysis. "Sillimullite" crystallizes in the orthorhombic space group *Pnam* with $a = 7.5127(4)$, $b = 7.6823(4)$, $c = 5.785(3)$ Å, $V = 333.88(4)$ Å^3, $Z = 1$. It has a complete Si/Al ordering at tetrahedral sites like sillimanite but with neighboring double chains of SiO_4 and AlO_4 tetrahedra being offset by ½ unit cell parallel to **c** relative to each other causing the change of the space-group setting from *Pbnm* (sillimanite) to *Pnam*. Difference Fourier calculations and refinements with anisotropic displacement parameters revealed the formation of oxygen vacancies and triclusters as known in the crystal structures of mullite. Final refinements converged at $R1 = 5.9\%$ for 1024 unique reflections with $F_o > 4\sigma(F_o)$. Fe was found to reside predominantly in the octahedral site and with minor amounts in one of the T* sites. Mg and Ti were not considered in the refinements. The crystal studied here is considered to represent a new mineral intermediate between sillimanite and mullite, named "sillimullite."

Keywords: Sillimullite, new mineral, crystal structure, electron microprobe, sillimanite, mullite