

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

REINHARD X. FISCHER^{1,*}, VALERIA TIKHONOVA¹, JOHANNES BIRKENSTOCK¹, LENNART A. FISCHER²,
KLAUS HERRMANN³, KURT MENGEL³ AND HARTMUT SCHNEIDER^{1,4}

¹Fachbereich Geowissenschaften, Universität Bremen, Klagenfurter Strasse, D-28359 Bremen, Germany

²Institut für Mineralogie, Leibniz Universität Hannover, Callinstrasse 3, D-30167 Hannover, Germany

³Institut für Endlagerforschung, TU Clausthal, Adolph-Roemer-Strasse 2A, D-38678 Clausthal-Zellerfeld, Germany

⁴Institut für Kristallographie, Universität zu Köln, Greinstrasse 6 D-50939 Köln, Germany

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 $\text{Al}_{7.84}\text{Fe}_{0.18}\text{Ti}_{0.03}\text{Mg}_{0.03}\text{Si}_{3.92}\text{O}_{19.96}$ and $\text{Al}_{8.28}\text{Fe}_{0.20}\text{Si}_{3.52}\text{O}_{19.76}$ (Fe is Fe^{3+}) corresponding to x -values of 0.02 and 0.12, respectively, in the solid-solution series $\text{Al}_{8+4x}\text{Si}_{4-4x}\text{O}_{20-2x}$ 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, $V = 333.88(4)$ Å³, $Z = 1$. 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 $\frac{1}{2}$ unit cell parallel to \mathbf{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