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Deposit Art Material for

Structural variations in the brownmillerite series $Ca_2(Fe_{2-x}Al_x)O_5$: Single-crystal X-ray diffraction at 25 °C and high-temperature X-ray powder diffraction (25 °C ≤ *T* ≤ 1000 °C)

Günther J. Redhammer,[1,*] Gerold Tippelt,[2] Georg Roth,[1] and Georg Amthauer[2]

[1]Institute of Crystallography, Rheinisch-Westfälische Technische Hochschule Aachen, Jägerstrasse 17/19, D-52056 Aachen, Germany
[2]Institute of Mineralogy, University of Salzburg, Hellbrunnerstrasse 34, A-5020 Salzburg, Austria
[3]Corresponding address: Neuhofen im Innkreis 224/1, A-4910 Ried im Innkreis, Austria

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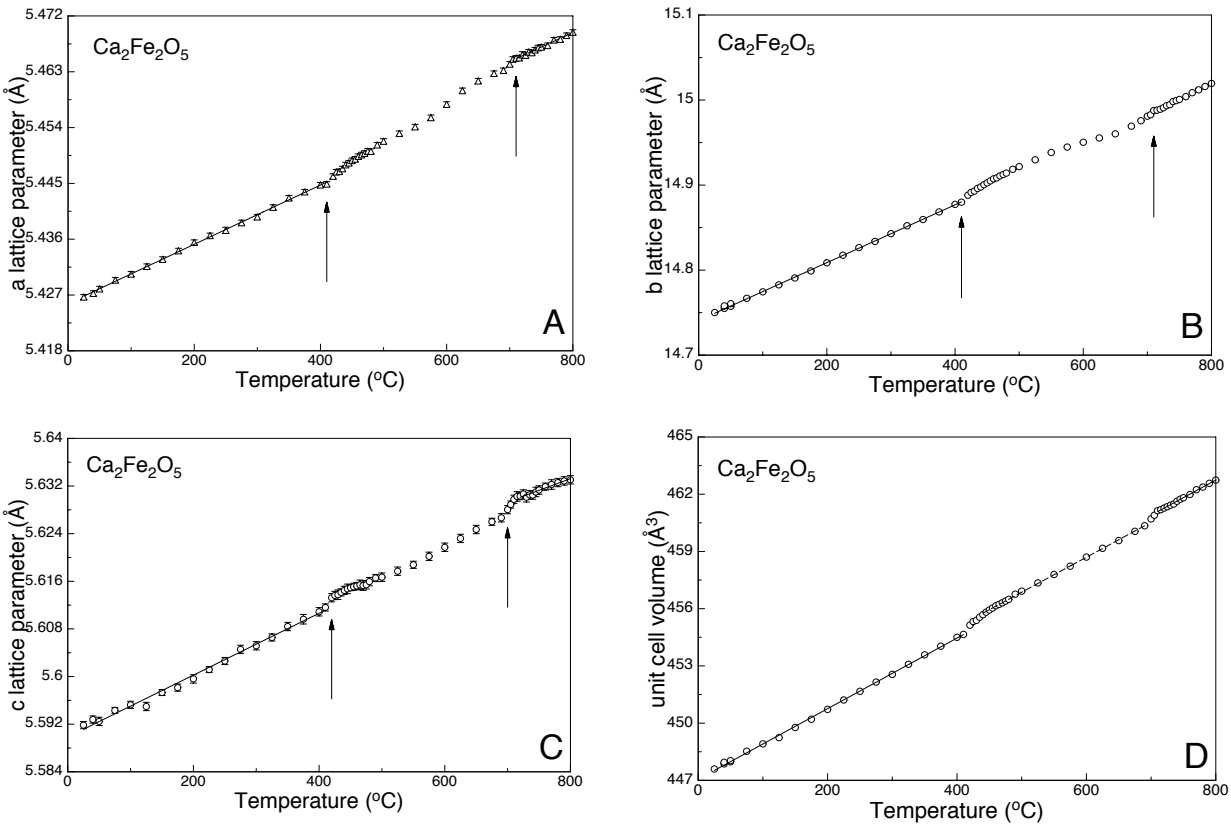
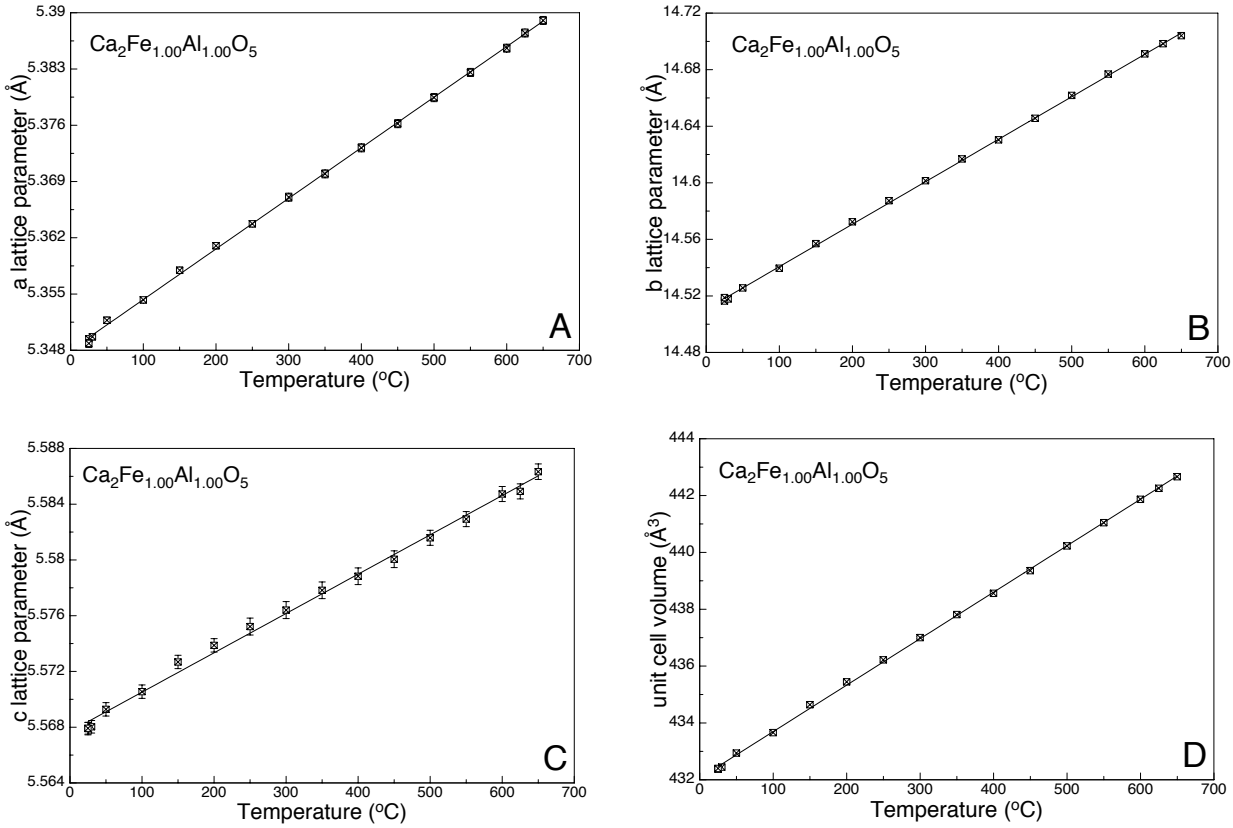
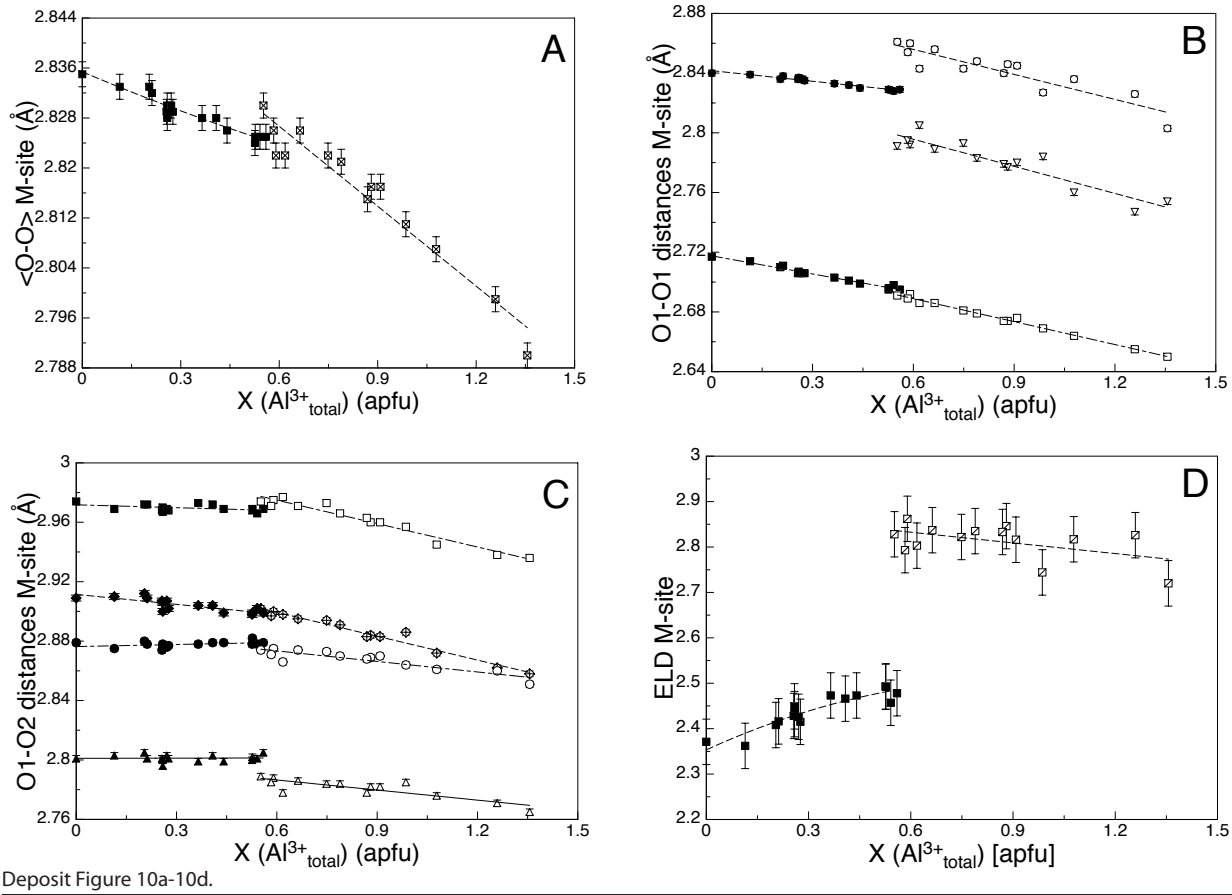


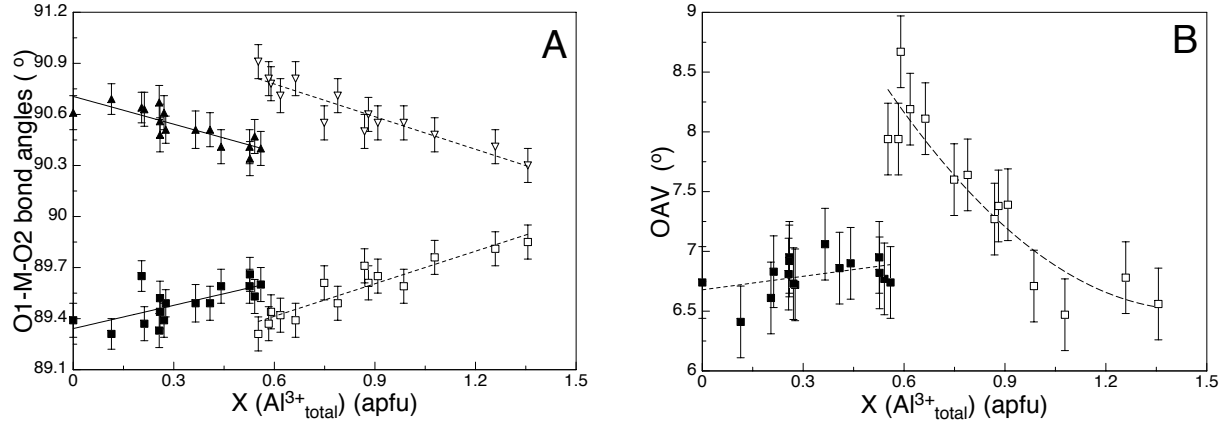
DEPOSIT FIGURE 5. Temperature-dependent evolution of the lattice parameters of $Ca_2Fe_2O_5$ ($x = 0.00$) as determined from powder X-ray diffraction data. Arrows indicate discontinuities related to the magnetic and the crystallographic phase transition ≈430 and 724(2) °C, respectively. Estimated standard deviations are smaller than the symbols.



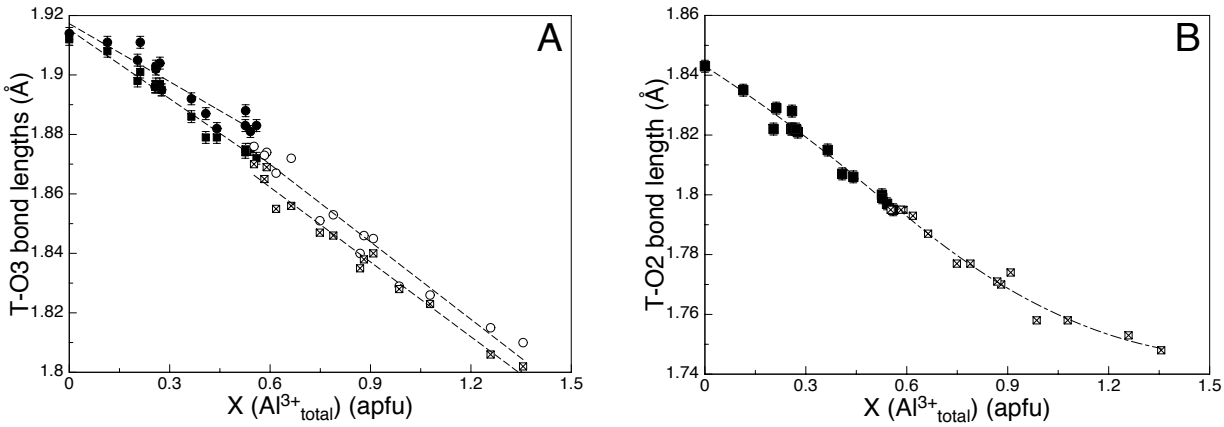
DEPOSIT FIGURE 6. Temperature-dependent evolution of the lattice parameters of Ca_2FeAlO_5 (x = 1.00) as determined from powder X-ray diffraction data.



Deposit Figure 10a-10d.



Deposit Figure 11. O1-M-O2 bond angles (**a**) and quadratic octahedral angle variance (OAV, Robinson et al. 1971) for the $Ca_2Fe_{2-x}Al_xO_5$ solid solution series at 25 °C. Regression curves are fitted to the data and serve as guides to the eye, and the filled and open symbols correspond to *Pnma* and *I2mb* symmetry of the samples.



Deposit Figure 13. Individual (**a**–**b**) and average T-O bond lengths for samples of the $Ca_2Fe_{2-x}Al_xO_5$ solid solution series at 25 °C. Regression curves are fitted to the data and serve as guides to the eye; if not visible, estimated standard deviations are smaller than the symbols, and the filled and open symbols correspond to *Pnma* and *I2mb* symmetry of the samples.

← **Deposit Figure 10.** Average (**a**) and individual O-O atom distances, defining the edge of the $(Fe^{3+},Al^{3+})O_6$ octahedron as well as edge length distortion (ELD) for the $Ca_2Fe_{2-x}Al_xO_5$ solid solution series at 25 °C. Regression lines are fitted to the data and serve as guides to the eye; if not visible, estimated standard deviations are smaller than the symbols, and the filled and open symbols correspond to *Pnma* and *I2mb* symmetry of the samples.