

SFCA-I-type solid solutions in the system $\text{CaO-Fe}_2\text{O}_3\text{-FeO-Al}_2\text{O}_3$ - structural investigations on an iron-ore sintering phase

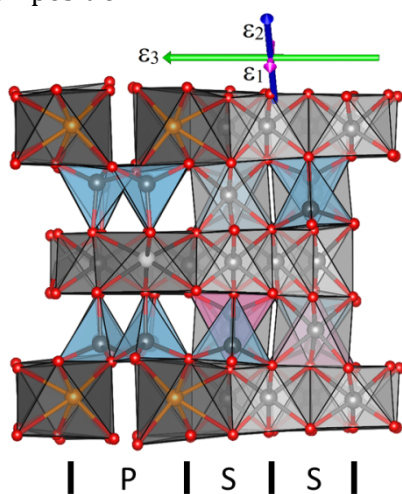
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The present investigation provides - for the first time - a detailed crystallographic analysis on the impact of chemical variations on a compound that is of relevance for the field of applied mineralogy related to the technologically important process of iron-ore sintering.

Effects of $\text{Fe} \leftrightarrow \text{Al}$ substitution on triclinic SFCA-I-type compounds with general formula $\text{A}_{40}\text{O}_{56}$ (A: Ca, Al, Fe^{3+} , Fe^{2+}) have been studied using single-crystal X-ray diffraction. Crystals of sufficient quality and size were synthesized in the temperature range between 1200 and 1300 °C. Six samples with $\text{Al}/\text{Fe}_{\text{Tot}}$ -ratios of 0.127, 0.173, 0.216, 0.310, 0.349 and 0.459, respectively, have been structurally characterized. SFCA-I can be described with a modular approach involving the stacking sequence $\langle \text{PSS} \rangle$ of "P" and "S" modules that can be imagined as being cut from the well-known pyroxene (P) and spinel (S) structure-types. Furthermore, SFCA-I is related to the sapphirine supergroup of minerals.

Within the present solid-solution series the contents in calcium show only minor variations (≈ 6.7 a.p.f.u.). The twenty crystallographically independent tetrahedrally (T) and octahedrally (M) coordinated cation sites exhibit considerable differences concerning the Al-uptake. Indeed, Al is preferentially incorporated into the tetrahedra belonging to the single-chains located in the pyroxene-modules. Ferrous iron, on the other hand, is restricted to one of the T-positions within the spinel-blocks. Most structural aspects, from unit-cell parameters and cell volumes to site occupancies, tetrahedral chain kinking as well as polyhedral distortions are defined by linear or nearly linear trends when plotted against the $\text{Al}/\text{Fe}_{\text{Tot}}$ -ratio. Analysis of the $\langle \text{T-O} \rangle$ and $\langle \text{M-O} \rangle$ distances showed a complex interplay between the different coordination polyhedra resulting in a contrasting behaviour of these values with positive or negative change rates as a function of composition.



Evaluation of the average chemical strain tensor derived from the sets of lattice parameters for the two limiting compositions of the series indicated that the major contraction with increasing Al-content is perpendicular to the pyroxene- and spinel-modules. Furthermore, the pyroxene-module seems to be more effected when compared with the spinel-block. There is evidence that the SFCA-I type solid-solution series is limited on both the Al- and Fe-rich sides.

Fig.1 Orientation of the principal axes of the compositional strain tensor for the SFCA-I solid-solution series and their relations to the pyroxene (P) and spinel (S) blocks. The size of the axes is proportional to the principal strains ϵ_1 , ϵ_2 and ϵ_3 .