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Non-ideality and defectivity of the åkermanite-gehlenite solid solution: An X-ray diffraction and TEM study

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Abstract

This paper reports a structure analysis of the åkermanite-gehlenite solid solution. This solution is non-ideal with a negative excess volume in the entire compositional range. X-ray diffraction shows anomalous behavior of the cell parameters close to the gehlenite end-member ($åk_{08}ge_{92}$, $åk_{35}ge_{65}$). This behavior is correlated with an excess of Si and deficiency of Al with respect to the Mg content, which implies a defective, non-stoichiometric structure with Ca vacancies. Electron microscopy images have confirmed an increase in the defectivity on the atomic scale for Al-rich compositions, and single-crystal structure refinements show a correlated decrease of the tetrahedral volume preferentially occupied by Si. The incommensurate modulation, characteristic of åkermanite, has been observed also in $åk_{95}ge_{05}$, and it is still visible as diffuse scattering in $åk_{75}ge_{25}$. (210) twinning has been observed in the entire compositional range.

Keywords: Melilite, solid solution, X-ray diffraction, electron microscopy