Incommensurately Modulated Structure in Natural Melilites

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Melilite-type compounds have general formula $X_2T1(T2)_2O_7$ (X = Ca, Sr, Pb, Ba, Na, REE; T1 = Be, Mg, Mn^{2+}, Fe^{2+}, Co, Cu, Zn, Al, Fe^{3+}, Si; T2 = Si, Ge, Al, Fe^{3+}, B, Be). Natural members mainly consists of solid-solution between gehlenite, $Ca_2Al_2SiO_7$, and åkermanite, $Ca_2MgSi_2O_7$. The structure, space group $P\bar{4}2_1m$, consists of a linkage of tetrahedral layers connected each other by eight-coordinated X cations. As with peculiar chemical compositions, at room temperature, synthetic melilite-type compounds exhibit weak satellite reflections indicating a two-dimensional incommensurately (IC) modulated structure. To date, the presence of IC reflections in natural samples was only observed in both hardystonite [1] and åkermanite [2]. TEM-EDX investigations proved hardystonite to be chemically slightly inhomogeneous, with detectable IC satellites in the regions where composition approaches the $Ca_2ZnSi_2O_7$ end-member. Stronger and sharper IC satellites were observed in åkermanite. Therefore, a five-dimensional refinement and *in situ* low- and high-temperature (100 - 773 K) studies were carried out using single-crystals of åkermanite. As already observed for synthetic $Ca_2MgSi_2O_7$ [3], the displacive modulation of the atoms is mainly related to a variation of the X cation coordination. On the other hands, with respect to the temperature dependence of the **q** value, strong differences were found between the natural and the synthetic compound.

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