Understanding the Dehydration and Rehydration Pathway of Calcium Monosulfoaluminate

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Calcium monosulfoaluminates ($Ca_4Al_2(OH)_{12}SO_4 \cdot nH_2O$), known in cement research as Alumino-Ferrite mono (AFm) phases, are significant components in Portland cements [1]. These phases form through reactions involving the clinker phase $Ca_3Al_2O_6$ and the hydrated phase ettringite ($Ca_6Al_2(OH)_{12}(SO_4)_3.26H_2O$) or through thermal decomposition of ettringite [2].

The AFm phases, specifically $Ca_4Al_2(OH)_{12}SO_4 \cdot nH_2O$, exhibit layered double hydroxide structures with interlayer variability in water content, with reported values 0<n>6 [3-4]. This structural flexibility allows for different hydration states which are influenced by temperature and relative humidity (RH).

This study investigates the dehydration and rehydration pathways of Calcium Monosulfoaluminate ($Ca_4Al_2(OH)_{12}SO_4 \cdot nH_2O$) using in-situ combined Powder X-ray Diffraction – Differential Scanning Calorimetry (PXRD-DSC), a unique capability in our X-ray diffraction facility, which allows the thermal properties of a material to be directly linked to crystal structure changes. Further investigations on the AFm phases using variable humidity PXRD, and Thermogravimetric Analysis (TGA) are also presented here.

Rehydration experiments using both variable humidity XRPD and variable humidity TGA demonstrated the reversibility of hydration between certain states, with a notable reversible transition between $Ca_4Al_2(OH)_{12}SO_4 \cdot 6H_2O$ (the so-called “12-hydrate” state) and $Ca_4Al_2(OH)_{12}SO_4 \cdot 4H_2O$ (“10-hydrate” state) under controlled humidity conditions.

These methods provide insights into the complex hydration states and their impact on cement microstructure. The research highlights the variability of hydration states with environmental changes and their potential to cause structural issues such as cracking, affecting the material's performance and durability.

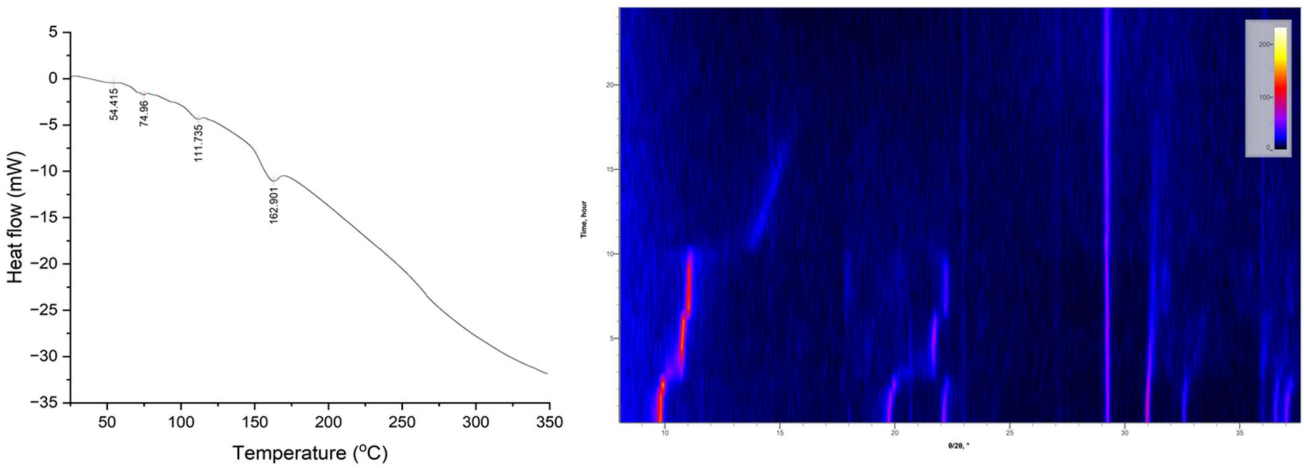


Figure 1. *DSC (left) and PXRD (right) data collected simultaneously on heating a sample of $Ca_4Al_2(OH)_{12}SO_4 \cdot 6H_2O$ from 25–350 °C*

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