Methodology and determination of water in important hydration phases of cements

Afm (LDH)-sulfate, carbonate,hydroxide phases

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Afm-phases play an important role during the hydration of cements and in hydrated building materials. The varying water content in hydrated minerals is accompanied by changes of the crystallographic dimensions, leading to a shift in X-ray peaks. The determinations of these different phases is therefore of high potential in practical applications as there is also an increase or decrease of the molar volume of these phases and the bound water. The composition based on a positive charged main layer and a negative charged interlayer can be described as follows:

$$Ca_4Al_2(OH)_{12}] \; [\,(X)_n \cdot n\,H_2O]$$

Depending on the existing surrounding conditions these layered strcutures show different hydration stages. Basically these phases are described with their water contents at room temperature and 35 % r.h. To describe the properties of these minerals it is necessary to control relative humidity and temperature and perform X-ray experiments at non-ambious conditions. Lamellar calcium aluminum hydrate phases with the anions carbonate, sulfate and hydroxide can form 3 monophases, 2 binary phases and 3 ternary phases, which can partially form solid solutions and form more than 20 different hydration states due to composition, rel. humidity and temperature. Also the coexistence or replacement with minerals of ettringite-type structure must be taken into account.
The following most important lamellar phases will be described :

Composition	Lattice parameters in Å	Space group
$[Ca_4Al_2(OH)_{12}][(CO_3)\cdot 5H_2O]$	**a_o=5.7747 b_o=8.4689 c_o= 9,923 α = 64.77° ß = 82.75° γ = 81.43°**	**P1**
$[Ca_4Al_2(OH)_{12}][(SO_4)\cdot 6H_2O]$	**a_o = 5.761 c_o = 26.831**	**$R\bar{3}$**
$[Ca_4Al_2(OH)_{12}][(2OH)\cdot 6H_2O]$	**a_o = 5.75 c_o = 95.05**	**$R\bar{3}$**
$[Ca_4Al_2(OH)_{12}][(OH)(0.5CO_3)\cdot 5H_2O]$	**a_o = 5.77 c_o = 49.199**	**$R\bar{3}c$**
$[Ca_4Al_2(OH)_{12}][(0.4OH)(0.8CO_3)\cdot 4H_2O]$	**a_o = 5.7534 (1) c_o = 46.389 (1)**	**$R\bar{3}c$**
$[Ca_4Al_2(OH)_{12}][(OH)(0.5SO_4)\cdot 6H_2O]$	**a_o = 5.755 c_o = 26.25**	**$R\bar{3}$**
$[Ca_4Al_2(OH)_{12}]$ $[(OH)(0.17SO_4)(0.34CO_3)\cdot 5.5H_2O]$	**a_o = 5.771 c_o = 49.52**	**$R\bar{3}$**
$[Ca_4Al_2(OH)_{12}]$ $[(0.17OH)(0.17SO_4)(0.66CO_3)\cdot 5.5H_2O]$	**a_o = 5.769 c_o = 49.205**	**$R\bar{3}$**

Tab. 1: Afm-phases with carbonate sulfate and hydroxide in the interlayer and the hydration state at 35 % r.h. and 25 °C