Local structure – bulk property relationship in the mineral Strätlingite

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Unlike carbon, silicon atoms tend to form single σ bonds with oxygen due to the fundamentally different nature of their 3p valence orbital compared to carbon's 2p orbitals. The ability to create covalent bonds with four neighbouring atoms, enables a wide spectrum of Si-O-Si bond angles thus causing extreme structural flexibility in 1, 2 and 3D-network formation. As a result, numerous silicate minerals: ordered, disordered or even amorphous, are surrounding us and extensively involved in various aspects of our lives. Thus, a deep understanding of the close connection between a minerals' crystal structures and their respective properties is essential for the design of cheap and affordable functional materials of the future. One of such promising minerals appears to be Strätlingite, whose peculiar morphology and chemical stability is believed to be responsible for the longevity of the roman concrete.

In this work we assess the fundamental details of the mineral Strätlingite ($Ca_2Al_2SiO_2(OH)_{10}\cdot 2.25H_2O$): its formation, average crystal structure, and local disorder phenomena. Combining conventional X-ray powder diffraction (XRPD) analysis and 3D (cryo) electron diffraction (3D-ED), we demonstrate, that Strätlingite is best described by $R\bar{3}$ space group, composed of two electrostatically connected layers: a positively charged brucite-like layer $[AlCa_2(OH)_6]^+$, and a negatively charged double-tetrahedra (DT) layer $[AlSiO_2(OH)_4]^-$ that contains occupational and positional disorder within Si(Al) tetrahedral sites.

The second part of our work is dedicated to the analysis of the defects' correlation in the DT-layer, and to a description of unique properties that such arrangement gives to the mineral. A reversible structural response to the changes in the humidity of the surrounding atmosphere is one of them, has been demonstrated by the *in situ* variable humidity XRPD experiment at different temperatures (Figure 1).

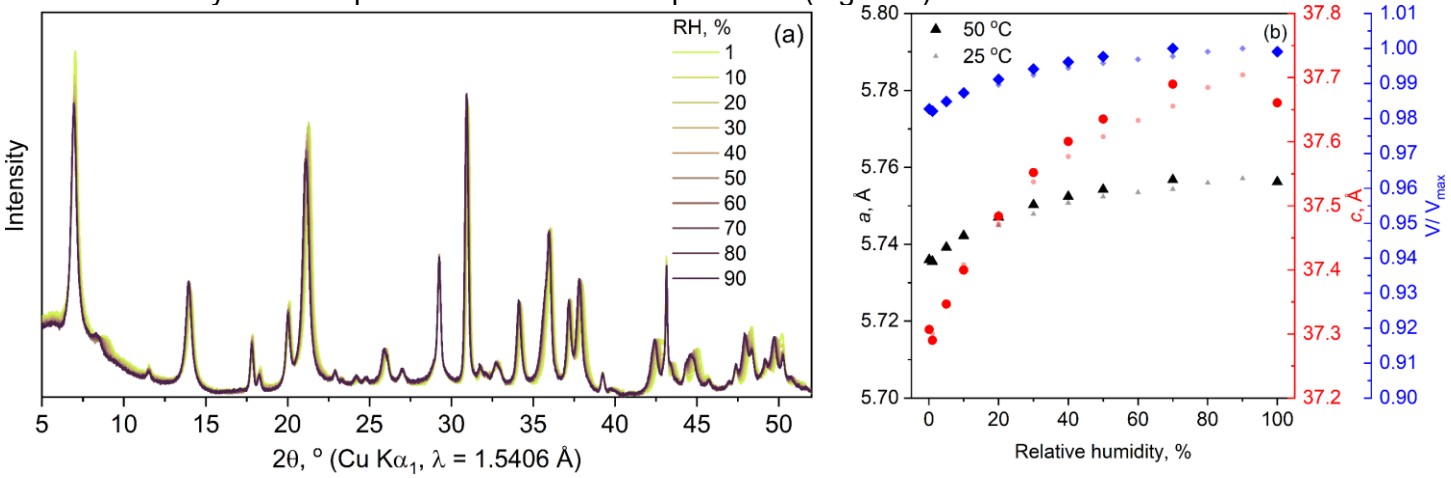


Figure 1. *Overlayed raw X-ray diffraction patterns under different air humidity (a), and respective lattice parameter changes vs relative humidity derived from the Pawley refinements [1].*

[1]. G. S. Pawley, J. Appl. Crystallogr. (1981).14, 357–361.