TEM INVESTIGATION OF AERINITE, COMPARED WITH SYNCHROTRON AND X-RAY POWDER DIFFRACTION DATA

D. Nihtianova[1], U. Kolb[2], Jixue Li[2], I. Queralt[3]
[1] *Central Laboratory of Mineralogy and Crystallography, Bulgarian Academy of Sciences, Acad. G. Bonchev Str., bl. 107, 1113 Sofia, Bulgaria.*
[2] *Institute of Physical Chemistry, Johannes Gutenberg-University, Welderweg 11, 55099 Mainz, Germany.*
[3] *Institut de Ciènces de la Terra. (CSIC) c/Solè Sabaris s/n, E-08028 Barcelona, Catalunya, Spain.*

Keywords: electron diffraction, HRTEM, computer simulation

Aerinite $(Ca_{5.1}Na_{0.5})(Fe^{3+}AlFe^{2+}_{1.7}Mg_{0.3})(Al_{5.1}Mg_{0.7})[Si_{12}O_{36}(OH)_{12}H][(CO_3)_{1.2}(H_2O)_{12}]$, a blue fibrous silicate mineral associated with the alteration of ophitic rocks in the southern Pyrenees, occurs in the Camporrells – Estopanyà area (Huesca – Lleida, Spain) and was commonly used as a blue pigment in most Catalan roman paintings between the XI – XV centuries. Its crystal structure was studied by TEM at 300 kV with a FEI Tecnai F30 ST. Unit cell parameters (a = b = 16.8820(9), c = 5.2251(3) Å, $\alpha=\beta=90°$, $\gamma=120°$) have been obtained through tilt series using a double tilt–rotation holder in nano diffraction mode [1] and confirm the values derived from powder diffraction by Rius et.al. [2]. Tilts were performed from the initial zone [100] around axis b*: [101], [10 $\bar{1}$], [10 $\bar{2}$], [201], [20 $\bar{1}$], [203], [20 $\bar{3}$], [301], [302], [304], [403]. The zone axes [210], [310], [3 $\bar{1}$ 0], [320], [410], [4 $\bar{1}$ 0], [430], [520], [5 $\bar{2}$ 0], [530], [540], [750] have been registered from an initial zone [100] around axis c*. HREM images were obtained in the following crystallographic orientations: [001], [101], [110], [$\bar{1}$ 11], [102], [120], [201], [122], [203], [301], [1 $\bar{1}$ 9], [$\bar{1}$ 24] but still four space groups were left over. Recently Rius et al. [3] have determined its crystal structure in space group P3c1 by applying the direct methods modulus sum function to synchrotron and X-ray powder diffraction data. Using the structure model of Rius et al. [3] and the program CERIUS 4.2 [4] the kinematically calculated electron diffraction patterns and the simulated HREM images gave a good agreement with experimental TEM data.

[1] U. Kolb and G. Matveeva, Electron crystallography on polymorphic systems, *Z. Krist*., **218**, 259-268, 2003.
[2] J. Rius, F. Plana, I. Queralt, D. Louër, Preliminary structure type determination of the fibrous alumosilicate “aerinite” from powder X-ray diffraction data, *Anales de Quimica Int. Ed*. **94**, 101-106, 1998.
[3] J. Rius, E. Elkaim, X. Torrelles, Structure determination of the blue mineral pigment aerinite from synchrotron powder diffraction data. The solution of an old riddle, *European Journal of Mineralogy*, Vol. **16**, No 1, 127-134, 2004.
[4] Cerius 2 version 4.2 MS, Molecular modeling environment from Accelrys Inc., 9685 Scranton Road, San Diego, CA 92121 – 3752, USA.