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Structure Determination of Donwilhelmsite by Electron Diffraction Tomography

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Calcium aluminium silicon oxide (CAS) phase, the new mineral "Donwilhelmsite" [1], formed in shock melt pockets in the lunar meteorite Oued Awlitis 001. This meteorite was found on January 15, 2014, in the Western Sahara (25.954°N, 12.493°W) as two individual stones totaling 432.5 g. The meteorite is classified as an anorthositic lunar melt rock [2]. Shock melt pockets 100 μm in size of roughly anorthitic chemical composition contain bundles of up to 20 μm long and less than 1 μm wide needle-shaped crystals (Fig. 1). The acicular habit and the very small size of these phases reflect rapid growth of the crystals during elevated shock pressures in less than tens of microseconds. In high-contrast BSE image, the acicular crystals appear slightly brighter and surrounded by a comparatively darker halo when compared with the adjacent anorthitic shock melt. This reflects a relative SiO_2 enrichment in the halo and relative SiO_2 depletion in the denser, high-pressure phase.

A lamella was cut out of the thick section NHMV-O104 with a focused ion beam (FIB) to study the structure of the needle-like crystals. It was investigated by Precession Electron Diffraction Tomography (PEDT) on a Philips CM 120 (LaB6, 120kV) equipped with a NanoMEGAS precession unit DigiStar and an Olympus SIS CCD camera Veleta (2048x2048px). The crystal was sequentially tilted by the step of 1 deg. from -50 to +50 deg., and at every tilt step a precession diffraction pattern in micro-diffraction mode was acquired using a precession angle of 1 deg. The data were processed in the PETS software. Structure solution and refinement were performed in the computing system Jana2006. The structure was solved by the charge flipping algorithm using the program Superflip, and refined using dynamical approach [3].

Eight datasets were collected with average lattice parameters a = 5.44(1) Å, c = 12.76(3) Å, space group $P6_3/mmc$. The structure is identical to the one of synthetic crystals experimentally produced at pressures of >15 GPa and temperatures of >1550 K by Gautron *et al.* [4]. The structure is composed of M1 octahedral sheets that contain Al and Si (Fig. 2). These are intercalated with two M2-octahedra occupied by Al, one larger site occupied by Ca coordinated by 12 oxygen atoms, and two Al-tetrahedra with 50% occupancy. The structure was refined dynamically to *R1(obs)* = 8.98%. The chemical composition derived from the structure model is $CaAl_4Si_2O_{11}$, which is in good agreement with chemical composition of $Ca_{1.02}Al_{3.92}Si_{2.06}O_{11}$ obtained experimentally [5].

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[4] L Gautron et al., Physics and Chemistry of Minerals **27** (1999), p. 47.
[5] The authors acknowledge funding from the Czech Ministry of Education, Youth and Sports (project LM2015087).

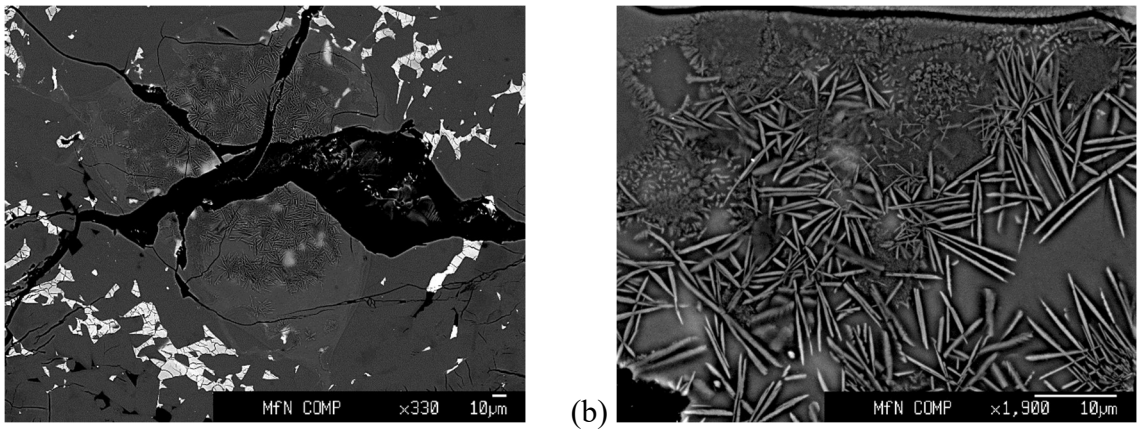

Figure 1. Backscattered-electron (BSE) images of a polished and carbon coated thick section of Oued Awlitis 001. (a) shock melt pocket, (b) needle-like crystals of Donwilhelmsite.

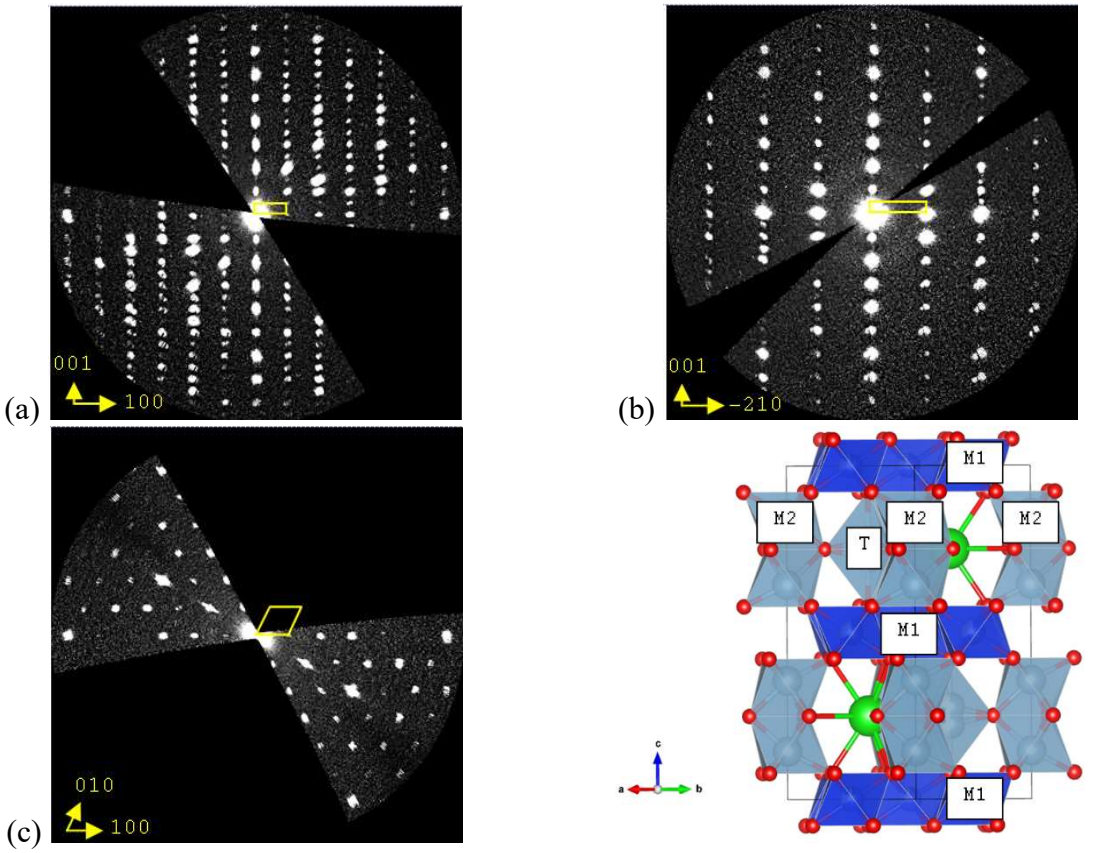

Figure 2. PEDT experiment. Reciprocal space sections (a,b,c). Structure of Donwilhelmsite (d).

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