SYNTHESIS, SYNCHROTRON DIFFRACTION STUDY AND TWINNING IN $Na_2Ca_4Mg_2Si_4O_{15}$ – A HETEROPOLYHEDRAL FRAMEWORK COMPOUND

Kahlenberg, V., Schmidmair, D., Hildebrandt, E., Ennemoser, P., Zöll, K. & Krüger, H.

Institut für Mineralogie und Petrographie, Universität Innsbruck, Innrain 52, 6020 Innsbruck, Austria
volker.kahlenberg@uibk.ac.at

The formation of polycrystalline $Na_2Ca_4Mg_2Si_4O_{15}$ from solid state reactions has been studied between 800 and 1050 °C. Single crystals of the compound have been grown in a closed platinum capsule by slow cooling in the temperature range between 1300°C and 1000°C. Basic crystallographic data are as follows: monoclinic symmetry, space group *P*12/*c*1, *a* = 7.1717(3) Å, *b* = 5.3512(2) Å, *c* = 16.4789(7) Å, β = 90.911(4)°, V = 632.33(4) $Å^3$, Z = 2.

A conspicuous feature of the crystals is an intensive lamellar non-merohedral twinning clearly observable already under a petrographic microscope. The diffraction pattern can be explained as a superposition of two reciprocal lattices with a two-fold axis parallel to [001] being the twin element. Using synchrotron radiation (X06DA beamline at the Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland) it was possible to solve the crystal structure of $Na_2Ca_4Mg_2Si_4O_{15}$ from a twinned data set. Least-squares refinements resulted in a residual of R(|F|) = 0.031 for 2899 observed reflections with $I > 2\sigma(I)$ and 127 parameters. The crystal structure contains both $[Si_2O_7]$-dimers and insular $[SiO_4]$-moieties. Tetrahedra and $[MgO_6]$-octahedra form a three-dimensional framework whose topological characteristics have been studied. The remaining calcium and sodium cations are distributed among four crystallographically independent positions located in voids of the network.

On a microscopic scale the twinning observed in the diffraction experiments could be explained by the existence of 2_1-screw axis parallel to [001] in (¼,0,*z*) mapping both domains onto each other. A comparison with related compounds having an $A^{+}_2B^{2+}_6Si_4O_{15}$ stoichiometry is presented.

More than 25 years after its first observation in refractories (HAUSNER & SUPPANER, 1992) our investigation clarifies the crystal structure of a silicate that is of relevance for both Materials science and high pressure research (BINDI et al., 2015).

HAUSNER, R., SUPPANER, M. (1992): Powder Diffr., 7, 36-37.
BINDI, L., SAFONOV, O.G., ZEDGENIZOV, D.A. (2015): Contrib. Mineral. Petr., 170, 14, 1-11.