X-Ray powder diffraction of synthetic Al-rich phlogopites: lattice parameters, polytypes, stacking faults, and implication of modulations

Fechtelkord, Michael[1] Langner, Ramona[1] Marler, Bernd[1] Friese, Karen[2] Grzechnik, Andrzej[2]
[1]Ruhr-Universität Bochum, Institut für Geologie, Mineralogie und Geologie, Universitätsstr. 150, 44801 Bochum, Germany [2]Universidad del Pais Vasco, Departamento de Fisica de la Materia Condensada, Bilbao, Spain

X-ray powder diffraction experiments of synthetic Al-rich phlogopites synthesized at 800 °C and 2 kbar were carried out. The grain size of the synthetic phlogopites ranges between particle diameters of 3 to 5 μm. The samples have already been well characterized by solid state NMR spectroscopy, and thus, possible impurity phases have been assigned.

As for all micas, the phlogopite structure can be described in terms of the OD-theory, where 2-d periodic layers can be stacked in different ways without changing the transition from one layer to the adjacent one (Nespolo and Ďurovič 2002).

One aim of the experiments was to study the change of lattice parameters with increasing F- and Al-content. Previous investigations have already shown that the c-lattice parameter decreases strongly with increasing F-content (e.g., Papin et al. 1997). From combined powder XRD and TEM investigations we expect to get detailed information on the polytypes which were formed during synthesis and on stacking faults in the mica structure. Up to now, many natural phlogopite single-crystals and synthetic powder samples have been characterized using XRD techniques. The most common polytype is the one-layer monoclinic polytype (1M) with space group symmetry C2/m. The other two possible polytypes, $2M_1$ (space group symmetry C2/c) and 3T (space group symmetry $P3_112$) are far less abundant (Brigatti and Guggenheim 2002).

Our first refinements indicate that all phlogopite samples consist of polytype $2M_1$. However, there may also be a mixture of polytype $2M_1$ and polytype 1M, leading to inelastic X-ray scattering. In some powder patterns with better resolution, satellite reflections surrounding hkl-reflections occur, which have not yet been reported and imply the presence of a modulated structure.

We expect that the X-ray diffraction results will be a valuable complement to our solid-state NMR investigations. While solid-state NMR spectroscopic investigations offer an insight into the local structure of the nuclei, the powder XRD patterns refinements may give new information about the long-range order of the tetrahedral and octahedral sheets. Combined with the TEM investigations, the results will contribute to a better understanding of stacking faults in the mica structure. Furthermore, this information may clarify the presence and type of modulations in the structure.

References

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