Routine definition of K-feldspar ordering degree in multiphase Rietveld refinements

Robert Möckel[1], Ulf Kempe[2], Stefan Richter[1,2], Jens Gutzmer[1,2]

[1]Helmholtz-Zentrum Dresden-Rossendorf, Helmholtz-Institute Freiberg for Resource Technology, Chemnitzer Str. 40, 09599 Freiberg, Germany
[2]TU Bergakademie Freiberg, Institute of Mineralogy, Brennhausgasse 14, 09599 Freiberg, Germany

Feldspars are the most common minerals in the Earth's crust, making up to 60 vol.%. Plagioclases ($(Na,Ca)[(Si,Al)_2Si_2O_8]$) are the most important of the feldspars, followed by potassium-feldspars ($K[AlSi_3O_8]$). They all belong to the tectosilicates with a SiO_4-tetrahedron framework and cations in the "interstitials" of the network (K^+, Na^+, Ca^{2+}, and subsidiary Ba^{2+}, Rb^+, Sr^{2+}). The charge excess is being compensated by replacing the respective amount of Si^{4+} by Al^{3+} in the tetrahedral sites. For compensation, four distinct sites are available, named T_1O, T_2O, T_1m, and T_2m. Their respective occupancy can be expressed as a statistical probability over the whole crystal structure, called t_1o, t_2o, t_1m, t_2m, respectively. The structure is fully disordered in the case that all positions are occupied with the same probability, which leads us in the case of K-feldspar to the high-temperature sanidine (monoclinic, 2/m). In case $t_1o= t_1m >0.25$ $t_2o= t_2m<0.25$, the mineral orthoclase (monoclinic, 2/m) is present. Alternatively, a fully ordered structure with all Al on the T_1O position will result in the formation of triclinic ($\bar{1}$) microcline. Intermediate ordering states are possible, leading to different degrees of monoclinic and triclinic ordering.

We included the calculation of the ordering degree following the method by Kroll & Ribbe (1987) into a microcline structure file for routine powder X-ray diffraction analysis. These calculations are basing on reciprocal lattice vectors, which can be easily achieved from the lattice parameters, released for refinement. For this purpose we used the BGMN/Profex Rietveld software bundle (Doebelin & Kleeberg 2015). It is shown that this procedure makes it possible to define routinely the triclinic ordering degree of K-feldspar and to estimate a statistical error deriving from the Rietveld procedure in a mixture of minerals (natural rocks samples).

The method was applied to K-feldspar bearing rocks from three locations. The ordering degree in the Khalzan Buregte rare earth element (REE) deposit in Mongolia was found to be significantly higher than in adjacent wall rocks, which supported a genetic model of secondary hydrothermal origin (Kempe et al. 2015). Similar findings in the Strange Lake REE deposit (Canada) gave assumption to comparable ore forming processes. We also used the model in a provenance study for building stones used in the historical part of St. Petersburg (Russia).

References:

Doebelin, N., & Kleeberg, R. (2015). Profex: a graphical user interface for the Rietveld refinement program BGMN. *Journal of applied crystallography*, *48*(5), 1573-1580.

Kempe, U., Möckel, R., Graupner, T., Kynicky, J., Dombon, E. (2015). The genesis of Zr–Nb–REE mineralisation at Khalzan Buregte (Western Mongolia) reconsidered. *Ore Geology Reviews* 64, 602-625.

Kroll, H., Ribbe, P.H. (1987). Determining (Al, Si) distribution and strain in alkali feldspars using lattice parameters and diffraction-peak positions: a review. *American Mineralogist* 72, 491–506.