Raman based study of the K-tourmaline zoning

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Tourmaline is a good petrogenetic indicator mineral due to its chemical resistance and extensive stability at a wide range of metamorphic grades. It often shows a strong compositional zoning, which can be used to reconstruct its crystallization environment. Unfortunately, ordered concentric core-to-rim zonation can be disturbed by the deformation, fluid-infiltration events or interactions with inclusions. As a result, the study of the thin section surface might be not enough to understand the full picture. Raman spectroscopy is a non-invasive technique which allows to estimate tourmaline properties and composition both at the crystal's surface and at depth. Several quantitative and qualitative tourmaline Raman-based classifications were developed recently, but none of these can estimate the amount of K. In the UHPM rocks from the Kokchetav massif, tourmalines are characterized by variations of K in their zoning pattern. In some zones K content reaches more than 0.5 apfu - half of the cation site which is usually occupied by Na, Ca or vacancy. That allows to distinguish another tourmaline end member - maruyamaite, found in nature as far only in this geological location.

We developed a new approach to estimate the amount of K in tourmaline based on the shape and the intensities of the Raman spectra in the region 650-850 cm-1 (silicate ring vibrations). We also discuss the influence of large K cations on the vibrational modes of Si_6O_{18} rings in tourmaline. We used Raman imaging to obtain spectral data from the studied area of the zoned natural tourmaline crystals from Kokchetav massif. Data were correlated with chemical composition determined by Electron Probe Microanalysis (EPMA). Our study demonstrates that Raman spectroscopy can be used as a reconnaissance tool for a semiquantitative discrimination of dravitic tourmalines with different X-site occupation. This approach can significantly help the studies devoted to reconstructing the PT conditions of the Kokchetav rocks. The study was supported by a grant from the Russian Science Foundation (RSF 18-17-00186).