

Abstract

This Ph.D. thesis was focused on the application of Raman spectroscopy as the main analytical method for the characterization of neo-formed minerals, notably sulfates, from burning coal waste dumps. This environment associated with subsurface fires gives rise to a variety of uncommon and rare minerals. The specific features of these minerals (metastability, hygroscopy, mixed aggregates) causes that the mineralogical investigation is a challenging task using traditional laboratory-based techniques. Advantages such as the non-destructive nature, the sensitivity to the changes in the hydration degree of sulfates, little or none pretreatment, and the option of measurements directly in the field were the main reasons for applying this spectroscopy method. The scarce availability of spectroscopic data of most gas-vent minerals can be considered as the disadvantage. Therefore, artificial prepared samples of six anhydrous sulfates, which are rarely found in nature, were analyzed by Raman laboratory spectroscopy and a miniature a Raman spectrometer, and specific Raman features as well the differences with hydrated counterparts are shown. Laboratory investigation of two natural hydrated aluminum sulfates, alunogen and khademite, were carried out using Raman spectroscopy and other methods in order to obtain Raman spectra of well-defined specimens. Since the hydration and other transformation of samples may occur after sampling, the performance of a miniature Raman spectrometer (785 nm) was tested for the detection of gas-vent minerals in the field. Despite the handheld instrumentation did not allow for ideal detection and discrimination of finely crystalline minerals in complex mixture, the general performance of the spectrometer was convincing. This work also reports preliminary results about occurrence and distribution of predominantly sulfates at two different burning coal waste dumps (Ostrava, Czech Republic and Alsdorf, Germany). A number of rare hydrated and anhydrous sulfates and halides were found within gas- vent encrustation. Among others, kremersite, sabieite, godovikovite, pyracmonite, millosevichite, or mikasaite were unambiguously identified by Raman spectroscopy in nature for the first time. However, several sulfate phases have remained unidentified. Results of distinct experiments as well as the application in the real environment of burning heaps carried out in this work proved that Raman spectroscopy is able to detect numerous sulfates and other minerals associated with fumarolic environment, including sulfate phases of the different hydration degree, chemically and structurally related phases, or intimately intergrown aggregates. Based on this work, a Raman spectral database of gas-vent minerals was also created.