Mineralogical interpretation discrepancies between infrared reflectance spectra and X-ray Diffractograms: An example from the Kuh Panj porphyry Cu mineralization, SE Iran

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Abstract

Laboratory measurements, including infrared reflectance spectroscopy and X-ray Diffraction (XRD), have been widely used to identify and discriminate hydrothermal alteration minerals. The molecular bonding mechanism within the first nanometers depth of the rock sample surface is measured as absorption features by Short-wave infrared (SWIR) reflectance spectroscopy. The lattice spacing of the crystalline structure of minerals within the interior structure of minerals is detected via penetrated X-ray beams. These differences in principles of measurements between infrared reflectance spectroscopy and XRD may result in discrepant mineralogical interpretations, depending on the mineral species involved. In a few studies, these inconsistencies have been indicated. However, the reasons for these discrepancies have been poorly investigated. This abstract aims to explain briefly why these conflicts have been observed.

Two rock samples from the different alteration zones and lithological units of Kuh Panj porphyry Cu mineralization within the southeastern part of Iran were used for the above-mentioned measurements. Flat surfaces were used to capture SWIR hyperspectral images from 940 nm to 2540 nm with 6 nm spectral resolution as the SPECIM camera setup. Then, to identify the rock samples' interior mineral composition with the SPECIM camera, the rock samples were cut into halves using a diamond saw. The SPECIM mineral maps were created using a decision tree that considers the wavelength position and the absorption features for classification. Montmorillonite lacks an absorption feature between 2300 to 2500 nm, while illite has two absorption features at approximately 2334 and 2443 nm. Montmorillonite has a deeper water absorption feature than illite at approximately 1900 nm. The mixture of montmorillonite and illite has a deeper water absorption feature at 1900 nm than the aluminum hydroxyl absorption feature at approximately 2200 nm and lacks an aluminum hydroxyl absorption feature at approximately 2443 nm. These spectral characteristics were used to create the decision tree. Afterward, the rock samples were powdered to collect whole-rock XRD from 6º to 80º (2θ) to identify dominant minerals and low angle XRD from 5º to 25º (2θ) on fractionated clay particles to determine clay mineral types. The pipette method as a gravitational separation method was used to separate the clay particles. In this method, the rock powders were dissolved with water and placed in a 1 L cylinder, and after 6 h, the top 200 ccs containing ≤2μm particles were collected, dried, and used as clay fraction powder XRD.

The presence of illite within both samples was confirmed with both SPECIM and XRD. The SPECIM mineral maps show montmorillonite on the surface of a sample while it was absent within the interior parts and XRD outputs. We believe that montmorillonite has been formed as a surface coating on a tiny surface rock due to the weathering process. A weak aluminum hydroxyl absorption feature at approximately 2443 nm for illite is a reason for the misinterpretation of illite (as correct interpretation) with a mixture of montmorillonite with illite (as incorrect interpretation). Also, there is no actual reflectance infrared spectroscopy threshold value for discrimination of illite from the mixture of montmorillonite and illite because of the gradual changes of the water absorption feature depth at approximately 1900 nm. SWIR spectra and X-ray beams penetrate approximately 2 and 0.0012 mm of particles with an approximate size of 63 microns. In one of the investigated samples, montmorillonite covers 6% of SWIR active weathered surface mineral proportion, which is approximately equal to 0.2 wt.% (0.256 mm SPECIM pixel length × 0.256 mm SPECIM pixel width × 900 number of montmorillonite pixels in weathered surface sample × 0.0012 mm spectroscopic penetration × 2.35 kg/m3 montmorillonite density) of the whole rock. XRD has a detection limit of 1-4 wt.%, and since montmorillonite has 0.2 wt.%, in the sample, which is below the XRD detection limit, it was not detected via XRD. Powder homogenization for the XRD measurement, which may have resulted in a lower concentration than the XRD detection limit, should also be added to the reasons for observing these discrepancies. The whole rock XRD result shows, semi-quantitatively an average of 50% phyllosilicates, 28% quartz, and 22% albite proportions within the rock powders. In contrast, the SPECIM mineral maps show that more than 70% surface area of the rock samples contain montmorillonite, illite, and their mixture. This disagreement occurs for two reasons: (a) any pixel with a small proportion of a SWIR active mineral has a SWIR active reflectance spectrum in SPECIM, and (b) SPECIM camera can only map SWIR active minerals. Therefore, although quartz and albite as non-SWIR active minerals exist within the rock samples were not included in the mineral proportions.