USING ORIENTATION-DEPENDENT INFRARED EMISSION SPECTRA OF SINGLE CRYSTAL QUARTZ TO STUDY MINERAL GRAIN ORIENTATIONS IN QUARTZ-RICH ROCKS

Hema Werner, Paras Angell, Thomas G. Sharp and Phil R. Christensen,
School of Earth and Space Exploration, Arizona State University, Tempe, AZ-85287. e-mail: Hema@ajnapress.com

Introduction: Quartz is an anisotropic mineral with orientation-dependent optical properties [1]. Quartz c-axis orientations, used to study crystallographic preferred orientations of naturally sheared rocks, are measured by a variety of techniques [2,3].

Thermal infrared emission spectroscopy is a non-invasive diagnostic tool for studying vibrational modes in minerals and rocks [4,5]. The goal of this study is to use orientation-dependent infrared emission spectra of single crystal quartz to evaluate mineral grains orientations and degree of shear of in quartz-rich rocks. This would have applications for measuring quartz c-axis fabrics in naturally sheared rocks.

Experimental Methods: Thermal infrared emission spectra were recorded between 200 cm^{-1} to 2000 cm^{-1} (25 µm to 5 µm) with the Nicolet iS50 spectrometer located in the Mars Space Flight Facility at Arizona State University [1]. Emission spectra were recorded from a large polished single crystal quartz along the c-axis and the a-axis. The spectra are plotted as emissivity vs wavenumber (cm^{-1}). Emission spectra from a suite of quartz-rich rocks which include sedimentary, metamorphic, and igneous specimens were recorded. These hand specimens include naturally weathered samples collected from the Granite Wash Mountains and South Mountains of Arizona.

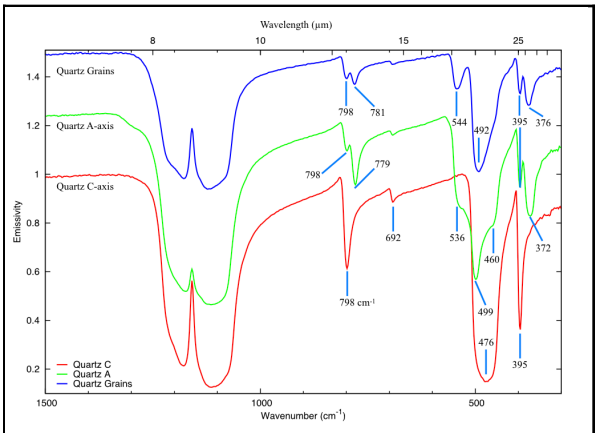

Figure 1. Infrared emission spectra of a polished quartz crystal measured along the c-axis and a-axis. The top curve is the emission spectrum of quartz grains. The spectra are offset along the vertical axis for clarity. The absorption features are annotated in cm^{-1} to illustrate the differences between the c-axis spectrum and a-axis spectrum of single crystal quartz.

Results: All these samples show the diagnostic quartz doublet absorption feature at 798 cm^{-1} and 779 cm^{-1} with a variation of ±2 cm^{-1}. Therefore this feature was selected for a detailed analysis to evaluate the proportions of quartz A and quartz C.

Differences in the spectral features of quartz A and quartz C

The emission spectra of quartz A shows the doublet feature at 798 cm^{-1} and 779 cm^{-1} (Fig. 1). However, in quartz C the 798 cm^{-1} feature is amplified in intensity and the 779 cm^{-1} feature is missing. Similarly, the doublet feature at 395 cm^{-1} and 372 cm^{-1} is present in quartz A. However the 372 cm^{-1} is absent in quartz C while the 395 cm^{-1} feature is stronger in quartz C.

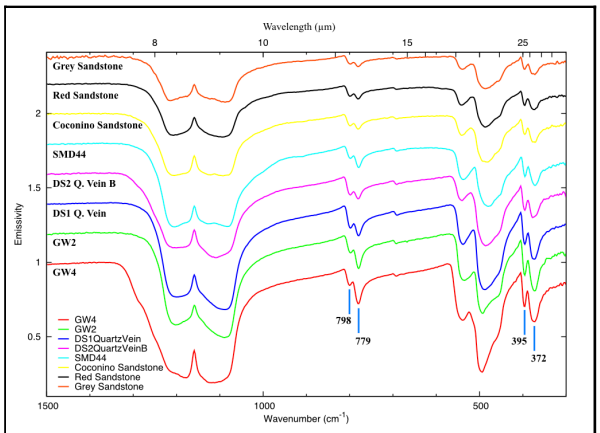

Figure 2. Infrared emission spectra of selected quartz-rich sedimentary, igneous and metamorphic rocks. The spectra are displaced vertically for clarity. Note the relative band depths of the annotated pairs of features around 800 cm^{-1} and 400 cm^{-1} change with the composition of the rock.

Spectral depth differences as diagnostic for quartz grain orientation

The difference in depth between the absorption features at 798 cm^{-1} (feature 3) and 779 cm^{-1} (feature 4) is 0.14 for quartz A. However, since the 779 cm^{-1} feature doesn't exist in quartz C, the presence of quartz C in a sample would contribute exclusively to the 798 cm^{-1} feature. Therefore, if a sample contains quartz grains oriented along the c-axis, the 798 cm^{-1} feature will be enhanced, and the depth difference, $\Delta d_{3\text{-}4}$, will be smaller than 0.14. Therefore, this depth difference, $\Delta d_{3\text{-}4}$, is an indicator of the orientation of quartz grains.

A similar analysis was carried out for the doublet feature around 395 cm^{-1} and 372 cm^{-1} (Figure 1).

Figure 2 shows the infrared emission spectra for the suite of quartz-rich rocks studied here. The depth differences, Δd_{3-4}, for the suite of quartz-rich rocks studied here are summarized in Table 1. Samples with Δd_{3-4} closer to 0.14 are expected to have a higher concentration of quartz grains with a-axis orientations. Examples include GW2 (0.11), GW4 (0.13), SMD44 (0.06).

Samples with mixed orientations of quartz a- and c-axes have a lower Δd_{3-4} , closer to 0.02. This result is illustrated in quartz grains which contain random mixed orientations of quartz in a- and c-axes, where Δd_{3-4} is 0.02. Other examples of samples which have a low Δd_{3-4} include: quartz vein 2, SM10, and the three sandstones (Coconino, red, grey). These samples are expected to contain both quartz a-axis and c-axis orientations.

Table 1. Variation in band depth differences for the pair of features around 800 cm^{-1} for quartz A, quartz C, quartz grains, and selected quartz-rich rocks.

Sample	Emissivity Features				
	3		4		d3-d4
	Wave#	Depth	Wave#	Depth	Δd
Quartz a-axis	798	0.85	779	0.71	0.14
Quartz c-axis	798	0.61	*		
Quartz Grains	798	0.89	781	0.87	0.02
Quartz Standard	798	0.92	781	0.91	0.01
Granite Wash GW2	798	0.86	779	0.75	0.11
Granite Wash GW4	800	0.85	779	0.72	0.13
South Mtn. SMD44	798	0.90	778	0.84	0.06
Quartzite	799	0.82	780	0.77	0.05
QuartzVein1	798	0.83	779	0.78	0.05
QuartzVein2	798	0.85	781	0.83	0.02
South Mtn. SM10	798	0.92	781	0.91	0.01
Coconino Sandstone	798	0.92	781	0.89	0.03
Grey Sandstone	798	0.93	781	0.91	0.02
Red Sandstone	798	0.92	781	0.90	0.02

Spectral Mixture Analysis (SMA)

SMA uses a linear mixing algorithm to build a composite model spectrum from a library of reference mineral spectra to yield a best fit to the experimental spectrum. Linear best-fit matches of the data are used to estimate the percent abundance of end-member minerals present in the sample [6].

Spectral mixture analysis (SMA) for quartz-rich rock samples was performed using a customized library of standard spectra with quartz c-axis and quartz a-axis spectra added, in two ways:

(a) with a custom library (b) with same library, excluding standards for quartz and chert in order to see if this analysis can give information about the amounts of a-axis and c-axis quartz present in the samples.

SMA of quartz grains (Δd_{3-4} = 0.02) yields a mineral abundance of 38% c-axis quartz and 62% a-axis quartz. Results of an example SMA are shown in Figure 3 for red sandstone (Δd_{3-4} = 0.02), which yields 24% c-axis quartz and 56% a-axis quartz. SMA of sample SMD44 (Δd_{3-4} = 0.06) yields 57% a-axis quartz, 27% K-rich glass, and 16% albite.

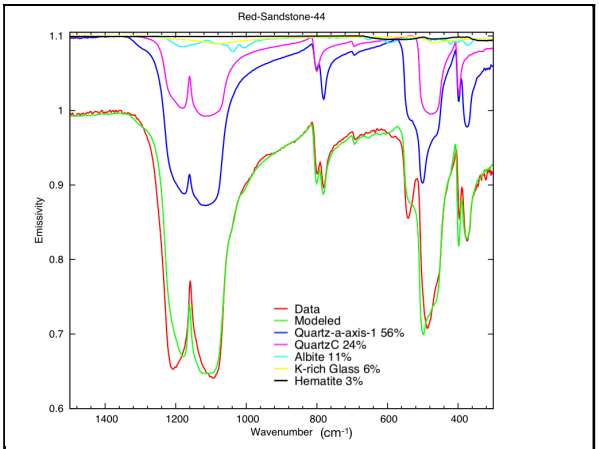

Figure 3. Spectral mixture analysis of the infrared spectra of red sandstone with a custom library with the standards for quartz and chert excluded. SMA yields mineral abundances of 56% a-axis quartz, 24% c-axis quartz, 11% albite, and 6% K-rich glass.

Discussion: Band depth differences between a-axis and c-axis infrared emission minima can be used as an indicator of quartz grain orientations in quartz-rich rocks. When the Δd_{3-4} is greater than 0.06, the samples could be composed primarily of quartz grains in the a-axis orientation. When the Δd_{3-4} is less than 0.05, the samples contain both quartz a-axis and c-axis orientations.

SMA can be used as an additional tool to estimate the proportions of quartz-grain orientations in sheared as well as sedimentary rocks by including quartz a-axis and quartz c-axis emission spectra as end-members in the SMA reference library.

Future Work: includes infrared emission spectral analysis of other naturally sheared rocks as well as optical microscopy studies of selected specimens to examine mineral grain orientations.

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