At site rock and mineral measurement using a handheld Agilent FTIR analyzer

Easy analysis with the diffuse reflectance geolibrary

Application Note

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Abstract

Agilent 4100 ExoScan and 4200 FlexScan FTIR systems facilitate fast rock and mineral identification in the field with little or no sample preparation. This is achieved by a diffuse reflectance sample interface coupled with an on-board Agilent diffuse reflectance geolibrary. In contrast to commercially available libraries that are specific to absorbance/transmittance measurements on a benchtop FTIR, the library is optimized for a diffuse reflectance field FTIR analyzer. For some minerals, spectra of both rough surfaces and smooth reflective crystal surfaces are included in the library. Users can also create their own libraries to meet specific requirements.

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4300 Handheld FTIR

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Introduction

Agilent introduced the first handheld battery operated Fourier transform infrared (FTIR) analyzers that have both the performance envelope and robustness to be used effectively in demanding field environments. A particularly useful application for this technology is in the geosciences. This application note discusses the use of the Agilent 4100 ExoScan and 4200 FlexScan FTIR systems (Figure 1) in the development of a rock and mineral library optimized for a field FTIR analyzer.

Figure 1. Agilent FTIR analyzer with diffuse reflectance sampling interface rapidly records the molecular spectrum of the sample with no preparation required

FTIR spectroscopy has been used for years in the study of rocks and minerals and there are a number of commercially available libraries containing geological samples. These libraries all have the common trait of being measured in classical absorbance/transmittance mode. This typically entails taking a small specimen of mineral and grinding it in KBr or nujol to make a suspension to record the spectrum of the mineral. The other common trait is that all of these spectra were recorded in a lab using a traditional benchtop FTIR spectrometer.

Diffuse reflectance sample interface

The complement to an at-site infrared (IR) analyzer is the ability to record a spectrum with little or no sample preparation. This allows the IR spectrum of an area of interest to be obtained, whether it is in an outcrop, ore body, drill core, or inside a mine. For this reason, Agilent have developed a diffuse reflectance sampling interface for Agilent handheld FTIR systems, which enables direct measurement of samples without sample preparation.

This form of reflectance measurements collects the diffusely scattered light from a sample and then returns the scattered light to the IR detector. Diffuse reflectance of neat rocks and minerals differ from transmittance spectra and thus a unique library is being created for this type of analysis method that is contained on-board the analyzer. Igneous/plutonic, metamorphic and sedimentary rocks and minerals are included in the library possessing various chemical compositions including nitrates, sulfates, oxides, silicates, aluminosilicates, phosphates, sulfides, borates, vanadates, tungstates, urinates, and so on. If a mineral possesses a chemical structure in which the atoms are covalently bonded, there is frequently a well defined IR spectrum that is obtained.

Depending on the particle size and crystallinity of the specimen, as well as the reflectivity of the surface being analyzed, there can be a specular component to the diffuse reflectance spectrum, which tends to alter the overall spectrum. Therefore, for certain minerals, spectra have been included in the library of both the rough surface and the smooth reflective crystal surfaces (Figure 2). The algorithm used by the analyzer accesses both types of spectra to predict the best match for a particular sample.

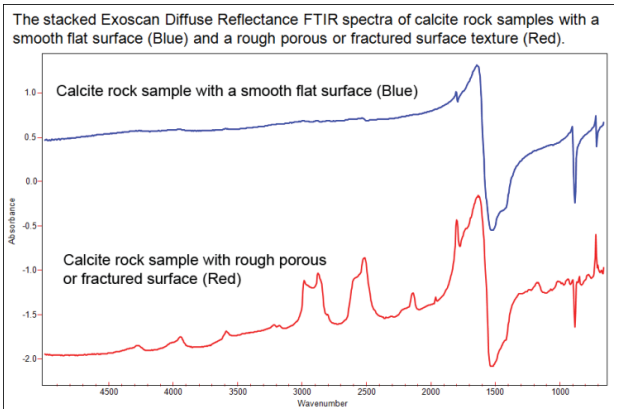

Figure 2. Stacked plot of spectra of calcite rock samples with a smooth flat surface (blue) and a rough porous or fractured surface texture (red) from representative mineral chemical composition classes. The spectra were recorded at 4 cm^{-1} resolution and consist of 128 scans co-added interferograms that take approximately 1 minute to collect and process

Diffuse reflectance geolibrary

The intuitive software of the Agilent FTIR analyzers enables the user to quickly ascertain the identity of a mineral in the field (Figure 3). The full spectrum of the specimen in question is stored and can be accessed for further investigation. As more referee specimens become available, Agilent will continue to expand the diffuse reflectance rock and mineral library. In addition to the on-board Agilent library, the 4100 ExoScan and 4200 FlexScan FTIR analyzers enable users to easily create their own library specific to their requirements.

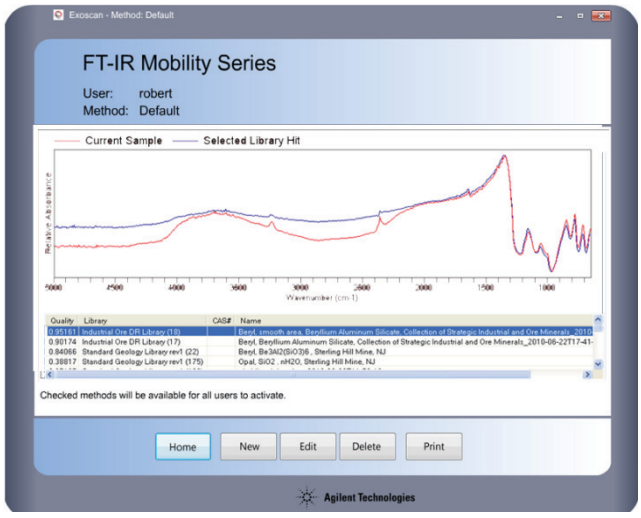

Figure 3. The IR spectrum of minerals measured neat may arise from diffuse and specular reflection and thus both types of spectra are included in the library, thereby maximizing the potential hit quality

Conclusion

The availability of a field-ready FTIR analyzer that provides molecular composition analysis of rocks and minerals with little or no sample preparation, coupled with an on-board library to assist in identification, is a powerful tool for the geoscientist, and an important complement to elemental analysis analyzers that are already in use in the field.

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