

ABSTRACT

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The RRUFF Project: Creating an Integrated Database of Oriented Raman Spectra, X-Ray Diffraction and Electron Microprobe Analyses of Minerals

Robert T. Downs, Bonner M. Denton, George R. Rossman

Recent advances in the miniaturization and optimization of Raman spectroscopic techniques provide the promise of handheld instruments that can be used to quickly and routinely identify and characterize the naturally occurring crystallized compounds. In fact, commercial probes are just coming to market now. These advances have benefited from research efforts funded by NASA to send a state-of-the-art miniature Raman instrument on one of the Mars Rovers to unambiguously identify the Martian minerals. For these reasons, we are building a database of Raman spectra that can be used to identify and characterize minerals. The samples are first subjected to X-ray diffraction to obtain cell parameters, constrain the symmetry, and provide identification. Electron microprobe analysis is conducted to obtain an empirical formula. Fragments of the characterized samples are then oriented in the directions necessary to measure the symmetry effects of orientation. These fragments are glued onto titanium pins and polished to ensure the highest quality spectra.

We envision about 15,000 samples in the database. The Raman spectrum of a mineral is like its diffraction pattern, inasmuch as it provides a unique fingerprint of the mineral, influenced by the crystal structure and the bond strengths of the constituent arrangement of atoms. Therefore, a complete library of spectra can be used to identify unknown samples. We also are investigating how well a mature Raman database can be used to estimate chemical composition, site occupancy and order-disorder, as well as to determine the orientation of the sample. The most intriguing aspects of a miniaturized handheld Raman instrument are that no sample preparation is required, acquisition time is about 10 sec, it is portable, and generally non-destructive. As such, it will be useful to jewelers, police, homeland security, and in a myriad of yet unforeseen circumstances.

Co-Authors

Name	Affiliation
Denton, M. Bonner	University of Arizona
Rossman, George R	California Institute of Technology