INTERLABORATORY AND CROSS-INSTRUMENT COMPARISON OF RAMAN SPECTRA OF 96 MINERALS

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Overview

The emerging importance of Raman spectroscopy for in situ planetary exploration requires an infusion of work into development of databases for mineral identification. Key to that endeavor is an understanding of the characteristics of various commercial and built-from-scratch instruments, their data processing software, and the presumption of consistency of spectra from identical minerals across varying instruments and platforms. This study tests the latter of these assumptions by presenting comparative results on a suite of 96 pure mineral powders from 15 different instrument/laser combinations using an array of geometries and laser energies. Our results assess the usefulness of existing databases built on powder or single crystal data and suggest work needed to align datasets from varying instruments to provide the deepest possible databases for impending Mars exploration use.

Methods

To date, we have collected 15 complete datasets on the 96-sample suite; additional measurements are in process at other labs:

- B&W Tek i-Raman (532 nm laser)
- B&W Tek NanoRaman (785 nm)
- Bruker Senterra (532, 633, and 785 nm lasers)
- Bruker MultiRAM 1064
- BRAVO (758 and 852 nm lasers simultaneously)
- An in-house system using a Holoplex grating, custom-gated thermo-electrically cooled mini-ICCD detector, and 2.5” Meade ETX-125 telescope at the University of Hawaii (532 nm laser)

Spectra were not baseline corrected so as to allow us to manipulate the algorithm used for data from each instrument.

Issues with Use of the RRUFF Database

Although the RRUFF database is the de facto standard for Raman data interpretation, there remain significant difficulties in using those data. These include:

1. RRUFF data are acquired at different laser wavelengths (514 nm, 532 nm, 780 nm, and 785 nm) and from oriented and un-oriented single crystal samples that are not always appropriate when matching against powdered samples.
2. 35.9% of RRUFF samples are without confirmed identifications by independent techniques, making those data useless.
3. By design, RRUFF focuses on representing a broad range of the ~4,000 known mineral species rather than on complete coverage of common rock-forming species.
4. Important mineral groups such as the pyroxene quadrilateral and the olivine solid solution are not well-represented in RRUFF.
5. Many RRUFF spectra are contaminated by mild to strong fluorescence features resulting from minor elements that give rise to fluorescence centers; these are not characteristics of the individual minerals, and have the potential to confuse matching algorithms.
6. RRUFF contains no data on mineral mixtures because it uses single crystals. Depending on the beam sizes used in planetary exploration, it is likely that mineral mixtures will be encountered on planetary surfaces.
7. The RRUFF database is no longer growing.

Although several mission concepts are currently being developed that will use Raman spectroscopy, much work remains to be done to provide appropriate and sufficient mineral and mineral mixture databases for calibration. A theoretical framework and improved software for mineral identification and un-mixing are also badly needed.

http://nemo.cs.umass.edu/54321/

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