Raman Technology

Raman instruments (which use many high resolution lenses and filters as well as high powered lasers) generally occupy the surface of a large table. To free this technology from the laboratory, it is necessary to miniaturize it. The result is a hand-held Raman instrument with point-and-click functionality. Using technology developed by the telecommunications industry, such a device can be constructed from “off-the-shelf parts,” including the same type of class 2 laser used in laser pointers.

Sample Detail

Perhaps already the largest publicly accessible database of its kind, it contains many hundreds of mineral entries. Each sample added to the database may be either a mineral not present in the database, or a variation in composition / locality, for a mineral already in the database.

Advantages to the database design include easy retrieval of multiple data sets for a given sample, and expandability to include data from alternative analysis and characterization. See documentation and references.

Going the distance

Our dedicated team of experienced professionals and enthusiastic students works hard to make this project noteworthy. It is our hope that this database, and a suitable miniature Raman device, will travel to Mars on a rover in the near future. There the spectral data will aid in planetary exploration, expanding the envelope of our scientific knowledge, and generously rewarding our efforts.

Closer look at the Database

To use the vibrational spectrum as an identification tool, it is necessary to have a complete set of high quality spectral data from well characterized minerals, and to develop the technology for sharing this information with the world. We hope that the RRUFF project will serve as a model for such an effort.

Equipment

For X-ray Powder diffraction, the RRUFF project uses the Bruker D8 Advance. The powdered sample is applied to a glass slide, and placed in the Bruker D8 Advance powder diffractometer where it is scanned from 5 to 80 degrees 2 theta at 2 seconds per 0.016 degree step at 20 degrees C. The data is searched matched with a program called Isis, and the unit cell is refined using h/k/l values from the Crystal Structure Database.

Raman Spectroscopy

Several Raman spectroscopists are sallying the various labs. The Downs group has a custom machine with a 174 nm laser and a Thermos Altera X8 single crystal diffractometer. The RRUFF research group uses a Bruker X8 single crystal diffractometer produce a 3x3 orientation matrix that describes the orientation of each crystal. Each crystal must be mounted on an adjustable goniometer head that is then transferred to a modified diffractometer, that we call “the orienter”. The orientation matrix obtained from the X8 provides the angles necessary for the orienter to drive to a cryogenic x-ray state. The crystal can then be affixed to a mount in a known crystallographic orientation.

X-ray Powder Diffractometer

Crystal orientations are determined using a Bruker Apex X8 single crystal diffractometer. Analysis of the diffraction spots from the Bruker X8 single crystal diffractometer produce a 3x3 orientation matrix that describes the orientation of each crystal. Each crystal must be mounted on an adjustable goniometer head that is then transferred to a modified diffractometer, that we call “the orienter”. The orientation matrix obtained from the X8 provides the angles necessary for the orienter to drive to a cryogenic x-ray state. The crystal can then be affixed to a mount in a known crystallographic orientation.

Rruff Project

The Rruff Project, now beginning its second year, continues working to collect a complete set of high quality spectral data from well characterized minerals, and to develop the technology for sharing this information with the world. We hope that our collected data will serve mineralogists, geoscientists, gemologists and the general public with identification of unknown minerals, earth and planetary exploration, as well as any number of other scientific inquiries.

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Software Development

Another task of the project is to develop a better tool for processing and comparing the various data sets. The program below (still under development) allows the user to remove background locate peak positions, and on powder patterns it can distinguish hkl from h0l peaks and store the data for a semi-automated cell refinement.

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