MITT.ÖSTERR.MINER.GES. 151 (2005)

DEVELOPMENT OF A HIGH QUALITY RAMAN SPECTRAL LIBRARY FOR MINERALS AND FLUIDS

Bakker, R. J., Piribauer, C. J. & Strauß, V.

Applied Geosciences and Geophysics, Mineralogy and Petrology, University of Leoben, Peter-Tunner Str. 5, A-8700, Leoben, Austria
e-mail: bakker@unileoben.ac.at

Raman spectroscopy has become a standard analytical technique within geological sciences. The obtained spectra of unknown minerals or fluids must be compared to standard Raman spectra to identify the phases. Commercial Raman spectral libraries (e.g. Thermo, Aldrich) mainly consist of organic materials. Libraries for Raman spectra of minerals and fluids are mainly available on the internet (e.g. http://minerals.gps.caltech.edu/files/raman/index.htm). The list of shortcomings of these online libraries include (1) too few spectra displayed; (2) no indication of accuracy, standards, deviation, relationship to crystallography or measurement conditions; (3) poor presentation of spectra (e.g. no peak values given in drawings); (4) bad quality of spectra (low peak-background intensity ratio, or no wave numbers given); (5) relatively high cut-off wavenumber (> 150 cm^{-1}); (6) absence of a search engine for spectra of unknown minerals; and (7) carelessly designed website. The aim of this study is to address these deficiencies and to present a large series of high quality Raman spectra of all mineral groups and fluids, including an interactive search engine for unknown mineral/fluid-spectra in a well designed website. Raman spectroscopic measurements were done with a LABRAM (ISA Jobin Yvon) instrument. The laser beam is focussed through an Olympus BX 40 microscope onto the object of interest, either mineral or fluid, using 40x or 100x magnification combined with a confocal optical arrangement, enabling a spatial resolution in the order of a cubic micrometre. The apparatus has a 100 mW frequency-doubled Nd-YAG laser with 532 nm wavelength (green), which is reduced to 38 mW at the measured object. A portion of the scattered light is collected through the microscope and focussed onto a diffraction grating. The grating selects the desired region of the Raman spectrum and reflects this onto a Peltier-cooled, CCD matrix detector. Wavenumber measurements have an accuracy of 1.62 cm^{-1} at low $\Delta\nu$ (Raman shift close to 0 cm^{-1}) and 1.1 cm^{-1} at high $\Delta\nu$ (around 3000 cm^{-1}). Measurements can also be performed at controlled temperatures between -190 and 600 °C, using the Linkam THMSG 600 heating-cooling stage. Silicium, calcite and Neon light have been used to calibrate wavenumbers. The Raman activity of the crystals compared to the power of the laser is expressed in a ratio of intensity of the main peak and measurement time (i.e. s^{-1}). The variation of non-isotropic minerals in spectra compared to crystallographic features (e.g. cleavage) has been registered. The search engine is based on the position of the most intensive peak of each material and allows a certain degree of variation to take into account chemical variation that is common in most natural minerals.