Poster

RamanCrystalHunter: a new program and database for processing, analysis, and identification of Raman spectra

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RamanCrystalHunter (RCH) is a new program that includes novel techniques for processing, interpretation, and identification of unknown Raman spectra through comparison with reference spectra in the new RamanCrystalHunter Database (RCHDB). RCH features a versatile and intuitive graphical interface where both specialist and non-specialist users can easily perform many visualization and processing operations (e.g., spectrum addition and subtraction, smoothing, noise reduction, and baseline corrections), and other interpretive operations (e.g., fitting, derivative calculation, and peak/spectrum comparisons). RCH was initially developed for Earth Science applications, i.e., processing the Raman spectra of minerals, but can be used for analysing the Raman spectra of any natural or synthetic, inorganic or organic material. Using the RCHDB, which currently includes >1000 high-quality mineral spectra, users can perform matching operations on their spectra to identify unknown materials or compare individual peaks or signals in specific, user-defined frequency ranges. In recent years, Raman spectroscopy has become commonplace in many planetology studies as it is one of the most efficient and accurate means by which extra-terrestrial materials, particularly meteoritic minerals, can be identified. However, the most important extra-terrestrial samples (e.g., diamonds, graphite, SiC, Al_2O_3 and ultra-high-pressure phases such as bridgmanite from meteorites and many other minerals), and exsolved high pressure terrestrial samples are often observed at the micro- to nano-scale and thus are difficult to reliably analyse and identify. This often results in complex, mixed Raman spectra that require rigorous pre-processing before accurate phase identification can be made. Here, we provide several examples of solutions that RCH offers for processing and identification of complex Raman spectra of meteoritic materials. The RCH program and the associated database of Raman spectra (RCHDB) can be downloaded for free at https://www.fabrizionestola.com/rch.