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DiadFit: An Open-SourcePython3 Tool for Raman Peak Fitting

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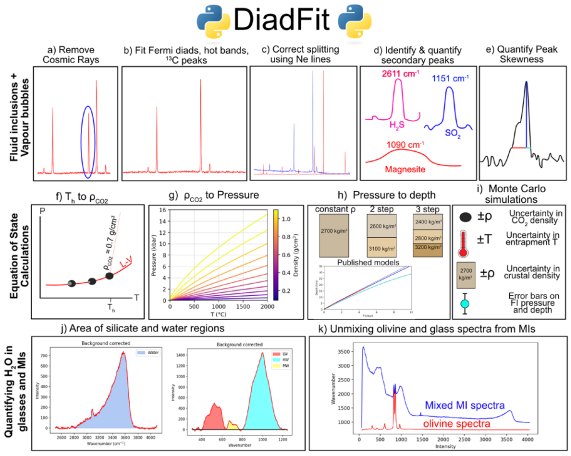

In recent years, Raman spectroscopy has gained popularity among igneous petrologists to perform non-destructive, in-situ measurements of the composition of fluids and melts – particularly to measure the density of CO_2-rich fluids in fluid inclusions and melt inclusion vapour bubbles to obtain accurate estimates of magma storage depths. Great strides have been made on optimizing calibration and analysis protocols for CO_2 rich fluids by Raman Spectroscopy while very little attention has been given to the software tools used to fit Raman spectral data. In fact, most studies use proprietary instrument software, paid subscription software such as OriginLab (~200 $/y) or have developed their own unpublished tools. Additionally, all these options along with Fityk, an open-source peak-fitting GUI, often involve fitting spectra one at a time and lots of manual clicking, which can quickly become tedious and a waste of resources ultimately harming reproducibility. We present a new Open-SourcePython3 tool, DiadFit, for efficient processing of Raman spectroscopy data for common volcanological workflows. DiadFit can automatically fit the Fermi diad of CO_2, hot bands, and the ^{13}C spectral peak for hundreds of spectra using Pseudovoigt or Voigt peaks combined with linear, polynomial and Gaussian backgrounds. Along with functions for performing cosmic ray filtering and Ne line corrections, this makes DiadFit the ideal tool for quantifying the density of CO_2 in melt inclusion vapour bubbles and fluid inclusions. DiadFit also contains numerous functions implementing different CO_2 equation of states, allowing microthermometry measurements to be converted to densities, and densities from Raman or Microthermometry to be converted to pressure and depths (with error propagation using Monte Carlo methods). There are also generic peak fitting functions (e.g., to quantify carbonate and S-rich phases), and functions to quantify the area ratio of the silicate vs. H_2O region of spectra collected on silicate glasses to determine H_2O contents (Schiavi et al., 2018). Documentation is available at ReadTheDocs (bit.ly/DiadFitRTD) and narrated examples are available on YouTube (bit.ly/DiadFitYouTube).