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A Raman model for determining the chemical composition of silicate glasses

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Raman spectroscopy is a spectroscopic technique based on inelastic scattering of monochromatic light which provides information about molecular vibrations of the investigated sample. Since the discovery of the Raman Effect (1928) in scattered light from liquids, the Raman investigation has been extended to a large number of substances at different pressure-temperature conditions. Recently, the Raman instrument setup has rapidly grown thanks to the progress in development of lasers, charge coupled devices and confocal systems (see Neuville et al. 2014 for a review). Here we present the first Raman model able to determine the chemical composition of silicate glasses.

In this study we combine chemical analysis from magma mixing experiments between remelted basaltic and rhyolitic melts, with a high spatial resolution Raman spectroscopy investigation; we focus on tracking the evolution of the Raman spectrum with chemical composition of silicate glasses.

The mixing process is driven by a recently-developed apparatus that generates chaotic streamlines in the melts (Morgavi et al., 2013), mimicking the development of magma mixing in nature. From these experiments we obtained a glassy filament with a chemical composition ranging from a basalt to a rhyolite. Raman and microprobe measurements have been performed on a filament of $\sim$1000 μm diameter, every 2.5-20 μm.

The evolution of the acquired Raman spectra with the measured chemical composition has been parametrized by combining both the Raman spectra of the basaltic and rhyolitic end-members.

Using the developed Raman model we have been able to determine the chemical composition (mol% of SiO_2, Al_2O_3, FeO, CaO, MgO, Na_2O and K_2O) of the investigated filament. Additionally, the proposed Raman model has been successfully tested using external remelted natural samples; reference glasses (Jochum et al., 2000), a remelted basalt, andesite from Etna and Montserrat respectively.

Finally, as the Raman spectrum depends on the silicate structure yielding information about network-forming structural units (Qn species, where n indicates the number of bridging oxygen), we combined the deconvoluted Raman spectra, in the rhyolitic field, with the chemical analyses and abundance of Qn species. This demonstrate how the evolution of silicate structure might control the bimodal eruptive style (explosive vs effusive) as shown by silica-rich volcanic systems.

References:

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D. R. Neuville, et al. 2014. Advances in Raman Spectroscopy Applied to Earth and Material Sciences. Rev. Min. Geochem., 78, 509-541.