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X-ray diffraction shines light on mineral inclusions: A natural high-pressure experiment

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From a mineralogical, geological and geodynamical point of view, mineral inclusions trapped inside another minerals are a treasure trove of information that can shed light on processes occurring at depth in the Earth. Entrapped at depth and protected by their host minerals during their ascent to the surface, inclusions are rare and provide pristine samples of regions of the Earth otherwise inaccessible with direct exploration methods i.e. hundreds of km against tens of km the deepest borehole drilling. Information on the environment of growth and the pressure and temperature conditions of formation can only be retrieved by performing in situ non-destructive measurements on the enclosed inclusions to prevent any possible loss of precious information.

Two techniques are the most common in this type of studies: Raman spectroscopy and X-ray diffraction (XRD). From these measurements phase identification allows to determine the environment of growth, whereas elastic geobarometric calculations allow to calculate the conditions of pressure and temperature of the entrapment, i.e. at the depth of formation for the pair, from the strain in the inclusion and the equations of state of both minerals.

Raman spectroscopy is a popular technique for characterising mineral inclusions, since it is quick and allows small portions of the sample to be probed. However, while phase identification for determining the environment of growth is quite straightforward, the relationship between the strains and the Raman peak position is not well established for several mineral phases. On the contrary, XRD directly measures the unit cell parameters and from their change with respect to a reference mineral is possible to calculate the strains acting on the inclusion trapped in the host at laboratory P and T.

We developed a methodology to calculate the strain from the Raman peaks, but it needed to be cross validated against direct measurements of the strains, such as the ones from XRD. Conventional laboratory set up do not allow us to measure inclusion smaller than 70 μm , because of the large X-ray absorption coefficient of the host minerals, and the 1-2 mm thickness required to preserve inclusion stress state. Unfortunately, inclusions of such dimensions are very rare in most natural rocks, so we extended our study using synchrotron light at the XPress beamline at Elettra (Basovizza, TS). Furthermore, XRD can be used to simultaneously extract a wide range of information. In fact, intensity data can be used for structural refinement for phase identification, allowing to infer the environment in which the host-inclusion system grew, and to characterize the structure of the entrapped mineral, which is under deviatoric stress, a condition very difficult to reproduce in a laboratory experiment in a controlled way. At the same time peak positions can be used determine the orientations matrices of both the host and the inclusion to enable modelling possible growth processes and scenarios.

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