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Elastic geobarometry: a comparison between experiments and numerical simulations

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Raman spectroscopy provides information on the residual strain state of mineral inclusions entrapped in other minerals, in terms of variation of the Raman shift (Murri et al 2017). This information, coupled with elastic geobarometry theory (Angel et al. 2015), can be used to constrain the P-T conditions during inclusion entrapment. Recently, Finite Element (FE) numerical simulations have theoretically shown that the geometry of the host-inclusion system may affect the residual strain on the inclusion (Mazzucchelli et al., 2018), therefore leading to incorrect estimates of the entrapment pressure (Ptrap).
To evaluate this effect, we performed Raman spectroscopy measurements on single crystalline inclusions of zircon and coesite while still entrapped in garnet megablasts and porphyroblasts from the UHP Dora Maira Massif. We selected inclusions located in fracture-free garnet hosts located well within their host (e.g. at least three times the radius of the inclusion from any free surface). Two main geometrical features have been considered: the shape of the inclusion and its proximity to the external host surface. In general, rounded inclusions exhibit homogeneous Raman shifts throughout their entire volume, whereas for angular elongated crystals the Raman shift is not constant and is mainly affected by the presence of corners and edges that act as stress concentrators. Chemical analyses with WDS microprobe have shown that the Raman shift variation within sharp inclusions is not related to variations in the chemical composition that, indeed, is rather homogeneous.
A step-by-step polishing of the host, performed on both rounded and prismatic inclusions show that the strain acting on the host-inclusion system is gradually released when the inclusion approaches the free surface of the host. The magnitude and the rate of the strain release depends on the elastic properties of the inclusion and its crystallographic orientation with respect to the host. Our experimental results closely match those from FE numerical models for the same geometry of the system using anisotropic elastic properties for both the host and the inclusion. This confirms that both the shape of the inclusion and its position within the host affect the residual strain, and these effects must be taken into account to retrieve the correct Ptrap through the elastic geobarometric approach.

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