Raman elastic geobarometry to infer unique P-T conditions of host-inclusion systems from UHPM rocks

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Raman spectroscopy applied to host-inclusion systems can provide key information on the residual strain state of the inclusion phases. However, to determine the strains for inclusions still trapped in their hosts, knowledge of the phonon-mode Grüneisen tensor for each Raman-active mode is mandatory.

To determine the phonon-mode Grüneisen tensor, we performed *ab initio* Hartree–Fock/Density Functional Theory simulations on alpha-quartz calculating its structure, elastic parameters and Raman-active vibrational modes as a function of different applied strains. These results coupled with the elastic geobarometry theory [1] allow us to infer the imposed stress at the moment of inclusion entrapment. As an example, we used these results to calculate the entrapment conditions for quartz inclusions in garnet within an eclogite xenolith from Mir pipe. The estimated entrapment conditions point at an elastic equilibration of the pair into the stability field of coesite at 3 GPa and temperatures between 925 and 1000°C [2].

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