MS15-P05 | Ab initio simulation and X-ray diffraction measurements of deviatoric stress in mineral inclusions

Morana, Marta (University of Pavia, Pavia, ITA); Murri, Mara (University of Pavia, Pavia, AUT); Girani, Alice (University of Pavia, Pavia, ITA); Angel, Ross J. (University of Pavia, Pavia, ITA); Alvaro, Matteo (University of Pavia, Pavia, ITA)

The behaviour of crystals under deviatoric stress is still poorly understood, despite that it plays an important role in reconstructive [1] and symmetry breaking [2] phase transitions. Even simple systems, such as an inclusion of an elastically anisotropic mineral entrapped in an elastically isotropic host, can develop deviatoric stresses. Since the experimental generation and measurement of deviatoric stress is difficult, we first performed *ab initio* hybrid Hartree–Fock/Density Functional Theory calculations to characterize how deviatoric stress affects crystal structures [3]. An ideal candidate for this study is quartz, since it has a simple and well-known structure, whose variation with pressure and temperature has been widely characterised, and it is one of the most common mineral inclusions. We compared the simulation results with X-ray diffraction data collected from a quartz crystal entrapped in a garnet host. Here we discuss how to overcome the experimental challenges related to the collection of intensity data from a crystal entrapped in another one, assess the quality of the results and the agreement between the experiment and the calculation.

[1] B. Richter, H. Stünitz, R. Heilbronner *Journal of Geophysical Research: Solid Earth*. **2016**, 121(11), 8015-8033.
[2] Bismayer, U., Salje, E., & Joffrin, C. *Journal de Physique*. **1982**, 43(9), 1379-1388.
[3] M. Murri, M. Alvaro, R.J. Angel, M. Prencipe, B.D. Mihailova *Physics and Chemistry of Minerals*, **2019**, 46(5), 487-499