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High Pressure Single-crystal Synchrotron XR diffraction of natural pyrochlores

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Accessory minerals are able to incorporate trace-elements whose content is affected by factors that include lattice strain, melt polymerization and the water content of the melt. Most of High Field Strength Elements (HFSE) including rare earth elements (REE), yttrium, niobium, and tantalum are used in a vast array of devices such as lasers, electronic screens, permanent magnets, battery alloys, and ceramics. The worldwide demand of HFSE supply raised constantly in recent time. In this framework, understanding the physical and chemical properties of REE- and REE-bearing minerals becomes critically important as, based on the available data, they are still far to be fully understood.
In particular, in order to understand the structural factors governing REE incorporation in host lattices and REE partition coefficients, is crucial to investigate the structural role of REE in crystalline structures of accessory REE-minerals.
In order to increase the available data on the physical and chemical properties of REE-minerals we studied the HP structural variation of natural pyrochlore by performing XRD data collections at increasing pressures in hydrostatic mode up to around 10 GPa at the XPRESS beamline (Elettra).
Pyrochlore-group minerals are among the most common HFSE-bearing minerals, they have a cubic structure (sp.gr. F-3d) characterised by a [8]-fold and a [6]-fold cations sites where HFSE can enter by a complex substitutions scheme. Na, Ca, Ba, Y, Ce (and other REE) may be hosted in the A site, whereas the B site may host Ta, Nb, Ti. The X and Y sites can host OH, F, H2O and vacancies.
We selected natural Na-pyrochlore from the Agua de Pau syenites (Azores islands, Portugal) particularly rich in Ba. The pyrochlore crystal was tested for crystallinity by single-crystal in-house XRD at the Dept of Physics and Geology (Perugia University) before the HP experiment.
The selected crystal is cubic, sp. gr. F-3d, with lattice parameter a = 10.3568(3) Å and a volume of 1110.91(6) Å3.
For the HP experiment we used a DAC assemblage prepared with a stainless steel gasket indented to 81 μm thick with a hole of 150 μm, and 600 μm culets diamonds. A mix of methanol:ethanol 4:1 was used as pressure transmitting medium. As pressure calibrant a ruby chip was loaded in the DAC. Pressure was measured before and after each data collection. Data collections were carried out by ±35 ω-rotation scan, angular step 1° and 5 sec scan time. We collected diffraction data at 16 pressure points up to ca. 9 GPa. Each collection data were processed by the CrysAlis software (Rigaku) to obtain the cell parameters and to extract the intensity for the refinements.
Pyrochlore crystal remained crystalline up to 9 GPa. A discontinuity in the lattice parameters and volume P-trends between 6 and 7 GPa suggests a phase transition.
We will present the bulk elastic parameters and structure modification up to the phase transition.
How the entering of REE correlates with physical properties like bulk modulus could help to better understand the pyrochlore cation partitioning at high pressure.

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