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Structural behaviour of CaZrO3 perovskite under pressure. Influence of pressure-transmitting medium

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Perovskite materials have been intensively investigated over last decades due to the interest for understanding their stability as a function of pressure and temperature as well as the establishment of correlations between crystal structure and physical properties. They cover many scientific and technological areas in Materials Science and Geophysics (structure of Earth's interior). In this regard, especial attention has been paid to phase transitions from the perovskite to the CaIrO3-type "post-perovksite"structure at high pressures, involving changes from corner sharing to edge sharing octahedral conformations.1,2 Such transition in MgSiO3 is hypothesized to be responsible for many seismic signatures of the Earth's lowermost mantle. Many structural studies have been conducted on ABX3 compounds in order to establish general models providing understanding on the distortion mechanisms of perovskites via polyhedral tilting. However, in spite of the efforts paid so far, there is no clear knowledge on the factors determining the destabilization of the perovskite structure. CaZrO3 is a very interesting system which has been proposed for possible applications in high temperature devices (refractory) and sensors, among others. In addition, this is a good candidate to investigate as a MgSiO3 analogue, i.e. to determine its distortion evolution under pressure and its stability limit in comparison with silicates. The idea is to establish guidelines to predict the structural evolution of perovskite materials in wide pressure ranges, explaining the equation of state (EOS) in terms of microscopic models, as well as to rationalize the propensity to form the post-perovskite structure. Thus, the structural behaviour of CaZrO3 has been studied as a function of pressure at ambient temperature by ADXRD. In addition the effect of different pressure transmitting media (methanol-ethanol mixture, paraffin and silicone oils) on the high pressure response has also been evaluated for this compound, focusing on the tilting evolution in the hydrostatic or quasi-hydrostatic regimes (below 15 GPa). Supplementary information has been obtained by means of Raman spectroscopy. Previous results on this and similar systems have been compared with present findings. The main conclusions will be presented at the conference.

References

1. A. R. Oganov and S. Ono, Nature 430, 445 (2004).
2. T. Litaka, K. Hirose, K. Kawamura and M. Murakami, Nature 430, 442 (2004).

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