XXI Brazilian Meeting on Inorganic Chemistry
X Brazilian Meeting on Rare Earths
III Workshop on Theoretical Bioinorganic Chemistry
Belo Horizonte, September 12 - 15th 2024

Bent and Fracture of δ-$CsPbI_3$ Single Crystal Under Hydrostatic High Pressure

Dieric S. Abreu (PQ)[1,4*]

[1]Laboratory of Materials & Devices (Lab MaDe), Department of Analytical and Physical-Chemistry (DQAFQ), Federal University of Ceará (UFC), Fortaleza-CE, Brazil
[4]Institute of Exact and Natural Science (ICEN), University of International Integration of Afro-Brazilian Lusofonia (UNILAB), Redenção – CE, Brazil
E-mail: dsabreu@ufc.br

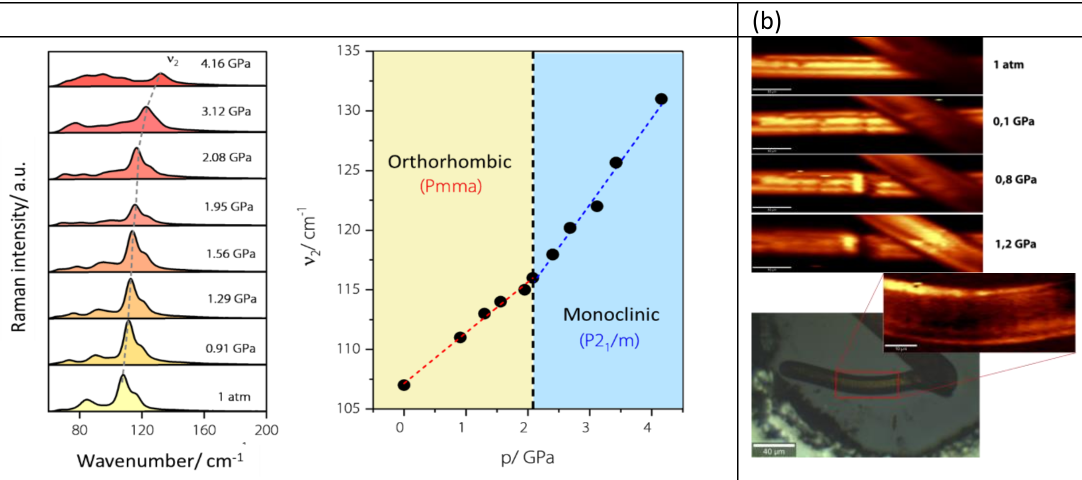
Thematic Area: Materials Chemistry

Keywords: Lead perovskite, Bent single crystal, High pressure

Lead-halide inorganic perovskites exhibit high stability against chemical degradation. However, the prototypical perovskite of this class, the dark phase α-$CsPbI_3$ (cubic, Pm$\bar{3}$m), undergoes spontaneous phase transitions under normal temperature and pressure conditions, eventually transforming into the non-perovskite yellow phase δ-CsPbI3 (orthorhombic, Pnma), thereby losing the connectivity of the three-dimensional network of $[PbI_6]^{4-}$ octahedra and consequently its main optoelectronic properties. Generally, such studies have been conducted on polycrystalline systems, where macroscopic structural effects are neglected. Therefore, this study aims to investigate in detail the evolution of the macroscopic structure of a δ-$CsPbI_3$ single crystal through Raman imaging under hydrostatic high-pressure conditions. Hydrostatic high-pressure Raman maps were obtained using a symmetric diamond anvil cell (DAC) with mineral oil as the compression medium. In addition to the observed transition (Figure 1.a b) from the δ-$CsPbI_3$ phase (orthorhombic, Pnma) to a lower-symmetry phase (monoclinic, P21/m), the δ-$CsPbI_3$ single crystal exhibited an anomalous longitudinal deformation phenomenon with transversely observed fractures (Figure 1.b). Such behavior is associated with martensitic phase transformation that lead to fracture and plastic deformation throughout the crystal.

Figure 1. (a) Raman spectra and (b) Raman maps (peak center at 126 cm^{-1}) of the single crystal of δ-CsPbI3 under hydrostatic loading.

(a) (b)



Acknowledgments: Acknowledgments: The author thanks to CAPES, CNPQ (407954/2022-8 and 407956/2022-0), FINEP (CV. 01.22.0174.00), and Rede VERDES FUNCAP (075480003/2023).