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Impact of high-pressure evolution of elementary distortions on the phase-transition of RFeO_3

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Rare-earth orthoferrites (RFeO3) have been intensively studied in last years, as they exhibit a variety of interesting physical properties, with a large number of works having addressed the underlying microscopic mechanisms [1]. The rare-earth size drives the cooperative rotations of the FeO6 octahedra, which is known to linearly scale with the octahedra tilt angles [1]. Their physics has been studied with hydrostatic pressure as external parameter. Though empirical rules regarding the pressure dependence of octahedral tilts and rare-earth displacements in 3:3 perovskites have been proposed [2], a systematic and detailed experimental study of the pressure evolution of the lattice distortions of a representative set of RFeO3 is still missing. Moreover, contradictory theoretical results have been discussed in literature, such as the prediction that the octahedral tilts and rare-earth displacements should decrease with pressure, via their trilinear coupling [2]. This decrease should yield a structural phase transition into a higher-symmetric structure at some critical pressure PC, which, in fact, is not the case of RFeO3, presenting a pressure-driven isostructural transition [3].
Our work reports on the evolution of the octahedral tilts and mean Fe-O bond lengths of RFeO3 (R = Nd, Sm, Eu, Gd, Tb and Dy) with applied hydrostatic pressure by Raman scattering and synchrotron XRD up to 55 GPa. We have found out that the octahedra tilts decreases with pressure for R = Nd-Sm, whereas it increases for R = Tb-Lu, affecting the displacement of the rare-earths due to trilinear coupling, and compression rate of the FeO6 octahedra [3]. EuFeO3 stands at the borderline, with nearly pressure-independent tilt angles. The surprising crossover between the two opposite pressure behaviors is discussed in relation with the general rules proposed from different theoretical approaches. The similarity of the pressure-induced isostructural insulator-to-metal phase transition, observed in the whole series, point out that the tilts play a minor role in its driving mechanisms. A clear relationship between octahedral compressibility and critical pressure is ascertained with respect to a critical volume of the FeO6 octahedra.

[1] E. Bousquet and A. Cano, J. Phys.: Cond. Matt. 28, 123001 (2016)
[2] H. J. Xiang, J. Íñiguez, J. Kreisel and L. Bellaiche, Phys. Rev. B 96, 054102 (2017)
[3] R. Vilarinho, P. Bouvier, M. Guennou, I. Peral, et al., Phys. Rev. B 99, 064109 (2019)

Summary

This work reports on the evolution of the octahedral tilts and mean Fe-O bond lengths of RFeO3 (R = Nd, Sm, Eu, Gd, Tb and Dy) with applied hydrostatic pressure by Raman scattering and synchrotron XRD up to 55 GPa, and their impact on the high-pressure structural insulator-to-metal phase transition.

Topic

1. Materials under high pressure

Primary authors: VILARINHO, Rui (IFIMUP, Departament of Physics and Astronomy, Faculty of Sciences, University of Porto); Dr GUENNOU, Mael (Luxembourg Institute of Science and Technology, rue du Brill, Belvaux, Luxembourg); Dr BOUVIER, Pierre (Université Grenoble-Alpes, CNRS, Institut Néel, 38000 Grenoble, France); Dr WEBER, Mads (Luxembourg Institute of Science and Technology, rue du Brill, Belvaux, Luxembourg); Dr PERAL, Inmaculada (Luxembourg Institute of Science and Technology, rue du Brill, Belvaux, Luxembourg); Prof. TAVARES, Pedro (Centro de Química, Universidade de Trás-os-Montes e Alto Douro, Vila Real, Portugal); Dr GARBARINO, Gaston (European Synchrotron Radiation Facility, 38043 Grenoble, France); Dr MEZOUAR, Mohamed (European Synchrotron Radiation Facility, 38043 Grenoble, France); Prof. KREISEL, Jens (Luxembourg Institute of Science and Technology, rue du Brill, Belvaux, Luxembourg); Prof. ALMEIDA, Abílio (IFIMUP, Departament of Physics and Astronomy, Faculty of Sciences, University of Porto); Prof. AGOSTINHO MOREIRA, Joaquim (IFIMUP, Departament of Physics and Astronomy, Faculty of Sciences, University of Porto)

Presenter: VILARINHO, Rui (IFIMUP, Departament of Physics and Astronomy, Faculty of Sciences, University of Porto)

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