

Structural transition and magnetism of $(\text{Sr}_{1-x}\text{Ba}_x)\text{FeO}_2$

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An unprecedented FeO_4 square planar coordination has been recently realized in SrFeO_2 by reducing perovskite SrFeO_3 with CaH_2 at low temperatures. The structure of SrFeO_2 is made up of corner-shared FeO_4 square planes intervened by strontium atoms and is isostructural with the IL structure SrCuO_2 . Surprisingly, first-principles calculations revealed that this new material is a thermodynamically stable phase. From the isomer shift of Mossbauer spectra, we found that the Fe^{2+} in SrFeO_2 is indeed more strongly bonded to neighboring O^{2-} than those of any other existing divalent ferrous compounds. The utmost feature allows this material to achieve a magnetic order well above room temperature ($T_N = 473 \text{ K}$) and explains why a spin-state transition is realized for the first time in a four-coordinated metal center. This feature is also responsible for dynamic structural manipulations during the hydride reaction. SrFeO_2 is susceptible of substantial positive chemical pressure: the substitution of the strontium site with calcium having a smaller ionic radius is possible up to as much as 80 %. A further and complete substitution to CaFeO_2 results in a considerable distortion of the FeO_4 square plane towards tetrahedron.

Here, we report on the negative chemical pressure effect on the structural and magnetic properties by the Sr-to-Ba substitution.

The neutron diffraction study and the synchrotron X-ray diffraction revealed that SrFeO_2 with the IL structure can tolerate only up to 30% substitution of Ba unlike the case of Ca-substitution.[1] Too long Fe-O distance caused by the Ba-substitution destabilizes the IL structure. The negative pressure effect does not drastically change the magnetic properties in contrast to the

theoretical anticipation, meaning that iron atoms are still very strongly bonded to oxide ion.

[1]T. Yamamoto, et al., *Inorg. Chem.* 49, 2010, 5957.

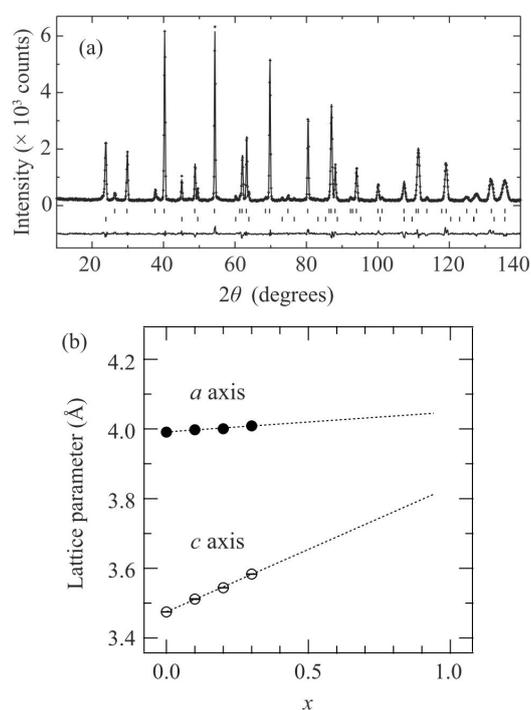


Fig. 1. Fig. (a) Structural characterization of $\text{Sr}_{0.2}\text{Ba}_{0.8}\text{FeO}_2$ ($x = 0.2$) by the Rietveld refinement of powder neutron diffraction data at room temperature. (b) The lattice parameters of $(\text{Sr}_{1-x}\text{Ba}_x)\text{FeO}_2$.