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Investigations of magneto-elastic coupling in a multiferroic ferrite by in-situ precession diffraction

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Imitate couplings among charge, lattice, and spin degrees of freedom are widely considered to breed rich emergent physical properties, like multiferroics and colossal magnetoresistance [1,2]. Deciphering the intertwined interplay among these degrees of freedom is one of the major themes at the core of condensed matter physics. Such an interplay is generally complex and can be further complicated especially at phase transitions, where delicate changes in different kinds of energy can induce prominent changes in different degrees of freedom and introduce emergent physical properties. A typical example is multiferroics, where atomic displacements at phase transitions can interact with charge and spin degrees of freedom and bridge the ferroelectric moment and the (anti)ferromagnetic moment, therefore bringing in the desired magneto-electric coupling [3]. Hence quantitatively determining how atoms move as a function of temperature and unraveling how they respond to the ferroelectric or (anti)ferromagnetic transition in multiferroics, as well as their influences on the electronic structure, can be of great importance to the community, allowing the in-depth understanding and fine control of the multiferroic properties.

In this study, we report a strong magneto-elastic coupling in a typical multiferroic ferrite, *h*-$Lu_{1-x}Sc_xFeO_3$ ($x \sim 0.5$), deciphering how lattice and spin interact and couple with each other at the atomic level. *In-situ* cooling precession electron diffraction results show the lowering of the in-plane symmetry right at the magnetic transition, manifested by the generation of a constellation of satellite reflections (Fig. 1(a)). Quantitative analysis of these satellite reflections reveals that their temperature-dependent intensities vary synchronously with the magnetic susceptibility, suggesting a close coupling between the lattice and spin. Furthermore, combining with the refinement of the *in-situ* neutron diffraction and synchrotron X-ray diffraction results, we quantitatively determine the temperature-dependent lattice parameters (Fig. 1(d)) and more importantly all the atomic positions and displacements of atoms in the unit cell (Fig. 1(e)), where Lu/Sc and O atoms show distinct anomalies at the magnetic transition. Especially for the in-plane oxygens (O3 and O4), they show the most dramatic *z*-axial displacement, which is as large as around ~ 0.1 Å (Fig. 2(e) and 2(f)). Such a displacement magnitude is almost comparable to the atomic displacement at Curie temperature in classic ferroelectrics, like $BaTiO_3$ (0.05-0.4 Å) [4]. While, interestingly, the Fe atoms remain at the high-symmetry position over the whole temperature range (Fig. 2(g)), which is in contrast to the behaviors of multiferroic hexagonal manganites [3]. This suggests that the magnetic-elastic coupling observed in the hexagonal ferrite is mainly governed by the atomic displacement of the oxygen rather than the transition metal. These movements of oxygens induce

different changes in different types of Fe-O bond lengths, which alters relative magnitudes of different magnetic exchange interactions and therefore accounts for the strong magnetic-elastic coupling. Our work not only quantitatively demonstrates the strong magneto-elastic coupling in multiferroic ferrites, but also clarifies its origin at the atomic level, insights from which advance our understanding of the underlying interactions between lattice and spin degrees of freedom [5,6].

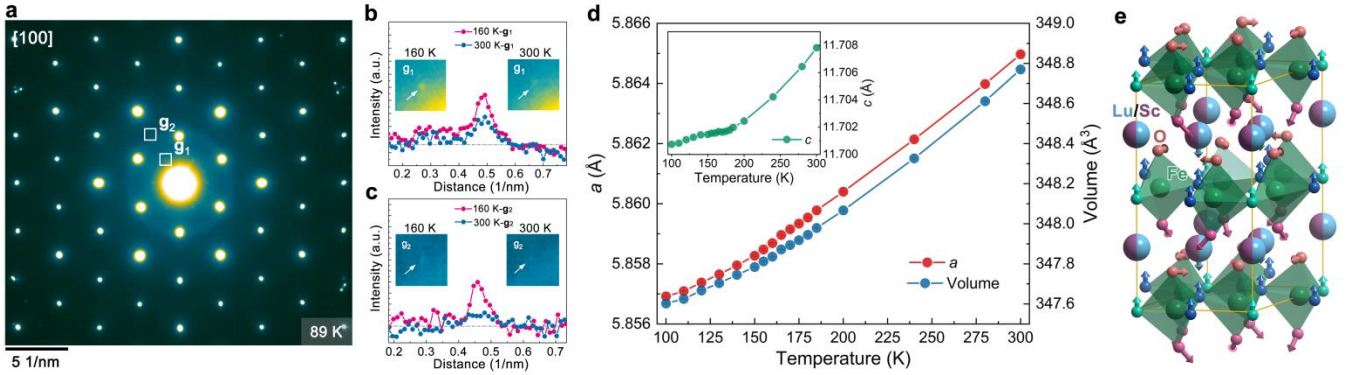

Figure 1. Characterization of the magneto-elastic coupling in Lu1-xScxFeO3. (a) Precession electron diffraction at 89 K. (b,c) Peak intensity for g1 and g2 at 160 K and 300 K. (c) Temperature-dependent lattice parameter and unit-cell volume. (d) Primitive unit-cell with arrows indicating experimentally observed atomic displacements.

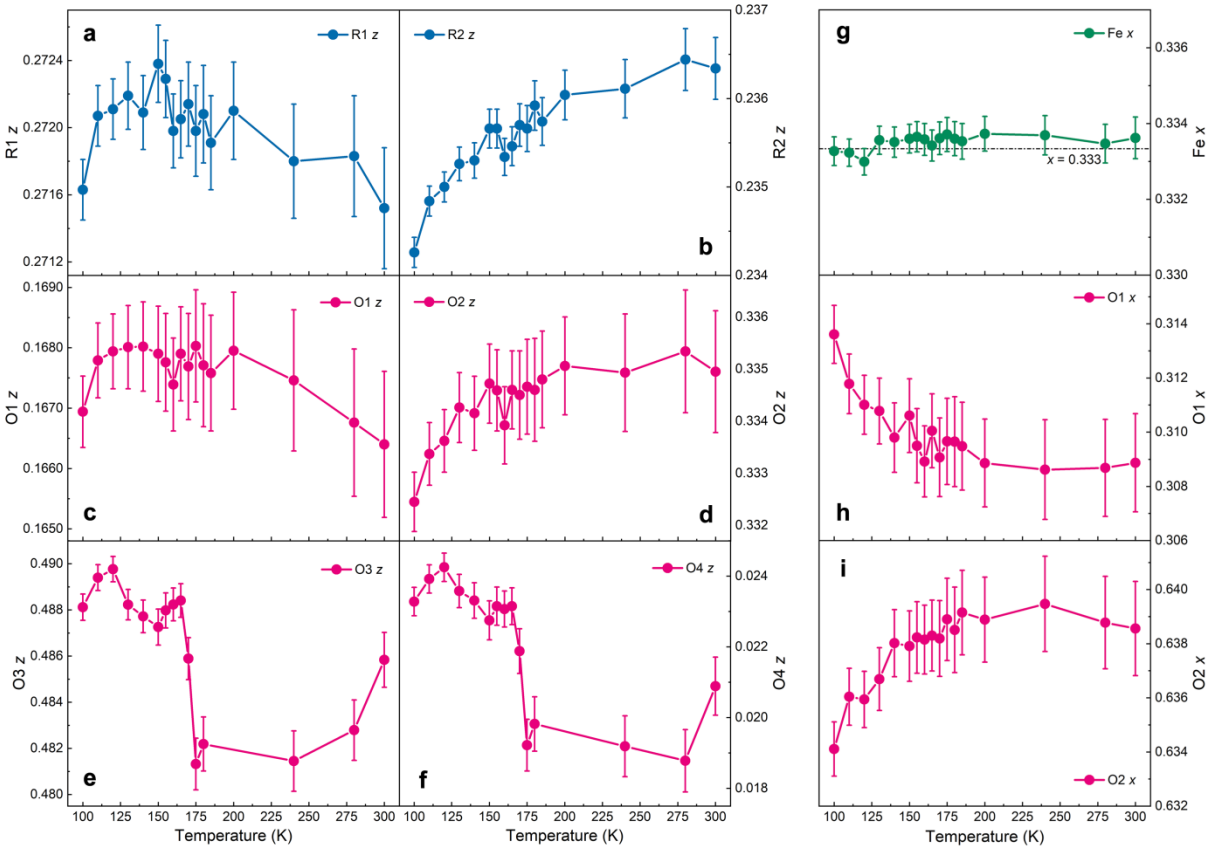

Figure 2. Temperature-dependent atomic positions of all atoms in a 30-atom unit cell. Temperature dependence of the z positions of, Lu/Sc atoms at two different crystallographic sites (a,b), and O atoms at four

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different crystallographic sites (c-f). All the Lu/Sc atoms and O atoms show distinct anomalies of atomic positions at TN. (g) In-plane positions of Fe atoms, which almost remain unchanged around x = 1/3 over the whole temperature range.

References

[1] E. Dagotto, Science **309** (2005) p. 257.
[2] S. Q. Deng *et al*, Phys. Rev. Lett. **122** (2019) p. 126401.
[3] S. Lee *et al*, Nature **451** (2008) p. 805.
[4] R. W. Wyckoff, Crystal Structures (Krieger Publishing, New York, 1986).
[5] S. Q. Deng, et al, *in preparation*, 2021.
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