

Pressure-Induced Structural, Magnetic and Transport Transitions in the Two-Legged Ladder Sr₃Fe₂O₅

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Introduction

The layered compound SrFeO₂ with an FeO₄ square-planar motif exhibits an unprecedented pressure-induced spin state transition ($S = 2$ to 1), together with an insulator-to-metal (I-M) and an antiferromagnetic-to-ferromagnetic (AFM-FM) transition [1]. Similarly, we also found the spin state transition ($S = 2$ to 1), together with an I-M and an AFM-FM transition in the structurally related two-legged spin ladder Sr₃Fe₂O₅ [2] at 34 GPa by ⁵⁷Fe Mössbauer and resistivity measurements. In this report, we have studied the pressure effect on the structural properties of Sr₃Fe₂O₅.

Experimental section

A powder sample of Sr₃Fe₂O₅ was synthesized by hydride reaction of a slightly oxygen deficient Sr₃Fe₂O_{7-x} ($x \sim 0.4$) with CaH₂ [2].

Synchrotron X-ray diffraction (XRD) experiments at high pressures up to 36.7 GPa were performed at the NE1A synchrotron beam line of the PF-AR. The incident X-ray beam was monochromatized to a wavelength of 0.41310 Å. A powder sample of Sr₃Fe₂O₅ was loaded into a 180 μm diameter hole of a pre-indented rhenium gasket of the diamond-anvil cell. Helium was used as a pressure-transmitting medium. The shift of ruby fluorescence was used to determine the pressure. The obtained synchrotron XRD data were analyzed by the Rietveld method using RIETAN-FP program [3].

Result and dissection

In the synchrotron XRD study, we unexpectedly found a drastic change in the diffraction pattern above 30 GPa. Below 30 GPa, all diffraction peaks could be assigned to an *I*-centered orthorhombic structure. The diffraction patterns above 30 GPa could be also indexed on the basis of the orthorhombic unit cell but have different extinction conditions. It follows that the new structure induced by pressure has an *A*-centered orthorhombic lattice. When pressure released, Sr₃Fe₂O₅ returned to *I*-centered orthorhombic structure.

The Mössbauer spectra indicated that the irons in the high-pressure structure are in a square planar geometry having only one crystallographically equivalent site. In addition, the structural transition is reversible with only small hysteresis, indicating that the two structures are

topotactically related with each other. All these observations led us to consider that the structural transition from the *I*- to *A*-centered space group is caused by a change in the stacking sequence of the two-legged ladder blocks as found in Figure a and b.

Assuming space group *Ammm* and the structure with Sr(1) to be at 2*c* (0.5, 0.5, 0), Sr(2) at 4*j* (0.5, 0.5, *z*), Fe at 4*i* (0, 0, *z*), O(1) at 2*a* (0, 0, 0), O(2) at 4*i* (0, 0.5, *z*) and O(3) at 4*i* (0, 0, *z*), we refined the structural parameters. The refinements converged well, providing $R_{wp} = 0.90\%$, $\chi^2 = 0.89$ (see Figure c). These small agreement indices as well as the small atomic displacement parameters *B* for all atoms suggest that the refined structure is reasonable.

In this way, we resolved the high pressure structure of Sr₃Fe₂O₅. It is interesting that the high pressure structure of Sr₃Fe₂O₅ undergoes several magnetic and transport transitions. For more details of the study, see the reference [4].

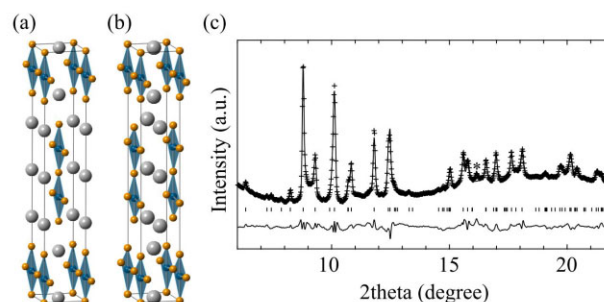


Figure. The structure of Sr₃Fe₂O₅ at (a) low pressure and (b) high pressure. White, blue, and orange spheres represent Sr, Fe and O atoms, respectively. Structural characterization of Sr₃Fe₂O₅ by the Rietveld refinement of the synchrotron XRD data at 36.7 GPa and RT.

References

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