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High pressure neutron and synchrotron X-ray diffraction studies of tetragonal $LaFeAsO_{0.9}F_{0.1}$

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We studied polycrystalline tetragonal $LaFeAsO_{0.9}F_{0.1}$ up to 9 GPa using time-of-flight neutron and synchrotron X-ray diffraction. Consistent with previous studies, the layer-structured $LaFeAsO_{0.9}F_{0.1}$ has a bulk modulus of 74–79 GPa, with the $c-$axis being twice as compressible as the $a-$axis. The refined structural parameters under pressure show non-monotonic variation with kink points at 4 GPa, well correlating with a maximum superconducting temperature (Tc) of 43 K previously reported for $LaFeAsO_{0.9}F_{0.1}$. At this pressure, however, both the As–Fe–As bond angle and anion height from the Fe layers deviate substantially from the respective ideal values of 109.47° and 1.38 Å for a regular $FeAs_4$ tetrahedron. These findings indicate that the correlation between the maximum Tc and the geometry of conductive Fe–As layers is material dependent and may also be sensitive to atomic doping in the parent Fe-based superconductors.

Keywords: neutron diffraction; high pressure; iron-based superconductivity; isostructure transition

1. Introduction

The discovery of superconductivity in iron-based materials has attracted extensive research interest over the past few years. The very first report in this new field was an '1111'-type $LaFeAsO_{1-x}F_x$ [1], which exhibits high superconducting temperature (Tc) without the CuO_2 structural units, commonly present in the Cu-based superconductors. This research ignited a firestorm of research to understand the mechanisms behind high Tc superconductivity and to unveil new superconductors in other iron-based systems. The '122' and '111'-type iron arsenides as well as '11'-type iron selenide with superconductivity have been discovered subsequently [2–4]. $LaFeAsO_{0.89}F_{0.11}$, with a Tc of 26 K at atmospheric pressure, has a layered structure crystallizing in a tetragonal $P4/nmm$ space group with lattice constants $a = 4.0397(4)$ Å

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and $c = 8.7553(9)$ Å. There are two structurally distinct layers in $LaFeAsO_{1-x}F_x$. The tetrahedral FeAs layers, intercalated by La–O (F) layers, serve as conductive carriers and are negatively charged. The positively charged La–O (F) layers function as the electron donors; they also confine the FeAs layers along the crystallographic c-axis, resulting in a strong interaction among the electrons. In general, the behavior of iron-based superconductors is sensitive to both composition and pressure [5,6,11]. Doping F^- on the O^{2-} site, for example, provides an extra positive charge in the La–O layer, leading to increased electron density in carrier layers, and is primarily responsible for the observed rise in the superconducting temperature. In the case of $LaFeAsO_{1-x}F_x$, the Tc at atmospheric pressure exhibits a parabolic-like dependence on F^- content, with the highest Tc of 26 K at 5–11 at.% F^- [1].

Pressure plays important roles in modulating the superconductivity of iron-based materials as it directly tunes the geometry of alternating layers and the associated electronic configuration [5–10,12–16]. Based on the electrical measurements under high pressure, Takahashi et al. [5] reported a maximum Tc of 43 K for $LaFeAsO_{0.89}F_{0.11}$ at the pressure of ~4 GPa, a 65% increase compared with its ambient-pressure value. However, in spite of several subsequent high pressure studies [6,17,18], the structural response of $LaFeAsO_{1-x}F_x$ to pressure and its correlation to the superconducting temperature have not yet been established. An investigation of these relationships will not only shed light on the mechanisms underlying iron-based superconductivity, but also guide the future pathways to formulate new superconductors. To further understand the relationship between pressure-induced structural and Tc evolution [2], we performed in this work *in situ* high pressure neutron and synchrotron X-ray diffraction on $LaFeAsO_{1-x}F_x$ with $x = 0.1$.

2. Experimental methods

The polycrystalline $LaFeAsO_{0.9}F_{0.1}$ sample was prepared using a two-step, solid-state reaction method [19]. First, Fe and As powders in an 1:1 atomic ratio were ground and pressed into a pellet. Then it was sealed in an evacuated quartz tube and heated at 750° C for 10 h. The resultant pellet was smashed and ground together with LaF_3, La_2O_3 (purity 99.9%) and La powders (purity 99.99%) in the stoichiometric composition of $LaFeAsO_{0.9}F_{0.1}$. They were then pressed into a pellet and heated in an evacuated quartz tube at 900°C for 2 h, followed by an annealing at 1150°C for 50 h and slow cooling to room temperature. High pressure neutron diffraction experiment on $LaFeAsO_{0.9}F_{0.1}$ was performed by using a 500-ton, toroidal anvil press (TAP-98) [20,21] at the flightpath of High Pressure-Preferred Orientation [22,23], Los Alamos Neutron Science Center. The time-of-flight neutron diffraction spectra of the powder sample were collected by three detector banks at a fixed Bragg angle of $2\theta = \pm 90°$. A mixture of $LaFeAsO_{0.9}F_{0.1}$ and NaCl powders was first compressed into a cylindrical pallet of 5.4 mm diameter and 7 mm length, and was then loaded into a high-P–T ceramic cell assembly specially designed for TAP-98 (see Ref. [24] for detail). The synchrotron X-ray experiment was conducted using a cubic anvil apparatus at beamline X17B2 of the National Synchrotron Light Source, Brookhaven National Laboratory [25]. An energy-dispersive X-ray method was employed with diffracted X-rays collected at a fixed Bragg angle of $2\theta \approx 6.48°$. A cubic mixture of amorphous boron and epoxy resin was used as the pressure-transmitting medium, and amorphous carbon was used as the furnace material. The starting $LaFeAsO_{0.9}F_{0.1}$ and NaCl powders were packed, in a volume ratio of approximately 1:1, into a cylindrical container of hexagonal boron nitride (BN), 1.0 mm inner diameter and 2.0 mm length. In both types of the experiments, we used NaCl as the internal pressure standard and Decker's EOS [26] to determine the pressure. The neutron diffraction data were analyzed by using the Rietveld method with the General Structure Analysis System [27].

3. Results and discussion

In Figure 1(a), we show an X-ray diffraction pattern for the as-prepared $LaFeAsO_{0.9}F_{0.1}$. A typical high-resolution transmission electron microscope (HR-TEM) image of $LaFeAsO_{0.9}F_{0.1}$ is shown in the inset. All strong diffraction peaks can be indexed by a tetragonal structure and also show excellent agreement with the calculated pattern. Therefore, the sample is dominated by $LaFeAsO_{0.9}F_{0.1}$ with only a tiny amount of impure FeAs, which was also revealed with similar relative intensities in the original work of Kamihara et al. [1]. The well-resolved microstructure at atomic scale coupled with sharp diffraction lines indicates that the as-prepared $LaFeAsO_{0.9}F_{0.1}$ is well crystallized. Figure 1(b), which was obtained through the VESTA software [28], illustrates a schematic crystal structure of tetragonal $LaFeAsO_{0.9}F_{0.1}$. Substitution of F^- on the O^{2-} sites

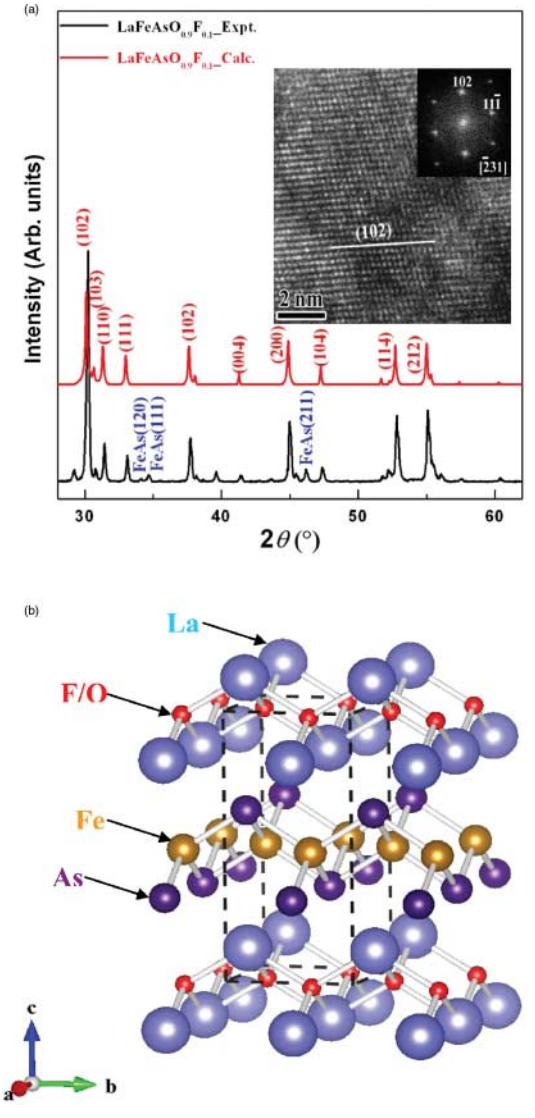

Figure 1. (a) X-ray diffraction patterns of $LaFeAsO_{0.9}F_{0.1}$. A typical HR-TEM image of $LaFeAsO_{0.9}F_{0.1}$ is displayed in the inset. (b) A schematic crystal structure of $LaFeAsO_{0.9}F_{0.1}$.

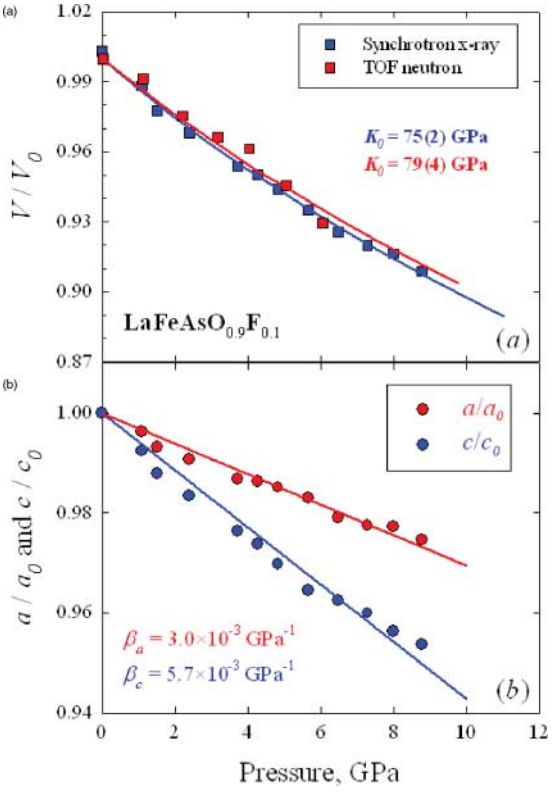

Figure 2. Pressure dependence of the normalized unit-cell volume (a) and lattice parameters a and c (b) for $LaFeAsO_{0.9}F_{0.1}$. The curves in (a) represent result of the least-squares fit using a second-order Birch–Murnaghan equation of state. The axial compressibility is obtained by linear fits of the data in (b).

makes the La–O layers to be more positively charged; in the mean time, the Fe–As layers become more negatively charged, which increases the electron density of the conductive layer.

Figure 2 shows the evolution of unit-cell volume and lattice parameters (a and c) of $LaFeAsO_{0.9}F_{0.1}$ as a function of pressure. At the highest experimental pressure of 9 GPa, the tetragonal structure with $P4/nmm$ space group is preserved with no phase transition. Also noted is that all three lattice parameters decrease monotonically with increasing pressure. The calculated bulk moduli based on a second-order Birch–Murnaghan equation of state (*i.e.* $K_0' = 4$) are 75(2) GPa with synchrotron X-ray data and 79(4) GPa using neutron data, which are in good agreement within the mutual uncertainties (Figure 2(a)). These results are also consistent with that of a previous study in diamond anvil cell (78 GPa in Ref. [18]). Similar to Cu-based high-Tc superconductivity (*e.g.* Ref. [29]), the crystallographic direction normal to the FeAs layer (*i.e.* the c-axis) is substantially more compressible than the direction parallel to the FeAs layer (Figure 2(b)). Linear fits of the normalized lattice parameters result in the axial compressibility of 3.0×10^{-3} GPa^{-1} along the a-axis and 5.7×10^{-3} GPa^{-1} along the c-axis, both of which are comparable to those reported by Takahashi et al. [17] for $LaFeAsO_{0.89}F_{0.11}$. This anisotropic compression is expected to lead to additional change in charge distributions and makes the layered $LaFeAsO_{0.9}F_{0.1}$ more easily tuned by the external pressure.

In order to study the pressure effects on crystal structure and the related electronic properties at the atomic level, we refined structural parameters using the Rietveld refinement method for all neutron diffraction data at various pressures [27]. The two key parameters, the As–Fe–As bond angle and the anion height, are plotted as a function of pressure in Figure 3. Here, the As–Fe–As

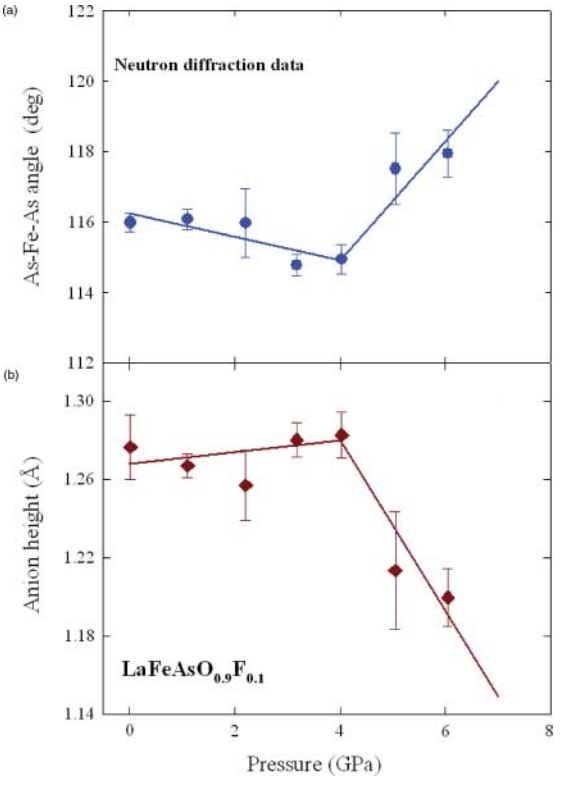

Figure 3. The As–Fe–As bond angle (a) and the anion height and (b) plotted as a function of pressure at room temperature. Straight lines are linear fits of the data for guiding the trends of variation.

bond angle refers to the angle α conventionally defined for a $FeAs_4$ tetrahedron and the anion height is the vertical separation between the As atom and the Fe layer. The β angle in $FeAs_4$ tetrahedron shows a similar trend of variation to that of the anion height and is hence not given in this article. As shown in Figure 3(a), the α angle decreases with increasing pressure; it reaches a minimum of 114.9° at 4 GPa and then rapidly increases at higher pressures. The anion height varies in different ways (Figure 3(b)) with a maximum value of 1.283 Å at 4 GPa, which is expected from the mathematical relationship for a tetragonal structure. The close relation between the angle α and the anion height indicates that the structural effects on Tc can actually be elucidated by one of these two parameters.

Previous studies on $LaFeAsO_{0.89}F_{0.11}$ show a positive dependence on pressure of Tc below 4 GPa, where it reaches the maximum of 43 K and then decreases rapidly with further increase in pressure [5,17]. This parabolic-type behavior between Tc and pressure has subsequently been reported for a number of Fe-based superconductors [7,8,16,30]. Of particular interest is that the highest Tc is typically achieved under pressure when a distorted FeAs tetrahedron becomes regular or 'optimized' at $\alpha = \beta = 109.47°$ [31]. On the other hand, based on the anion height – Tc systematics of different types of Fe-based superconductors [32] – a parabolic-like correlation was also revealed with the highest Tc corresponding to the anion height of 1.38 Å. This finding indicates that the anion height in a given Fe-based superconductor may show a similar parabolic-like evolution with pressure. Indeed, recent experiments on $Na_{1-x}FeAs$ [16] and $SmFeAsO_{1-x}F_x$ [30] demonstrated that the highest Tc concurs with an anion height of ∼1.38 Å under identical pressures. The structural parameters are closely tied to the optimal Tc in all these instances because a regular or a less-distorted charge reservoir layer would lead to a shorter electron conductive path to

the donor layers [33]. In addition, the antiferromagnetic superexchange interaction (J_2) between the next nearest neighbor Fe–Fe atoms is involved in the electron pairing between the hole-type Fermi sheet around the Γ point and the electron-type Fermi sheet around the *M* point [34]. The J_2 interaction is bridged by the As atom through the covalent bonding between the Fe and As atoms. Therefore, this interaction is sensitive to the local geometry of Fe–As bonding and will ultimately affect the Fermi surface and the electrons distributions and hence the superconducting temperature.

The present findings in Figure 3 are qualitatively in line with the pictures described in the preceding paragraph. First, the refined Fe–As–Fe bond angle and anion height both vary with pressure toward a less-distorted tetrahedron. Second, the kink points around 4 GPa are unambiguously defined for both parameters, which correlates well with a Tc maximum of 43 K at the same pressure for $LaFeAsO_{0.89}F_{0.11}$. Last but not least, at pressures above 4 GPa, the FeAs tetrahedron becomes progressively more distorted, consistent with the observed drop in Tc. However, at 4 GPa, both the As–Fe–As bond angle and anion height from the Fe layers deviate substantially from the observed values of 109.47° and 1.39 Å for a regular $FeAs_4$ tetrahedron in $SmFeAsO_{0.81}F_{0.19}$ [30]. This earlier work also showed that at the same pressure of 0.6 GPa, the 'optimized' structural parameters are well correlated with a maximum Tc of 55.2 K. The difference between La and Sm iron arsenide indicates that the correlation between the maximum Tc and the geometry of conductive Fe–As layers is material dependent. This correlation may also be sensitive to the exact nature of atomic doping in the parent Fe-based superconductors. In the work of Garbarino et al. [18], for example, the superconducting temperature for $LaFeAsO_{0.9}F_{0.1}$ was found to decrease monotonically at all experimental pressures up to 20 GPa (*no parabolic-type behavior!*). It was speculated that this unusual behavior may be attributed to 'over-doping' of F^{-1} relative to the nominal stoichiometric composition. Defects and impurities associated with atomic doping may further complicate the matter in this regard.

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