The New Fe-based Superconductor

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Abstract

The discovery in fluorine doped LaFeAsO superconductor with *TC* = 26 K was reported in February of 2008[1]. This discovery inspired researchers around the globe to study this unusual family of materials, which contain as their essential feature a square net of iron in the formal oxidation state Fe^{2+}. In the following month of 2008, hundreds of papers were published on these and related compounds and they have been analyzed with almost every imaginable experimental technique. A group in Beijing reported their $ReFeAsO_{1-\delta}$ (Re =Sm, Nd, Pr, Ce, La) superconductor which is prepared by high-pressure synthesis and without fluorine doping. The highest T_C they obtained so far is 55K in $SmFeAsO_{1-\delta}$ which suggests an unconventional pairing mechanism may be at work [3][4]. Several related families of materials with different crystal structures (still containing the square nets of formally divalent iron) were examined, and superconductivity has been found in almost every case. These fascinating families of compounds will be introduced in this paper and their crystal structure, physical properties of the superconducting and undoped "parent" phases will be discussed.

Introduction

Iron-based superconductors contain layers of iron and a pnictogen such as arsenic or

phosphorus, or chalcogens. Most undoped iron-based superconductors show a tetragonal-orthorhombic structural phase transition followed at lower temperature by magnetic ordering, similar to the cuprate superconductors. The magnetic parent compounds of the iron arsenide family of superconductors crystallize in tetragonal structures, with LaFeAsO [1] forming in the tetragonal ZrCuSiAs structure. As Y. Kamihara's report,

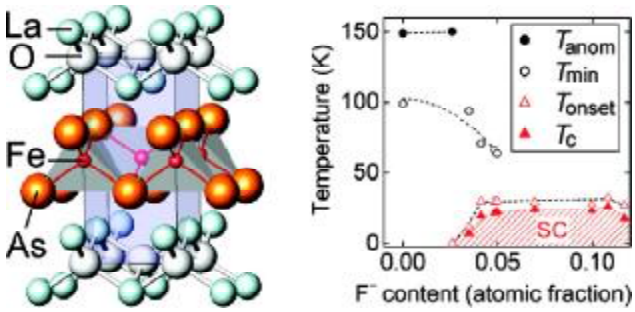

Fig1. (a) Crystal structure of LaOFeAs. (b) *T*c, *T*onset, and *T*min in the F-*T* curves as a function of F- content (*x*) for $La[O_{1-x}F_x]FeAs$. *T*c is defined as the temperature where the F value becomes half of that at *T*onset. *T*anom values for the undoped and $LaO_{0.97}F_{0.03}$- FeAs are also shown. Dotted curves are guides for eyes.

They discovered this iron-based compound which undergoes superconducting transition under doping with F^- ions at the O^{2-} site. As shown by Fig1[1], its *T*c exhibits a trapezoidal shape dependence on F^- content, with the highest *T*c of ~26 K at 5-11 atom %. The analysis of undoped compounds, such as LaOFeAs, is expected to provide important information toward the understanding of the superconducting state reached by ~10% F doping. People have studied the phonon density of states (PDOS) in $LaFeAsO_{1\_x}F_x$ with inelastic neutron scattering methods [3]. The PDOS of the parent compound (x= 0) is very similar to the PDOS of samples optimally doped with fluorine to achieve the maximum Tc (x ~0.1).This is unlike copper based superconductor. Neutron scattering experiments have provided evidence of magnetic order in LaOFeAs at 134 K: Fe spins order into ferromagnetic ‘‘stripes’’ that are aligned antiferromagnetically [5–7]. In the two-dimensional (2D) square lattice notation, the LaOFeAs magnetic structure factor has peaks at wave vectors q ~(0,π), (π, 0) [5–7]. Assuming a smooth continuity between the undoped and F-doped compounds, the pairing mechanism could be magnetic in origin and triggered by this unusual magnetic state [8]. More evident shows that Superconductivity in LaFeAsO emerges from specific structural and electronic conditions in the $(FeAs)^{\delta-}$ layer.

However, if only the iron arsenide layer is essential, also other structure types could serve as parent compounds. Another important compound in iron based family is $BaFe_2As_2$, which is called the "122" superconductor (see Fig2)[14]. The undoped parent phases LaFeAsO and $BaFe_2As_2$ have FeAs square-lattice sheets, and itinerant electrons in these layers undergo antiferromagnetic long range order (AFLRO) below modest temperatures, TSDW ~140 K[5]; electron or hole doping suppresses the AFLRO and induces superconductvity.

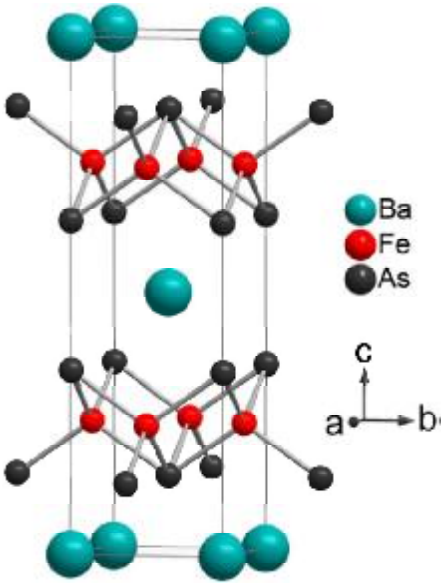

Fig.2 Crystal structure of $BaFe_2As_2$ ($ThCr_2Si_2$-type structure, space group I4=mmm)

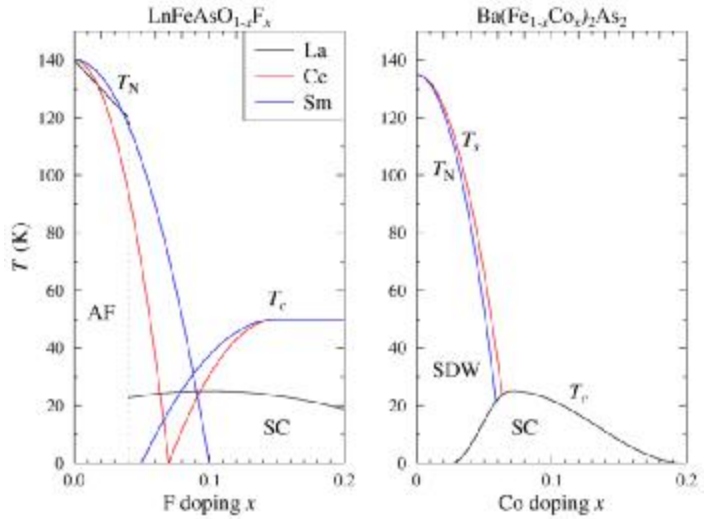

Fig.3. Simplified doping dependent phase diagrams of iron-based superconductors for both Ln-1111 and Ba-122 materials. The phases shown are the antiferromagnetic/spin density wave (AF/SDW) phase close to zero doping and the superconducting phase around optimal doping.

Iron based superconductor are poor metals rather than Mott insulators and have five bands at the Fermi surface rather than one. The phase diagram emerging as the iron-arsenide layers are doped is remarkably similar, with the superconducting phase close to or overlapping the magnetic phase. Strong evidence that the T_c value varies with the As-Fe-As bond angles has already emerged and shows that the optimal Tc value is obtained with undistorted $FeAs_4$ tetrahedra.

Theoretical Calculations

Many theoretical calculations have been done to understand the properties of the iron based superconductor. Such as band structure calculations that have shown the relevance of the 3d levels of Fe [9,10]. A metallic state involving a Fermi surface (FS) made out of disconnected small pieces (‘‘pockets’’) was predicted [9]. To understand some of the properties of the undoped limit, electron correlations appear to be important [10]. In K. Haule’s paper, they compute the electronic structure, momentum resolved spectral function and optical conductivity of the new superconductor LaO1_*x*F*x*FeAs within the combination of the density functional theory and dynamical mean field theory. They find that the compound in the normal state is a strongly correlated metal and the parent compound is a bad metal at the verge of the metal insulator transition. And they argue that the superconductivity is not phonon mediated. And some calculation showed that the optimized position of As atom doesn’t agree with experimental structure [12].Fe magnetic moment vary sensitively to As position. Two-orbitals descriptions [11, 13] and other models have been proposed, and a variety of approximations have led to several unconventional pairing channel proposals [8].

Experimental Method and Result

Many experiments have been done on the iron based superconductor to investigate its properties. In this paper I’ll give some experimental results which are quite important. At high temperatures LaFeAsO is a low carrier concentration metal with conduction dominated by electrons and with no local magnetic moment. Recording to Michael A. McGuire’s report, upon cooling, this material undergoes a tetragonal orthorhombic crystallographic phase transition at ~160 K followed closely by an antiferromagnetic ordering near 145 K. Temperature dependent powder x-ray and neutron diffraction

measurements(Fig5,6) is used to analysis these phase transitions. A magnetic moment of ~0.35μB per iron is derived from Mössbauer spectra in the low-temperature phase. Evidence of the structural transition is observed at temperatures well above the transition temperature (up to near 200 K) in the diffraction data as well as the polycrystalline elastic moduli probed by resonant ultrasound spectroscopy measurements [14]. A dramatic increase in the magnitude of the Hall coefficient below 160 K is also reported (Fig4). The results suggest that the structural distortion leads to a localization of carriers on Fe, producing small local magnetic moments which subsequently order antiferromagnetically upon further cooling. Evidence of strong electron-phonon interactions in the high-temperature tetragonal phase is also observed.

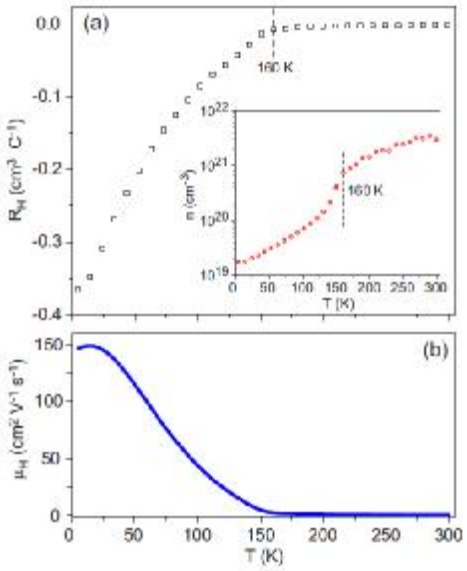

FIG.4 Results of Hall-effect measurements on LaFeAsO showing the remarkable decrease in inferred carrier concentration and high mobility at low temperatures. (a)The measured Hall coefficient and inferred carrier concentration (inset). (b) The Hall mobility calculated from the carrier concentration in (a) and the electrical resistivity.

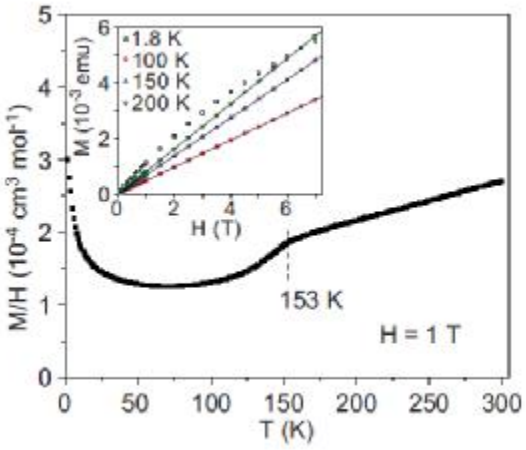

FIG. 5 The temperature dependence of *M*/*H* (per mole of formula units) for a PXRD pure polycrystalline
LaFeAsO sample. The inset shows *M*(*H)* data at four different temperatures.

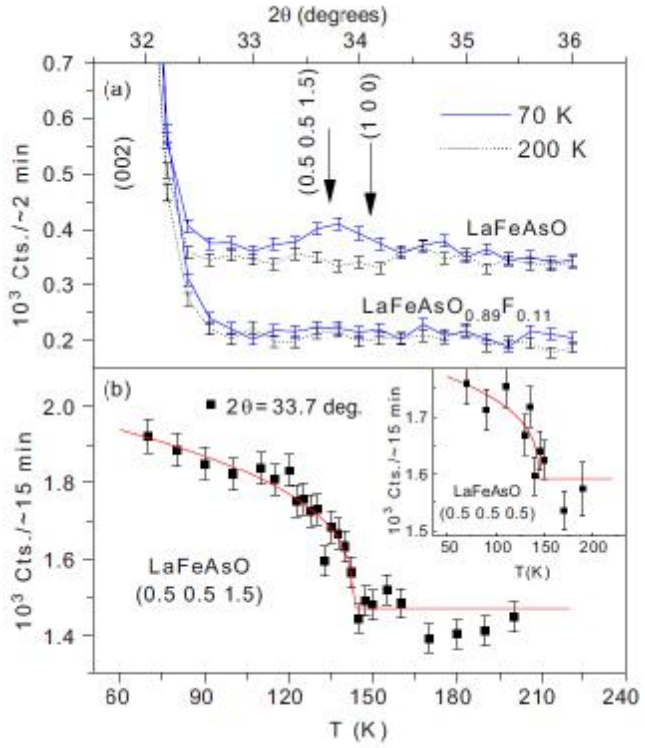

FIG. 6 (a) Neutron diffraction data for LaFeAsO and $LaFeAsO_{0.89}F_{0.11}$ at 70 and 200 K. Arrows indicate the angular position of the (1 0 0) and (0.5 0.5 1.5) wave vectors. For clarity, the data for LaFeAsO have been displaced by 150 counts. (b) The temperature dependence of the (0.5 0.5 1.5) and (0.5 0.5 0.5) (inset) positions. The wave vectors are labeled using the tetragonal setting. The lines are a guide to the eye.

In Clarina de la Cruz's paper, they reported the neutron-scattering experiments that demonstrate that LaOFeAs undergoes an abrupt structural distortion below 155 K, changing the symmetry from tetragonal (space group P4/nmm) to monoclinic (space group P112/n) at low temperatures, and then, at 137 K, develops long-range SDW-type antiferromagnetic order with a small moment but simple magnetic structure. Doping the system with fluorine suppresses both the magnetic order and the structural distortion in favour of superconductivity. Therefore, like high-Tc copper oxides, the superconducting regime in these iron-based materials occurs in close proximity to a long-range-ordered antiferromagnetic ground state.

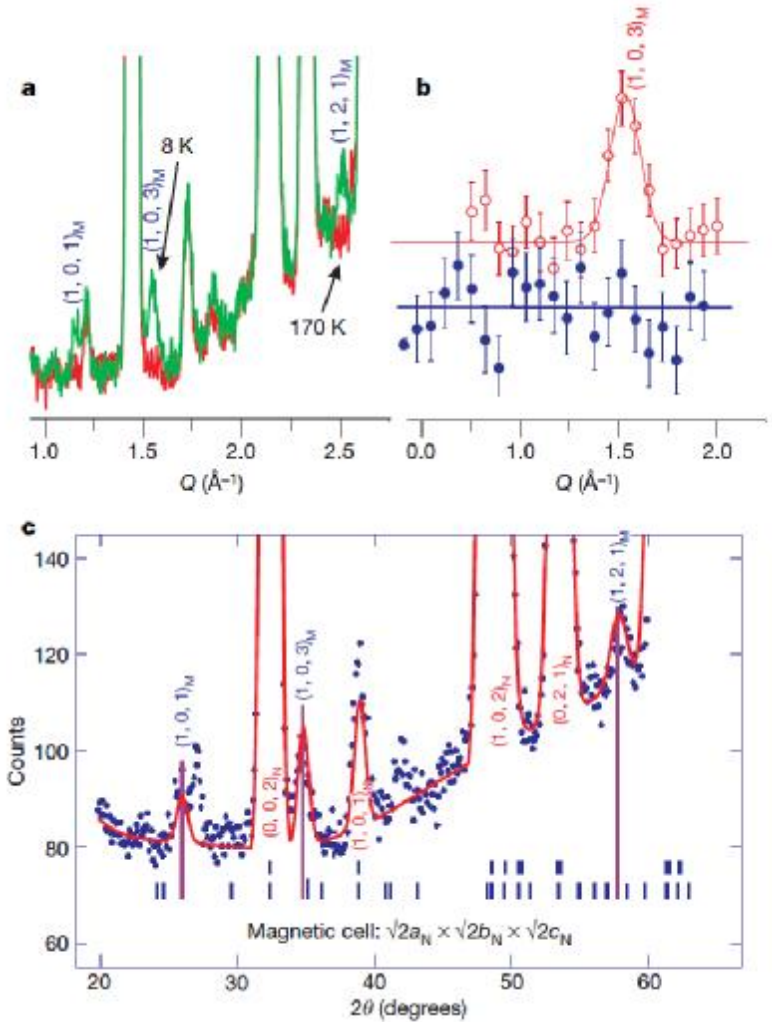

Fig.7. [5] Temperature dependence of the magnetic scattering for LaOFeAs and $LaO_{0.92}F_{0.08}FeAs$. a, LaOFeAs data clearly showing (marked) magnetic peaks at 8K that disappear at 170 K, counting 1 min per point. b, The temperature difference spectra (8–170 K) measured using the HB-1A spectrometer for LaOFeAs (red) and $LaO_{0.92}F_{0.08}FeAs$ (blue), counting 4 min per point. The magnetic (1, 0, 3) peak is missing from the $LaO_{0.92}F_{0.08}FeAs$ scan. Error bars, 1 s.d. c, LaOFeAs data again showing both magnetic and nuclear Bragg peaks (data, crosses; Bragg peak positions,

short vertical lines) together with the model fit (solid line), at 8 K. Data in a and c were collected using the BT-7 spectrometer with an incident beam wavelength of λ =2.44 $\mathring{A}$, a PG(0, 0, 2) monochromator and a PG (pyrolytic graphite) filter. Data in b were collected using the HB-1A spectrometer with λ =2.36 $\mathring{A}$ and a PG filter.

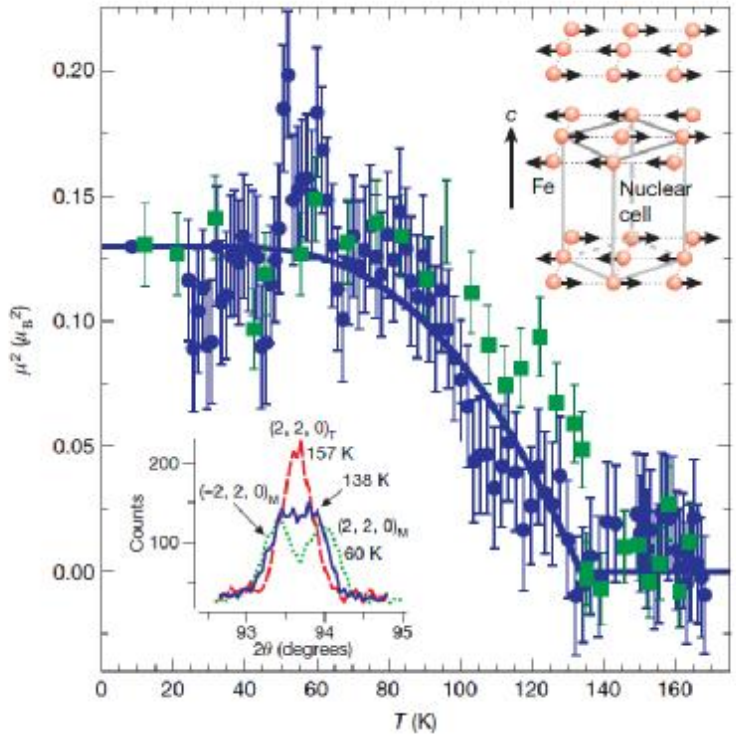

Fig.8. [5] Temperature dependence of the order parameter at Q=1.53 $\mathring{A}^{-1}$, obtained using the magnetic structure we determine for LaOFeAs. Blue circles, BT-7 spectrometer data; green squares, HB-1A spectrometer data. The solid line is a simple fit to mean field theory that gives a Ne´el temperature T_N=137(3) K. The bottom-left inset shows the temperature dependence of the nuclear (2, 2, 0) peak obtained using the BT- 1 diffractometer. It is clear that the lattice is distorted at 138 K, before the long-range static antiferromagnetic order sets in at ~137 K. The top-right inset shows the antiferromagnetic structure of the system, giving a $\sqrt{2}a_N \times \sqrt{2}b_N \times 2c_N$ unit cell with moment directions parallel to the planes of iron atoms. To determine the magnetic structure, we note that three magnetic peaks with h+k+l=2n, where h, k and l are Miller indices and n=0, 1, 2, …, suggest that the spin configuration has a body-centred symmetry. Our refinements including the spin direction with a c-axis component revealed that the c component converged to 0. Because of the very small difference (0.002 $\mathring{A}$) in the a and b lattice constants in the orthorhombic magnetic unit

cell (see Supplementary Information), it was not possible to determine the spin direction in the a–b plane. Error bars, 1 s.d.

Conclusion and result

Compare to copper based superconductor, similarly, iron based superconductor, such as LaFeAsO has a layered structure. Their Superconducting is associated with magnetism. But, iron based superconductors are itinerant metals, not Mott insulators. Its Superconductivity is competing with the spin wave density state. SC and SDW may coexist in underdoped samples. Many questions remain, such as, what is the nature of the fluctuating of magnetism in high temperature? How is the magnetism and As position related? Further work is needed to investigate on this new type superconductor. People are confident that this new class of materials will open new avenues of research regardless of the origin of the electron pairing and superconductivity

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