The Study on Superconducting Mechanism of Iron Based Superconductors ($LaFe_{1-x}Mn_xAsO_{0.89}F_{0.11}$)

BY: Minase Dirbaba

A **Graduate Project** submitted to the Applied Physics Program,

School of Applied Natural Science

Presented in partial fulfillment of the requirements for the degree of Master Of Science in Physics

Office of Graduate Studies

Adama Science and Technology University

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ADAMA SCIENCE AND TECHNOLOGY UNIVERSITY

DEPARTMENT OF PHYSICS

The undersigned hereby certify that they have read and recommend to the Faculty of Science for acceptance project entitled “The **Study on Superconducting mechanism of iron based superconductors**

($LaFe_{1-x}Mn_xAsO_{0.89}F_{0.11}$)

By: Minase Dirbaba Master of Science.

Dated: December.2017

Advisor:

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Dr.Mesfin Asfaw

Readers:

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ADAMA SCIENCE AND TECHNOLOGY UNIVERSITY

Date: **DECEMBER.** 2017

Author: ***MINASE DIRBABA***

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Signature of Author

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Minase Dirbaba

December, 2017

Abstract

This project is well organized review of new class of high-Tc superconductors i.e. iron-based layered compounds such as iron pnictides (‘FePn’, Where Pn is As or P) and include iron chalcogenides (‘FeCh’, where Ch includes S, Se and Te). All of which are becoming superconducting with the current maximum Tc up to 56K. The crystal and electronic structure, pairing mechanism, doping, Tc, Ts, Tsdw, applications and magnetic properties of all these compounds were discussed. In this project, the superconducting properties of such systems are reviewed in detail, including the dependence of Tc on the doping level, and external pressure. We analyzed the magnetization measurement data taken from IFW Dresden, Germany on ($La_{1-x}AsO_{0.89}F_{0.11}$).We found that Mn has a strong suppression effect even for a small amount. On the other hand Y has a favoring effect on Tc. The result is in agreement with already reported properties. We also discussed the progress and potential application of iron based superconductors.

Chapter 1

Introduction

From macroscopic point of view one can define superconductivity as a phenomenon of zero electrical resistance in certain materials when cooled below its critical temperature T_c [1]. The mechanism of high –temperature superconductivity in the iron –based superconductors remains an outstanding issue in condensed matter physics. The electronic structure plays an essential role in mechanism of superconductivity.

Superconductivity is a quantum mechanical phenomenon, hence the electronic and magnetic properties of superconductors cannot be understood simply by classical physic of perfect conductivity. The exclusion of interior magnetic field can be explained by the Meissner effect ,while the absence of the electric resistance in a superconductor and the microscopic properties can be explained through the electron pairing via the electron –phonon interaction in the crystal in the crystal lattice as explained by J.Bardeen, Leon, and Robert Schrieffer,(BCS).

I

t was found that certain materials undergo a phase transition to a state with zero electrical resistance $R= 0$,at a certain critical T_c, The electric resistance is defined from the Ohm's law resistivity $R=v/I$,where v is the voltage and I the current .The conductivity unit length in wire ,is the inverse of the resistivity $J=\sigma E$ where E is the electric field .In order to obtain zero resistance in the sample ,the voltage across the sample must be zero. Then, this sample exhibits the character of a perfect conductor with finite current flow without any energy loss. It was also found that at relatively low temperature $T<T_c$, the magnetic field inside the sample is zero. Any applied magnetic field on the sample was also found to be deflected from the samples. The phenomenon of the perfect conduction the exclusion of magnetic field in material is called superconductivity and the material that carries this phenomenon is known as a superconductor. Hence superconductor can be distinguished from a perfect conductor by two very simple characteristics, which is the zero electrical resistance in the sample and the exclusion of the interior magnetic field.

The discovery of a new class of high -temperature superconductors iron based layered compounds aroused a significant interest at the beginning of 2008 gave hope for progress in the synthesis of novel high-temperature superconductors (HTS) up to room-temperature superconductors [2]. The nature 0f high-temperature superconductivity is not completely understood yet. The principal task of solid state physics is the creation of superconductors which would ensure superconductivity at room temperature .Therefore, the large-scale search for such high-temperature superconductors is proceeding and intensified .The crucial role in the explanation of physical properties of superconductors is played by calculations of the electronic structure from the first principles. It is worth noting that one of the basic properties of high – temperature superconductors is the presence of a lot of bands [3].

The electronic structure of the iron –based compounds usually consists of hole-like bands near the Brillouin zone center and electron like bands near Brillouin zone corners, leading to proposals that the electron pockets around the Brillouin zone corners is viable mechanism for electron pairing in the iron –based superconductors[4] Compounds of iron has been relevant to superconductivity due to its strong local magnetic moment, a number of superconducting compounds containing iron were discovered. In fact, Fe Itself under pressure is a superconductor. From a basic physics point of view, is that the superconducting pairing mechanism may be related to the coexistent magnetism in the phase diagram. Current thinking is that the pairing is not primarily phonon mediated, although due to the coupling of the magnitude of the Fe moments to the Fe-Pn/Ch bond length and the presence of an isotope effect. Theoretical alternatives to phonon coupling include various *electronic* excitations that could mediate the superconducting pairing [5] e. g. spin fluctuations or inter-orbital pairing.

Different materials superconductivity at different critical temperatures exhibit different phase transitions, while keeping the general properties. Hence superconductors can be further classified in to two different types, which can be easily distinguished by their unique electronic and magnetic properties. Namely the Type I superconductor and Type II superconductor. Type I superconductors generally superconductivity at lower temperature and lower critical field while the type II superconductors superconductivity at a higher temperature range with higher critical field with two critical fields. Most of the pure metals in the periodic table such as mercury, whereas most alloys like Lead-bismuth alloys, barium-copper-oxide ceramics and highly –doped semiconductors exhibit type- II superconductivity.

The highest Tc observed so far in the Fe-based systems is 55K[1,3,5].Pressure has been found to be a power full tool for superconducting properties of these compounds, since the application of external pressure can induce or enhance superconductivity. Superconducting mechanism in iron based superconductor has been investigated theoretically and experimentally, however ;the mechanism of superconductivity in iron based superconductors has not yet been settled with consensus with regard to the pairing symmetry and the superconducting gap function, the vast majority of experiments support the existence of spin-single sign-changing *s*-wave SC gaps on multi-bands.

Here, we are interested to study effect of magnetization on the critical temperature of $LaFeAs0_{0.89}F_{0.11}$ compound. We have analyzed data to investigate critical temperature of the doped compound, specifically using manganese dopant.

General objective

The main aim of the study is to review superconducting mechanism in iron pnictides/chalcogenides in way to study the magnetic measurement in

$LAFeAsO_{0.89}F_{0.11}$ .It is meaningful to investigate how magnetization influences,

doping and its critical temperature .

Specific objectives:

To review, the theoretical and experimentally

superconducting mechanism of $LaFeAsO_{0.89}F_{0.11}$ Manganese

doped superconductor. To analyze $LaFeAsO_{0.89}$F0.11 data to determine Tc.

To show that magnetism and superconductors interrelated.

Chapter 2

2. Review of Literature

2.1 Overview of superconductivity

The superconducting phenomenon is known to occur in about two thousand kinds of materials, including elements, alloys, various metallic compounds, and organic materials. Of various metallic compounds, Fe-based compounds are available at higher Tc as superconducting materials. After the investigation of La-O-Fe-P superconductors, the ongoing search for new superconductors has yielded as a family of LaO1-xFxFeAs oxypnictides composed of altering LaO1-xFx and FeAs layers with Tc of 26K in 2008, and this Tc value raised to 56K by replacing La with Sr and Sm [6].This rapid sequence of discoveries captured the attention of the high temperature superconductivity community.

A large variety of other iron pnictides and chalcogenides have been shown to be superconductors with some reports of Tc as high as 100K [3,7].The symmetry and the structure of the superconducting gap in FeSCs, their evolution And possible change with doping are currently subjects of intensive debates in the condensed matter community. The basic crystallographic element of the iron based(FeSC) is the FeAs (where instead of As one can also have P, Se or Te. Most of the researchers believe that the superconductivity in FeSC is of electron origin and results from the screened coulomb interaction enhanced at particular momenta due to strong magnetic fluctuations or orbital's fluctuation. It is generally agreed that magnetism plays an important role in superconductivity of iron superconductors (FeSC) [8] pnictides FePn and Fe-chalcogenides FeCh [2, 9]. The former can further be classified into four categories whereas the later into two, giving rise to a total of six categories of Fe-based materials based on their chemical composition and crystal symmetry.

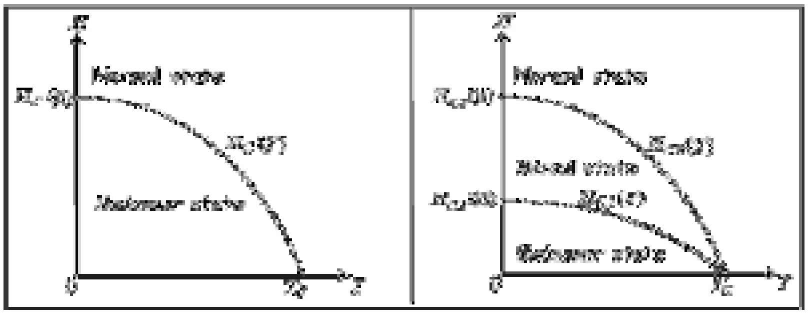
Families	**Formula**	**Appropriate elements for combination**
1111	**R FeAsO**	**La,Ce,Sm, Nd**
122	**AFeAs**	**Ba,Ca,Sr**

111	**AFeAs**	**Na,Li**
21311(42622)	**Sr_2MO_3FePn**	**M=Sc,V,Cr and Pn=P,As**
11	**FeM**	**Se,Te**
122*	**$A_{0.8}Fe_{1.6}Se_2$**	**K,Rb,Cs,Ti**

Table 2.1 The Six Family of iron pnictides or chalcogenides

Superconductors that can be explained by BCS theory or their derivatives are called conventional superconductors and those which cannot be explained by BCS theory are called unconventional superconductors. They can also be differentiated on the basis of dimensional structure. Although most superconducting materials are three dimensional, some organic compounds and single walled carbon nano tubes are found to exhibit two and one dimensional superconductivity, respectively. Properties of superconductors in external magnetic fields and the way in which magnetic flux can penetrate a superconductor.

In 1957 the discovered that superconducting materials can be separated into two groups ***type-I* and *type-II superconductors*** [10, 11]. Type I superconductors show abrupt transition from superconducting meissner state to normal state above a particular external field which is its ***critical field*** (***HC***), whereas for type-II superconductors there are two critical fields, the ***lower critical field* (*HC1*)** and the ***upper critical field* (*HC_2*)**. If the external magnetic field is lower than HC_1, the field is completely expelled and the material behaves the same as a type-I superconductor. By increasing the field above HC_1 up to HC_2, the flux partially penetrates into the superconductor as ***vortices***. As the field increases above HC_2 the flux totally penetrates the whole sample, and it returns to the normal state. A significant breakthrough then was made in 1986 by George Bednorz and Alex Müller, when they made a ceramic superconductor LaBaCuO with a critical temperature of 30 K [12]. Subsequently, by substitution of yttrium for lanthanum another ceramic superconductor with a critical temperature of 92 K was discovered [13]. Since the critical temperature of the material was considerably higher, it facilitated the use of liquid nitrogen, a cheaper refrigerant.



a) ***type-I-superconductors*** ***b) type-II-superconductors***

2.1.1 Existence of Superconductivity

superconductivity is widely regarded as one of the great scientific discoveries of the 20th Century[14].This miraculous property causes certain materials, at low temperatures, to lose all resistance to the flow of electricity .This state of" losslessness" enables a range of innovative technology applications. The era of low-temperature physics began in 1908 when the Dutch physicist Kamerlingh Onnes first liquefied helium, which boils at 4.2K at standard press Three years later, in 1911, in the Leiden laboratory of Kamerlingh Onnes and one of his assistants discovered the phenomenon of superconductivity while studying the resistivity of metals at low temperature. At that time it was noticed that the resistivity of Hg metal vanished suddenly at about 4.2k.The macroscopic quantum phenomenon at which the electrical resistivity of many metals and alloys drops suddenly to zero at particular temperature called critical temperature Tc is known to be superconductivity. At a critical temperature Tc, the specimen undergoes a phase transition from a state of normal electrical resistivity to a superconducting State. Below Tc resistivity is zero, not just close to zero. In Figure 2.1 it was shown that the Historical electrical measurement of superconductivity in mercury in 1911.According to Onnes, Mercury has passed into a new state, which on account of its extraordinary electrical properties This is called the super-conductive state [15].

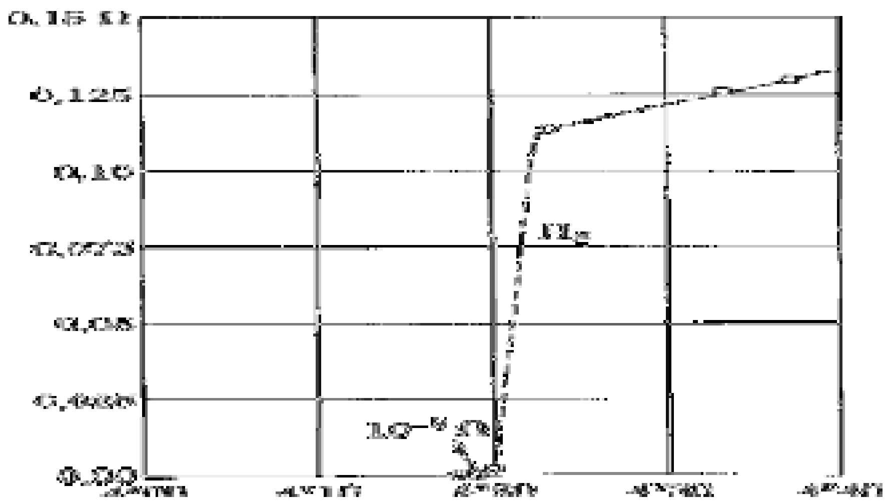


Figure 2.1: (Tc-RΩ) The critical temperature of Hg drops to 4.2K and it becomes superconductor.

There are below this temperature as discovered by Kamerlingh Onnes in1911. After this discovery a number of superconductors involving elements alloys, and compounds were invented at different critical temperature such that some of them are listed below [13,15].

Material	Ti	Al	Hg	Sn	Pb	Nb	Nb_3Sn	NbGE	Mg_2	$YB_2Cu_3O_6$
Tc(K)	0.4	1.14	4.15	3.72	7.9	9.2	18	23.2	39	90

Table :2.2 Tc of different element and alloy of compound.

Two most striking features of superconducting materials [23]

1. Perfect conductivity: zero resistance (no power loses).
2. Perfect Diamagnetism: strong repulsion in magnetic field.

Superconductivity of a material can be destroyed by application of sufficiently large magnetic field as well as if the current exceeds a critical current[2,3,16].The magnetic field above which the Superconductor becomes normal state is critical field (Hc).This critical field is related Thermodynamically to the free energy difference between the normal and superconducting states in zero field, the so called condensation energy of superconducting state[25],which is more Precisely named as thermodynamic critical field (Hc).It can be determined by equating Energy $\frac{H2}{2\pi}$ per unit volume, associated with holding the field out against the magnetic pressure With the condensation energy as follow:

$\frac{H2}{8\pi}$ = $f_n(T)$ -$f_s(T)$ where fn and fs are the Helmholtz free energy per unit volume in the res phases of zero field and Hc (T) is found empirically through approximation by a parabolic law [16].

Hc (T) = Hc (0) [1- $(\frac{T}{Tc})^{2]}$

2.1.2 Meissner Effect

One of the properties of superconducting material is expelling magnetic fields from its interior by generating electrical currents on the surface which is known as the Meissner effect [2, 4,17]. It is very suggestive that the process of expulsion of magnetic field and transition to the superconducting state of a macroscopic sample occurs through radial expansion of small superconducting regions [18].It was discovered in 1933 without any theoretical basis, by W.Meissner and R.Ochsnfield .This happens due to the screening currents, which are currents that the superconductor makes with its super currents, to screen out any magnetic fields attempting to penetrate the material. That is what causes the materials to expel the magnetic field [2,3,19].When a superconductor below Tc is placed under weak external magnetic field B, it repels the magnetic flux (field) B completely from its interior .By expelling the field and thus distorting nearby magnetic field lines, as shown in Figure 2.2, a superconductor will create a strong enough force field to overcome gravity. Superconductors in the Meissner state exhibit perfect diamagnetism, which means that the total magnetic field is close to zero deep inside the superconductor. By Lenz’s law a current generated, which opposes the flux and cancel out any magnetic field from the superconductor .The repulsion occurs only if the strength of the applied magnetic field does not exceed the value of critical field Hc of the superconductor. As the resistance is zero the current will continue to flow with constant strength as long as the external field is kept constant and consequently the bulk of the superconductivity will stay field-free [30].

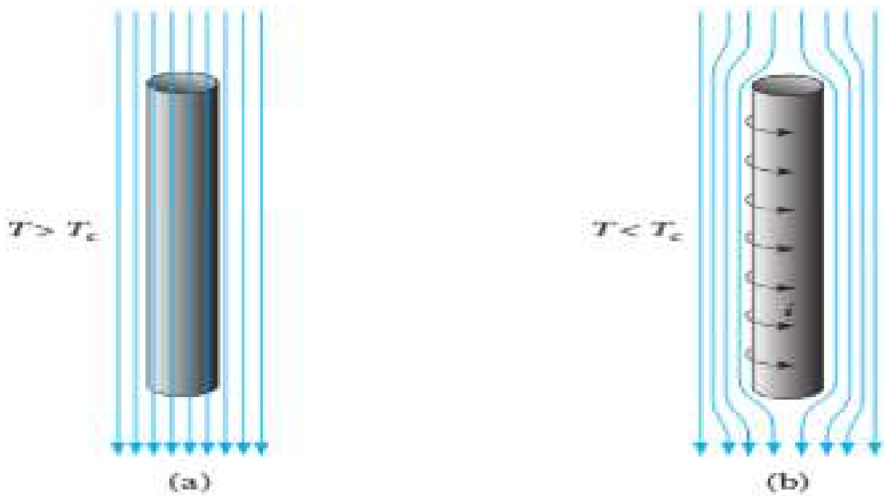


Figure 2.2: A superconductor in the form of a long cylinder in the presence of an external magnetic field. (a) At temperature above Tc, the field lines penetrate the cylinder because it is in its normal state. (b) When the cylinder is cooled to T < Tc and becomes superconducting, magnetic flux is excluded from its interior by the induction of surface currents [20]. Exhibition of perfect diamagnetic property of superconductors B=μ (H+M)(2.3)Where; M is magnetization, H is magnetic field and μ is permeability of free space from which the magnetic susceptibility χ can be found as ; $\chi = \frac{M}{H}$ by combining (2.3) and (2.4)

$$B=\mu H\,(1+\chi) \qquad (2.5)$$

2.1.3 Ginzburg Landau Theory (GLT)

The GLT was proposed in 1950 which concentrates entirely on the superconducting electrons rather than excitations [23]. Ginsburg and Landau were investigate the phenomenological theory of superconductor by using the order parameter Ψ(r) in order to introduce the concept of coherence length ξ [3,23].The attraction of the GLT are the natural introduction of the coherence .length ξ the wave function used in the theory of the Josephson effect. Through their theory,they introduce the constant ξGL known as Ginsburg Landau coherence length that is a measure of distance within which the superconducting electron concentration cannot change drastically in spatially-varying magnetic field which is given by:

$$\xi_{GL} = \left(\frac{\hbar 2}{2M\,\alpha}\right)^{1/2} \qquad (2.18)$$

Ginsberg and Landau proposed that the ratio $K = \frac{\lambda\, l}{\lambda\, GL}$ is called Ginsberg-Landau parameter r

[3,24]. If there was a mixed states like Bc1 < B <Bc2, based on the value of K superconductor materials can be classified into type I and type II superconductors. Accordingly when:

1.K<1 $/\sqrt{2}$ the material is type I superconductor.

2. K > $1/\sqrt{2}$ the material is type II superconductor.

2.1.4 London Equation

The electrodynamics equations of superconducting state were given by the two brothers H. London F. London in 1935 which was given the name London equations [25].The current to the Electromagnetic field around a superconductor can be related by the London equations. The London equation proposes that the supercurrent is proportional to the vector potential. Experiment shows that B is not uniform inside the superconductor and the field gets exponentially damped as we go into the bulk material from the external surface. [29]. If we define. The London penetration depth (λL) Can be written as [27]

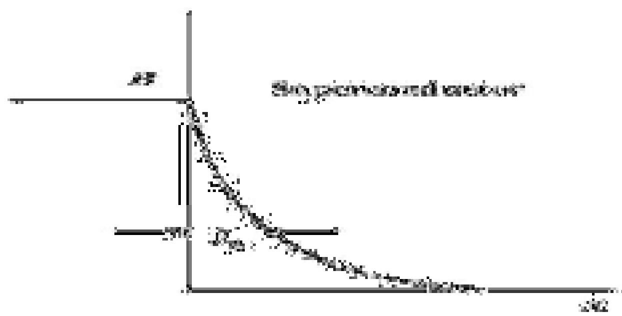


Figure 2.3: The magnetic field penetrates the superconductor within the range of as the Meissner Effect is established in the superconductor which is thicker than [30] weak external magnetic

Field, the field penetrates the superconductor only at a small distance of the London penetration Depth λL, decaying exponentially to zero within the bulk of the material.

2.1.5 Isotope Effect

Co-existence of superconductivity and magnetism in FePn superconductors, show a strong Sensitivity to the crystal lattice, suggesting the possibility of unconventional electron–phonon Coupling. Liu et al.(2008) reported the effect of oxygen and iron isotope exchange on and the spin density wave (SDW) transition temperature (T_{SDW}) in the SmFeAsFO1-xFx and Ba1-x

$KxFe_2As_2$ systems [30]. They also conclude that the impact of oxygen isotope effect is Very small whereas iron isotope effect exponent α is about 0.35 (for full isotope effect αc =0.5 another important thing is that exchange of iron isotope affect and same way. So electron phonon interaction plays a significant role in these FePn superconductors but strong magnon phonon coupling creels conventional electron-phonon coupling and makes it unconventional.

Isotope effect in Fe-based superconductors is currently controversial. It has been found that value of isotope effect exponent α for Fe-based superconductors may be negative as well as positive and in few cases it exceed αBCS=0.5 value .Associated with Fe –isotope substitution structural changes occur simultaneously causing changes α in and pnictogens height and thence the associated change in Tc.As a result, Fe isotope exponent contains two parts;

$$\alpha_{Fe} = \alpha_{\mathrm{Fe}}^{\mathrm{int}} + \alpha_{\mathrm{Fe}}^{\mathrm{str}};$$

one is related to structural changes and other is intrinsic. These experimental results convinced physicists a microscopic theory of superconductivity must involve the electron-phonon interaction to explain the isotope effect.

2.1.6 The BCS theory of superconductivity

The basis of a quantum theory of superconductivity was laid by the classic1957, papers of Bardeen, Cooper, and Schrieffer which is a BCS theory of superconductors for which they Received the Nobel Prize in 1972.According to the BCS theory, the interaction between electrons and phonon (the vibrational modes of the positive ions in the crystal lattice) causes a reduction in the Coulomb repulsion between electrons which is sufficient at low temperatures to provide a net long-range attraction [25]. This attraction causes the formation of bound pairs of remote electrons of opposite momentum and spin, the so-called Cooper pairs which is the central feature of the BCS theory [3,26]. A net attraction can be achieved if the electrons interact with each other via the motion of the crystal lattice as the lattice structure is momentarily deformed by a passing electron.The theory has been very successful in explaining the characteristic superconducting properties of zero resistance and flux expulsion [27].Because one cannot reduce the momentum of a single cooper pair, without reducing the momenta of all other pairs by scattering [28].The cooper pairs appear only at $T < Tc$ near the EF and the temperature dependent energy gap $\Delta(T)$ Decreases momentarily with T from $\Delta(T = 0)$ to $\Delta(T = Tc) = 0$.

The BCS theory with wave theory along with a BCS wave function, which include [28,]:

1. An attractive interaction between electrons can lead to a ground state separated from excited States by an energy gap (Δ). (The critical field, the thermal properties, and most of the Electromagnetic properties are consequences of the energy gap.

2. The electron-lattice-electron interaction leads to an energy gap of the observed magnitude. The indirect interaction proceeds, when one electron interacts with the lattice and deforms it, a Second electron sees the deformed lattice and adjusts itself to take advantage of the deformation to lower its energy. Thus the second electron interacts with the first electron via the lattice deformation.

3. The penetration depth and the coherence length emerge as natural consequences of the BCS Theory. The London equation is obtained for magnetic fields that vary slowly in space. Thus the central phenomenon in superconductivity, the Meissner effect, is obtained in a natural way. 4. The criterion for the transition temperature of an element or alloy involves the electron density of orbital D (EF) of one spin at the Fermi level and the electron-lattice interaction U estimated from the electrical resistivity measure of electron phonon interaction in room temperature. For D(EF) U << 1, The BCS theory predicts Tc as follow:

$$Tc=1.14\Theta \exp\left(\frac{-1}{UD(EF)}\right) \quad (2.6)$$

Where; Θ = hω/KB is the Debye temperature and UD (EF) is the coupling constant. In the same way the superconducting, energy gap at T=0 could be, written, as

$$\Delta(0)=2\hbar\omega \exp\left(\frac{-1}{UD(EF)}\right) \quad (2.7)$$

5. Magnetic flux through a superconducting ring is quantized and the effective unit of charge is 2e rather than e. The BCS ground state involves pairs of electrons; thus flux quantization in terms of the pair charge 2e is a consequence of the theory. It is clear that Tc or the zero temperature variation parameter Δ (0) depends on material properties such as phonon spectrum ~ω, the electronic structure D (EF) and the electron-ion coupling strength U [28]. Of various thermodynamic ratios. It is possible to form $\frac{2\Delta(0)}{Tc}$ =3.53 for weak coupling which is the most relevant for conventional superconductors. The temperature dependence of the gap Δ (T) near Tc can be computed numerically using the equation which is the universal function of T/Tc.

$$\frac{\Delta(T)}{\Delta(0)} = 1.74(1-\frac{T}{Tc})\frac{1}{2} \quad (2.8)$$

Where, Δ (0) = 1.76KBTc, and 1− T Tc << 1 in order to achieve this universal relation.

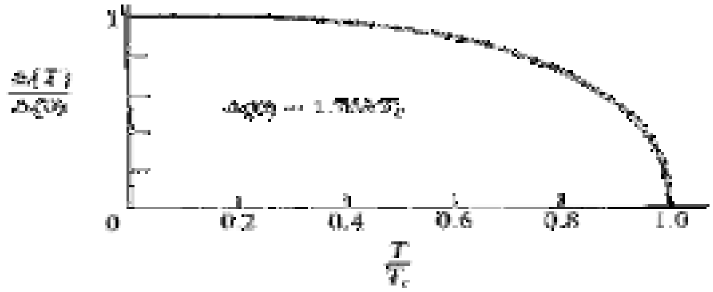


Figure 2.4: Behavior of the energy gap parameter Δ (T) for a superconductor in the BCS theory and weak coupling limit. The energy gap decreases monotonically from its zero T value to zero at Tc as shown in Fig 2.4. At very low temperatures Δ is nearly constant which can be physically interpreted as the fact that a significant number of quasi particles have to be excited before the energy gap value is affected by temperature variations? The pairs with opposite spins act like bosons and leave an energy gap Δ between the BCS ground state and the first excited state; $\Delta = 2\hbar\ \omega\ De$

(2.9)

Where ωD is Debye frequency, VO is coupling potential and NEf is density of states of electron at the Fermi energy. In its simplest form, BCS gives the superconducting transition temperature in terms of the electron-phonon coupling potential and the density of states of electron at the Fermi energy.

$$T_cK_B = 1.14\hbar\ \omega De(\frac{-1}{vo})N_{Ef} \quad (2.10)$$

2.1.7 Electron-Phonon Interaction

The usual treatment of ion movements in crystalline solids starts from the hypothesis that these movements are generally small-amplitude oscillations around the equilibrium positions that define the crystal structure [60]. This hypothesis is consistent with observed X-ray diffraction spectra consisting of very narrow lines [26].These oscillations are commonly called lattice vibrations. Because interactions keep ions connected to one another, the vibrations are collective motions, and should be analyzed in the context of normal modes of the whole system[26-27].The electron-phonon interaction causes superconductivity in many metals and influences the transport properties of every metal by describing coupled motions of electron and nuclei[26].This model for the interaction explains classic physical phenomena, such as conventional superconductivity, and plays an important role in many active fields for instance, Charge transport in molecular junctions.

The most natural environment in physics for implementing quantum gates is solid state systems where fermions (electrons) are subject of numerous interactions that concern and compromise quantum coherence. In particular, electron-electron and electron-phonon interactions are of central importance [29], because the attractive interaction between two electrons is caused by the electron-phonon interaction supported by the discovery of isotopic effect on Tc showed that electron-phonon interaction plays an essential role in conventional superconductivity. The interaction between electrons and phonon by itself is strongly affected by the disorder of the electron system [30].This is due to the attractive electron-electron interaction is mediated by phonon via the following mechanism [31]:

- ❖ An electron carries negative charge, and thus an electron will attract nearby nucleons. As a result, the spacing between the nucleons will be reduced around an electron (this is a lattice distortion). Because nucleons carrier of positive charge, smaller lattice spacing means that there is a higher positive charge density in this region near an electron.

- ❖ Electron mass is much smaller than nucleons, so electrons move much faster than nucleons. When electron flies away, the lattice distortion will not recover immediately (because nucleons move much slower). Locally, there is a higher density of positive charges here, which will attract other electrons.
- ❖ Combining the two facts mentioned above, we found that an electron will attract other electrons via lattice distortions. Because lattice distortions are described by phonon ,this effect is known as phonon mediated attraction between 2e’s

2.2.Iron Based Superconductors

2.2.1. Structural Electronic Properties Tc and its Correlations.

All of the iron pnictides and chalcogenides superconductors have structural and physical Properties in common. First the structure is crucial in any attempt to understand the superconductivity, particularly since there is aspects of the structure in the FePn/Ch which Influence Tc, similarities and correlations have been found. Then the structural phase transition Temperature TS and TSDW as a function of doping. There appear to be two distinct kinds of Phase diagrams is whether the magnetism is suppressed by doping before superconductivity is Induced. Further, in the 'coexistent' kind of phase diagram, there are again two distinct types. These are distinguished by whether the magnetic transition temperature, T_{SDW}, ever sinks down to Tc at a given composition or whether T_{SDW} remains larger than Tc. The important topic of Microscopic vs phase-separated coexistence of the magnetism and the superconductivity after the experimental evidence for coexistence in is established. Coexistence is obviously of interest for understanding the pairing mechanism. Finally, the pressure and field dependence of Tc reviewed.

2.2.2. Crystal Structure of six Family of iron FePn/ch

1111 family

Fe-based materials as presented in Fig.2.5a First category of Fe-based materials, known as 1111 Compounds, is made up of the combinations of elements, rare-earth (La, Sm, Gd… etc.)-Transition metal (Fe, Co, Ni--) pnictogens (As, P)-oxygen; more than 150 such compounds are Possible [50] out of which several are superconductors. In Fig. 2.5a.crystal structure of LaFeAsO which is representative of 1111 family. They have the Tetragonal, tp8 (''t'' means tetragonal, ''p'' means ''primitive '(8 atoms per unit cell) ZrCuSiAs (prototypical compound) structure with 2D layers of FeAs. They belong to space group with space p4/nmm group number 129 (tetragonal). These Materials undergo tetragonal to orthorhombic structural transition and have space group Cmma or P112/n or p2/c in the orthorhombic phase

122 Family

The most studied and probably the largest numbers of superconductors are in the122 families which are made up of combinations of metallic alkaline earth (Ba, K Ca Sr…)-transition metal (Fe, Co, Ni…)-pnictogens (As, P). More than 450 Compounds are possible within these combinations. These materials do not have any oxygen, tetragonal with 2D FeAs planes, was K-doped $BaFe_2As_2$, with the tetragonal tI10 with=38 K [32] .The ternary iron arsenide $BaFe_2As_2$, with the tetragonal $ThCr_2Si_2$-type structure space group (space group In 2.9. 4/nmm) contains practically identical layers of edge-sharing FeAs4=4 tetrahedral, but they are separated by barium'atoms'instead'of'LaO'sheets.

This Structure is shown in Fig 2.5b .

111 Family

The third FePn Superconducting structures to be discovered, Fig 2.5c also with 2D planes (FeAs) Were the MFeAs, 111M=Li, Tc=18 K) with the tetragonal tP6 Cu2Sb structure and the iron LiFeAs crystallizes into a Cu2Sb-type tetragonal structure containing FeAs layer with an average Iron valence Fe2+ like those for 1111 or 122 parent compounds. This structure is shown in figure 3.0[33]. In the layered structure, iron pnictide and Li or Na layer are stacked alternately. Fe Atoms are in a four-fold coordination, forming a FeAs (p)4 tetrahedron.

11 Family

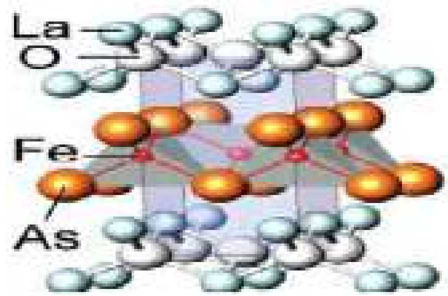
The iron PbO. FeSe ('11') Family (Tc=8 K) with the tetragonal tP4 structure. The PbO-type FeSe crystal structure is shown in Fig 2.5d [53].

21311 Family

The fifth Structure with FePn planes to join this superconducting set of materials is the so-called 21311 structures. The first member found, Sr_2ScO_3FeP [54] in (Fig 2.5e) had a17K While the pink open circle Fe vacancies are on the Fe1 site (4/unit cell) (fig 2.5e) with Cr or V, & P with has increased the Tc up to 37K in Sr2VO3FeAs), while Sr2Mg0.2Ti0.8O3FeAs has Tc=39 [55]. Intercalation of further layers of atoms between the FeAs layers to try to increase by expanding the c-axis has so far) resulted in Tc's up to 47K [56].

122∗ Family:

The most recent FePn/Ch structure discovered (Fig.2.5f) with superconductivity (Tc≈32 K) is an Ordered-defect alteration of the 122 $BaFe_2As_2$ structure (the '122*' written $A_{0.8}Fe_{1.6}Se_2$ (A=K, Rb, Cs, Tl), where the ordered arrangement of Fe vacancies below TS on the in equivalent Fe sites (ideally Fe2 sites are fully occupied, while Fe1 sites are not) has important influence on the measured properties including superconductivity state[57] .



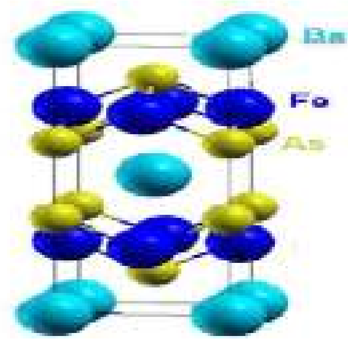
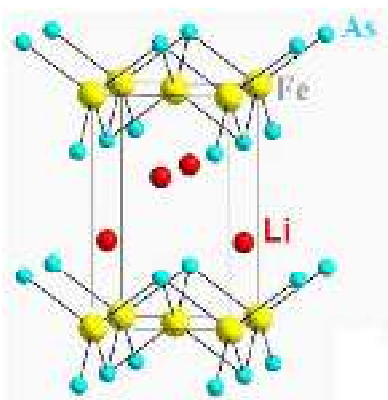


Figure-2.5a from Kamihara et al (2008) The lattice structure of 1111 LaFeAsO

Fig. 2.5b Shein and Ivanovskii (2009a). lattice structure of 122 $BaFe_2As_2$.



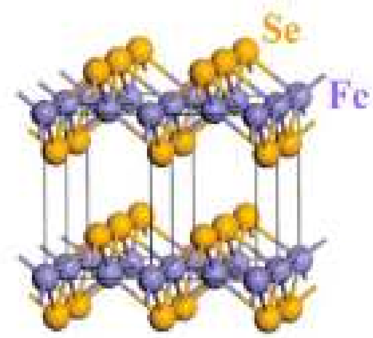
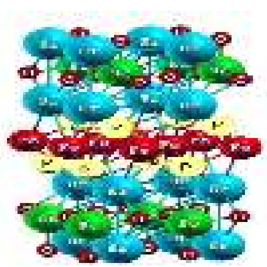


Fig2.5c structure of 111 LiFeAs

Fig.**2.5d.Structure of 11 FeSe**



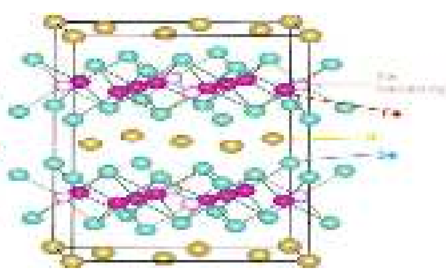


Fig.2.5e (21311) Sr_2ScO_3FeP

Fig. 2.5f (122∗) $K_{0.8}Fe_{1.6}Se$

All of the discovered FePn/Ch superconductors are tetragonal with planes of tetrahedral of Fe and either As or P (pnictogens) or S, Se or Te (chalcogenides). Fe-Fe Spacing's insure that the 3d Fe electrons take part in band formation. Varies calculations of the electronic structure result in these Fe d-bands dominate large density of states near the Fermi energy [34]; together with nesting on the Fermi surface, these Fe bands lead to magnetic ordering[35].

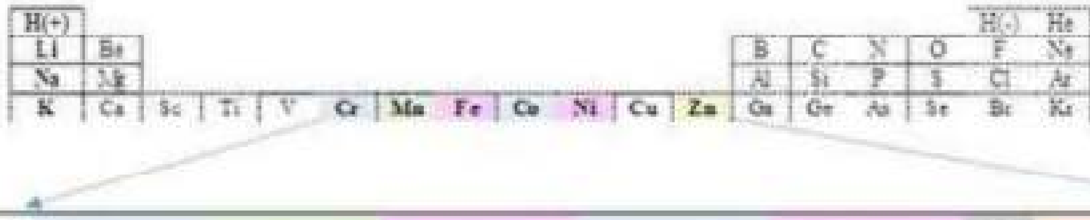
Compounds	Fe-Fe distance in Å
1111	2.85
122	2.7 Theory
122*	2.77
11	2.67
21311	2.84
111	2.6819

Typical, Fe-Fe, distance in iron based compound

They are small indicating that the Fermi surface would principally be made of Fe-3d.

2.2.3 3d Transition Metal Oxypnictides

IBSC was first discovered in LaFePO with Tc =~4K in 2006.Subsequently superconductivity was found in LaNiAsO with Tc=2.4K in2007 and then Tc jumped to 26K in early 2008 for LaFeAsO1-xFx [61].The electromagnetic properties of 3d transition metal (TM) oxypnictides vary drastically with TM [36] .Figure.2.1summarizes the properties of LaTMPnO, where TM= $3d^4$ transition metal, Pn=P or As). One may see that electric and magnetic properties of layered TM oxypnictides strongly depend on TM. The synthesis of early TMs and Cu oxypnictides was tried but unsuccessful even using high pressure up to ~9GPa and no distinct correlation was found between the stability of the 1111-type compound and the kind of TM. Bulk superconductivity appears in TM=Fe2+and Ni2+ both of which have even number of 3d electrons but no superconductivity has found in TM=Cr2+ [37] with 3d4 electronic configuration. Undoped LaFeAsO is an antiferromagnetic metal but does not exhibit superconductivity. For TM=Mn, an exceptionally high electron doping is possible by applying H[38] in place of F- as a substituent for the oxygen site and transition of antiferromagnetic insulator to ferromagnetic metal was observed but no Tc appeared.



TM^{2+} (3d electron number)	Cr(4)		Mn(5)		Fe (6)		Co(7)		Ni(8)		Cu (9)	Zn(10)	
Pn	P	As	P	As	P	As	P	As	P	As	P,As	P	As
Elect. Prop.		Metal	Mott Insulator		Superconductor		Metal		Superconductor			Semiconductor	
Magnetism		AF(CB)	AF(CB)				FM					Non-magnetic	
E_g		-	~1 eV		-		-		-			~1.5 eV	
T_c(SC)					Undoped 4K	F-doped 26K			Undoped 3K	Undoped 2.4K			
T_{mag}(Mag)		> 300K	> 400K				43K	66K					
Ref.	S-W. Park et al. IC (2013)		Yanagi et al. JAP (2009)		Kamihara et al. JACS (2006) Kamihara et al. JACS (2008)		Yanagi et al. PRB (2008)		Watanabe et al. IC (2007) Watanabe et al. JSSC (2007)			Kayanuma et al. PRB (2007) Kayanuma et al. TSF (2008)	

unsuccessful to synthesize   CB: checker board type

Table 2.3: The properties of LaTMPnO, where TM= 3d transition metal, Pn=P or As).

2.2.4 Parent Materials

Since the paper reporting Tc=26K in LaFeAsO1-xFx, several superconducting materials have been reported in layered iron pnictides or chalcogenides. These materials contain a common building block of square lattice of Fe^{2+} ions which take tetrahedral coordination with Pn (where P and/or As) or chalcogenides ions of a simplified classification of these parent compounds is shown in Table 2.3.Since the Fermi level of each parent compound is primarily governed by Fe five 3d-orbitals, iron plays the central role of superconductivity. These compounds have tetragonal symmetry in the superconducting phase, are Pauli Para metals in the normal state and undergo crystallographic/magnetic transition to orthorhombic or monoclic, tetragonal symmetry in the superconducting phase, are Pauli Para metals in the normal state and undergo crystallographic/ magnetic transition to orthorhombic or monoclic.

2.2.5 Phase Diagrams

*Different behaviors of un*doped parent compounds of iron-based superconductors are either superconducting or antiferromagnetic at low temperatures. LaFePO, LiFeAs, and FeSe, for example, are nonmagnetic and superconducting even without doping. In contrast undoped LaFeAsO and $BaFe_2As_2$, for example non-superconducting antiferromagnetic metals, electron or hole doping suppresses the magnetic order and induces superconductivity. Phase diagrams of different classes of Fe-based superconductors are presented in Fig. 2.6. Phase diagrams (a) to (d) correspond to various 1111 materials. Figures 2.6. (e to f) correspond to various122 materials [39].Out of all these, phase diagrams of 122 materials are well established due to availability of good quality samples. These materials (122) are also most extensively studied and very large number of materials exists in this family, as one can dope on any of the three sites M (e), Fe (f) or As (g). These phase diagrams are obtained through resistivity, spin Susceptibility, μSR measurements. These materials have well established magnetism and Superconductivity coexistence. The magnetism is caused by spin density wave (SDW) type transition seen in resistivity, spin susceptibility and neutron scattering measurements. It is worth Noting that there exists structural transition (Ts) together with the T_{SDW} transition and for M site doped material they are identical or nearly identical whereas for Fe-site doping (with Co) it differs as doping increases. The trend is also similar in case of As-site doped materials. These constitute the central theoretical and experimental studies of Fe-based materials.

In 1111 materials while SDW and structural (tetragonal to orthorhombic) transitions are present but there are no significant coexistence between the SDW and superconductivity (SC) is observed. While Structural transition is always slightly higher than the T_{SDW} transition, phase diagram for the Sm-compound came as a surprise; the TS is way above T_{SDW} transition, casting doubt about earlier understanding that the structural, magnetic and superconducting transitions are intertwined. Below is a detailed comparison of Ts and $_{TSDW}$ among 1111 and 122 along with other Fe-based compounds.

It is noticeable that for 122, 11 un-doped compounds they are Identical where as the difference between them decreases as sample quality improves for1111compound.Landau theory states that two simultaneous phase transitions that interact with each other (*i.e.*, are not simultaneous due to coincidence) and break different symmetries result in a first order transition. Wilson *et al.* (2009), in their neutron scattering experiments on a highquality single crystal of $BaFe_2As_2$, found that both the structural and magnetic transitions at136K are second order. Tegel *et al*. (2008) [40] argued from their measurements of the lattice order parameter p= [$\frac{a-b}{a+b}$] where a and b are the orthorhombic axes' lengths] in (M=Sr (Ts=203K and Eu(Ts=190K) that, despite their measured cell volume discontinuity at Ts in $SrFe_2As_2$, all of MFe_2As_2 the starting compounds undergo in fact second order structural phase transitions. In light of the prediction of Landau theory, then both the simultaneity of Ts and Tsdw are coincidental or there should be some higher temperature precursor of one of the transitions that breaks that transition's symmetry at a higher temperature. Ghost *et al.*, (2012) ,showed that if is due to orbital modulations and is inter orbital in origin due to nesting of Fermi Surface then they can occur simultaneously.

Material	T_S (K)	T_{SDW} (K)
LaFeAsO	158	134
PrFeAsO	154	135
CeFeAsO	155	140
	151	145
NdFeAsO	150	141
	143	137
SmFeAsO	130*	135*
GdFeAsO	135	
SrFeAsF	180	133
CaFeAsF	134	114
$BaFe_2As_2$	142	—
$SrFe_2As_2$	205	—
$CaFe_2As_2$	171	—
$EuFe_2As_2$	190	—
$Na_{1-\delta}FeAs$	50	40
FeTe	72	—
$K_{0.8}Fe_{2-y}Se_2$	578/551	559/540
$Rb_{0.8}Fe_{2-y}Se_2$	540	534
$Cs_{0.8}Fe_{2-y}Se_2$	525	504

The table 2.4 shows the correlation between Ts and Tsdw of undoped Families ofFePn/Ch.

LaFeAs compounds are easy structure, of alternating layers of Fe-As and La-O layers where FeAs layers are believed to be responsible for superconductivity. The main compound of these systems is not superconducting itself and exhibits both a structural and magnetic phase transition. This structural phase transition alters the crystal symmetry from tetragonal (space groupP4/nmm) to orthorhombic (space group Cmma) and leads to antiferro magnetic order with a spin structure, which is shown in Figure (2.6). However, the first direct existence of SDW order in LaFeAsO came from neutron-scattering experiments.

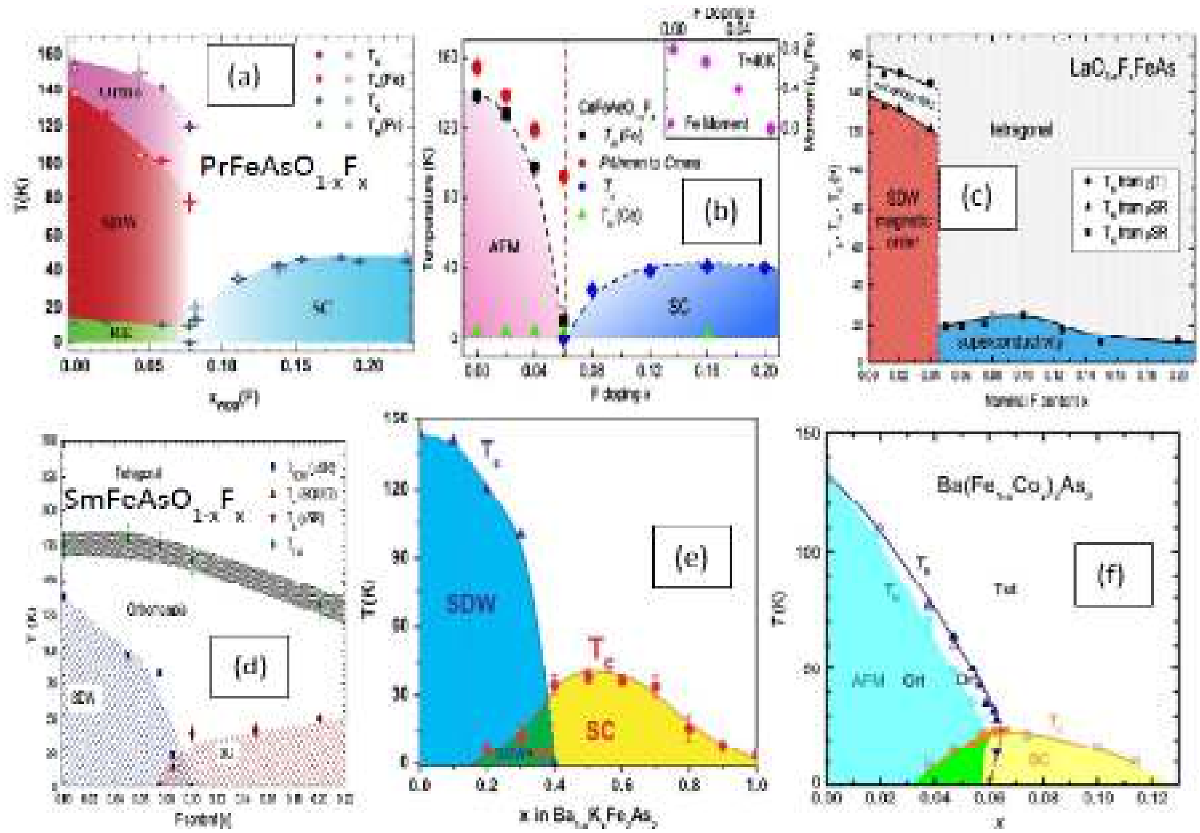


Fig.2.6 *Phase diagrams of Fe-based materials: 1111 (a-d), 122 (e-f), (taken from [68, 69, 70]*

2.2.6 Coexistence of S.D.W and Superconductivity

The FeAs based new superconductors have generated great enthusiasm, since the superconducting transition temperature Tc of these alternating layer materials increases to above 40K and finally reaches about 55 K. In addition to the superconductivity, a closely related electron pair imbalance on the Fermi surface, the spin-density wave (SDW), has been deduced from the nesting Fermi surface and recognized directly in neutron diffraction experiments in both LaFeAsO (1111) and $BaFe_2As_2$ (58) classes of materials [64]. It is hard to visualize that the same Electronic state would take part in both the superconducting and spin-density wave (SDW) Electron pairs instability of the Fermi surface, and indeed the electron and hole-like Fermi sheets In ($BaFe_2As_2$) have been observed in the angle-resolved photo-emission spectroscopy (ARPES) Study to be inuenced by either the SDW or superconducting i.e. x = 0.4 compound, Thus, it would be extremely significant to examine the relationship between the two correlated electronic states in the phase diagram.

The parent compounds of many of the pnictides are antiferromagnetic metals, which referred to

Here as the spin density wave (SDW) state. On doping, the magnetic order is decreased where as Superconductivity emerges. Coexistence of spin-density wave (SDW) and superconductivity in Multiple pnictide materials have been reported. For example, in Ba1-xKxFe$_2$As$_2$ an extended Region of coexistence with $0.2 \geq x < 0.4$ with a maximum superconducting transition temperature Inside this region of ~28 K are observed.

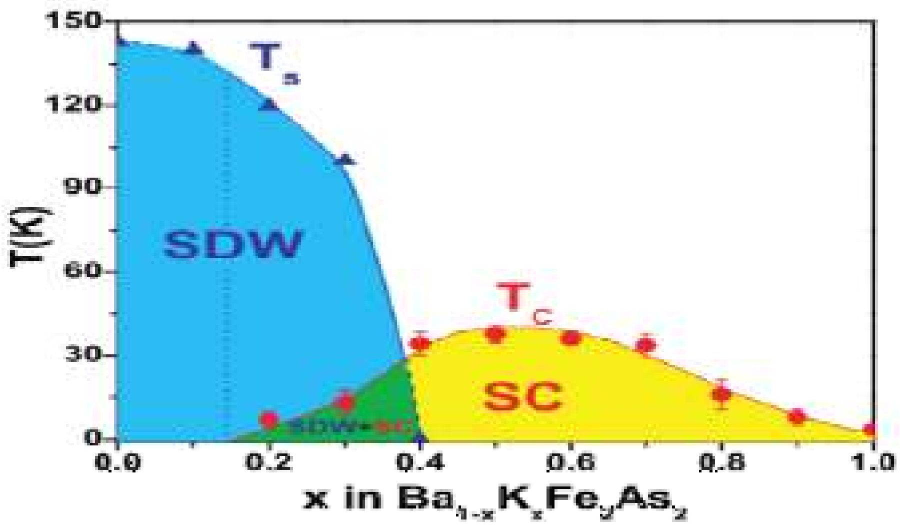


Fig.2.7 The composition-T (k) phase diagram, showing the magnetic and Superconducting transitions denotes the magnetic transition and Tc the superconducting .

There is strong evidence experimentally for microscopic coexistence coming from the same Fe 3d electrons, particularly in Co-doped BaFe$_2$As$_2$ which has excellent Sample homogeneity. At lower temperatures that all the domains in the sample are antiferromagnetically ordered. Thus the theorists' proposals that superconductivity in the FePn/Ch's is intimately connected with, magnetism/spin, fluctuations.

2.2.7 Tc vs doping: - Carrier doping to induce Tc

Most of the parent materials listed in section 2.6is antiferromagnetic metal and supercondu - Ctivity is induced by appropriate carrier doping or structural modification. Although some of the Parent phases exhibit superconductivity without doping, the Tc value of such a material was lowas exemplified by LaFePO with Tc=~4K, implying the occurrence of close relationship between magnetic ordering in the parent phase and resulting Tc. Metal iron with bcc structure is a Ferro-magnet with a Curie temperature of 1043K, but high pressure phase with hexagonal structure loses ferromagnetism & exhibits superconductivity of Tc=~0.4K under15-30GPa [41].We may understand in a sense that high Tc IBSCs are obtained by eliminating long range spin ordering in layered iron pnictides using carrier doping in place of applying high pressure to metal iron. Three types of carrier doping described below are possible for the parent compounds of iron based superconductors.

Electron Doping and hole doping

Substituting of oxygen atom by fluorine or by oxide vacancies, an extra electron goes into the FeAs layer, such situation is commonly referred to as electron doping. Redistribution of Electrons between the doped LaO and FeAs layers gives rise to a conductivity of compound another remarkable fact was a discovery of high-Tc superconductivity in the compounds LaOFeAs without Fluorine doping, but under oxygen deficiency. Thus, H. Mukuda et al reports
A detection of high Tc values in LaO0:6FeAs (Tc =28K), LaO0:75FeAs (Tc = 20 K) and NdO0:6FeAs (Tc=53K). The table below represents the different rare earth materials shows different transition temperature with Fluorine doping and with oxygen deficiency. The Original compound is $LaF_xO_{1-x}FeAs$ with Tc =26K.
The resulting compound, $La_{1-x}Sr_xOFeAs$, at x = 0.13 becomes superconducting with Tc=3325 K [42]. This was the first superconductor in the FeAs based superconductors, obtained by hope doping, as has been confirmed by measuring the Hall coefficient. A system Pr1, xSrx O FeAs is an example of the hole doping, on substituting Pr3+ by Sr_2+ [43].A superconductivity of Tc = 16 .3K was achieved at the Sr concentration x ≈0:20 - 0:25.Electron and Hole doping is also possible for ternary Iron Arsenide ($A_2+Fe_2As_2$), such as by doping $BaFe_2As_2$ with potassium. The charge carriers in Ba1-xKxFe_2As_2 are holess, which is confirmed by Hall Effect measurements. A unique characteristic of doping into IBSCs is Isovalent doping. Two typical examples are introduced. One is partial substitution of Fe_{2+} site by Co_{2+} and another is replacement of As site by P . The former is understood in term of electron doping because the Co_{2+} ($3d_7$) has an excess electron compared with Fe_{2+} ($3d_6$) .

Rare-earth elements

In ReOFeAs compounds the superconductivity was identified in LaO1-xFxFeAs with 26K with F-doping. After that many group substituted La with other rare earths like, Sm, Nd, Ce, Gd, Pr, Tb and Dy according to the simple chemical formula RE+3O-2Fe+-2As-3.exchanging lanthanum

With rare earth ions of smaller atomic radii in LnOFeAs, Tc was found to increased. According to report from experiment the lattice constants, hence the volume, decrease monotonically as the atomic number increases, but Tc increases only from La to Gd, where upon drops for heavier Rare earths. Electronic calculations for Ce, Nd and Gd show similar DOS and band structure with LaOFeAs.

2.2.8 Correlation between Tc, TS and TSDW vs pressure.

] It is a general trend that the optimal Tc is higher in the order 1111>122>11. This result implies that the optimal Tc is enhanced by the interlayer spacing of FeAs layers. The phenomenological correlation between the Tc an Ts becomes worse compared with that between the optimal Tc and Ts but the tendency still remains. However, data on the 11system and the first dome in LaFeAsO1-xHx are far from this empirical rule. This discrepancy is due to that the Tc is not determined only by the local structure of FePn (Ch).Kuroki et al. [44proposed a model that the pnictogens height (h) from the iron is a Good structural parameter. Associated with strength of spin fluctuation and the Tc is enhanced by increasing h the correlation between the h value.

It was found that pressure has a large effect on iron pnictides /chalcogenides so that some parent Compounds can become superconducting by simply applying pressure, we remark that the Tc of The original system LaO1-xFxFeAs went up from 26 K to ~43 K by applying a pressure of ~4GPa [68]. Indeed, in ReOFeAs compounds the atoms of rare-earth element have smaller radius than La and Tc in these compounds is markedly higher, exceeding 50 K. In a subsequent work, the measurements of electrical conductivity in LaO FeAs under high pressures, up to 29 GPa, have been done [45].As is seen from Fig. 2.8, the maximal Tc = 21 K in stoichiometric compound LaFeAs is achieved at the pressure of 12 GPa. As regards the variation of Tc with pressure in doped compounds, it first rises with pressure, passes through maximum and falls down. A similar behavior of Tc under pressure is observed in LaO1-xFxFeAs of a different composition, a similar trend shown in oxygen deficient LaFeAs compounds [46].

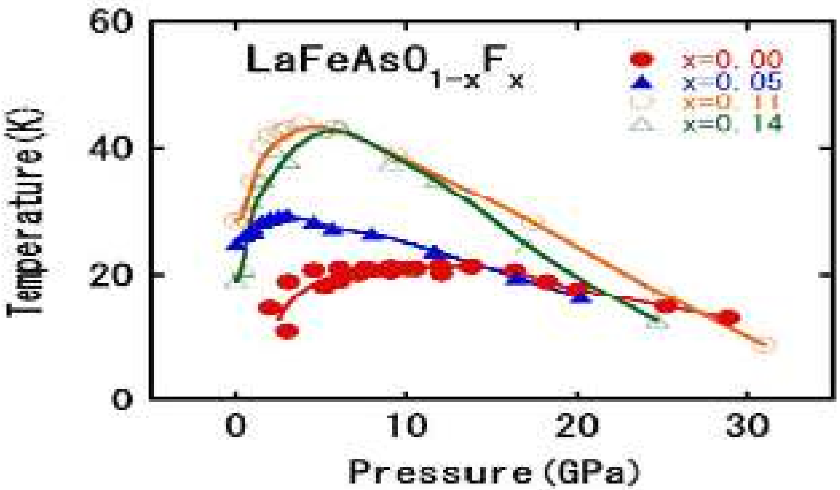


Figure 2.8: Variation of Tc with pressure in LaO1-xFxFeAs compounds.

A relation between the changes of Tc under pressure and variation of the lattice parameter at High pressures (P>10GPa), the lattice parameters and Tc for the compound investigated LaO0:9F0:1FeAs do decrease linearly [48] to the right of the Fig.2.8 peak inTc with increasing A-axis, pressure first increases Tc, followed there after by a decrease. In AFe2As2 compounds the application of pressure suppresses both the structural and the magnetic transitions and leads to the superconductivity. The high pressure experiment indicates that superconductivity appears at approximately 2 GPa to 6 GPa for $BaFe_2As_2$ and has a peak of Tc = 29 K near 4GPa [49], SrFe2As2 was first reported to super conducts at 2.5 GPa pressure with Tc =27 K and Tc decreases to below 20K with further increasing pressure up to 5.2 GPa. The main effect of pressure on the crystal structure of AFe2As2 is to shorten the Fe-Fe and Fe-As bond length and As-Fe-As bond angles.

The discovery of superconductivity in the 122 structure was via K-doping (whole doping) of BaFe2As2 [50]. Three other non-superconducting MFe_2As_2 (M=Sr, Ca, Eu) host compounds were quickly also discovered, where both hole doping on the M-site and electron doping on the Fe site, as well as more recently P doping on the As-site, succeeded in causing superconductivity. Table 2.2.9 for a complete listing. Clearly, the variety of dopant that achieve superconductivity in the 122's is quite large. In addition to doping-induced superconductivity, three Fe-containing 122 compounds super conduct without doping, KFe_2As_2 (Tc~3.8 K, $RbFe_2As_2$ (Tc~2.6 K,) and CsFe2As2 (Tc=2.6K).Comparing the effect of pressure and P-doping on the superconducting phase diagram of BaFe2As2, including the effect of pressure on

BaFe2As2-zPz, and conclude from the similarities between P doping and pressure that impurity scattering is not limiting Tc in the doped samples. The variety of dopant that achieve superconductivity in the 122's as in table (2.6).

Material	M-site dopant	T_c(K)/x y=z=0	Ref.	Fe-site dopant	T_c(K)/y x=z=0	Ref.	As-site dopant	T_c(K)/z x=y=0
$BaFe_2As_2$	K	38/0.4	1	Co	22/0.2	9	P	30/0.7
	Rb	23/0.1	2	Ni	20.5/0.1	10		
				Pd	19/0.11	11		
				Rh	24/0.11	11		
				Ru	21/0.9	12		
				Pt	25/0.1	13		
$SrFe_2As_2$	K	36.5/0.5	3	Co	20/0.2	14	P	27/0.7
	Na	35/0.5	4	Ni	10/0.15	15		
	Cs	37/0.5	3	Pd	9/0.15	16		
	La	22/0.4	5	Rh	22/0.25	16		
				Ru	13.5/0.7	17		
				Ir	22/0.5	16		
				Pt	16/0.16	18		
$CaFe_2As_2$	Na	33/0.66	6	Co	17/0.06	19	P	13/0.3
				Ni	15/0.06	20		
				Rh	18/0.1	21		
$EuFe_2As_2$	K	32/0.5	7				P	26/0.6
	Na	35/0.3	8					

Table 2.5 Tc vs Composition in M1-xAxFe2-yTMyAs2-zPz

Superconductivity [51] while Mn substituted for Fe in SrFe2As2 up to x=0.3 is relatively in effective in suppressing TS and TSDW [52] .phase diagrams are shown here for selected dopant. Despite the hole doped Ba1-xKxFe$_2$As$_2$ being the discovery superconductor in the 122's. This phase diagram shown in Figure 2.6 Within the resolution of the early neutron scattering.Determinations of TS and T_{SDW} determinations of TS/T_{SDW} the structural and magnetic transitions remained at the same) until both transitions are suppressed in Ba1xKxFe$_2$As$_2$.The discovery of superconductivity in the 122* materials, with the large local moment (3.3μB/Fe [53] and different Fermi surface (no hole) seems at present to argue against the s± direction

2.2.9.Superconducting Pairing Symmetry

The excitation (spin fluctuations) being exchanged to produce the coupling is repulsive it can still lead to attractive pairing if the excitation is being exchanged between parts of the Fermi surface with opposite signs of the order parameter. If Δk = - Δk+Q then a repulsive interaction with wave vector Q (Fig.2.9) can be attractive due to the Sign reversal in the order parameter Δ. This is a realization, specific to the FePn/Ch materials' Fermi surface with several small pockets separated by Q, of the general spin fluctuation pairing

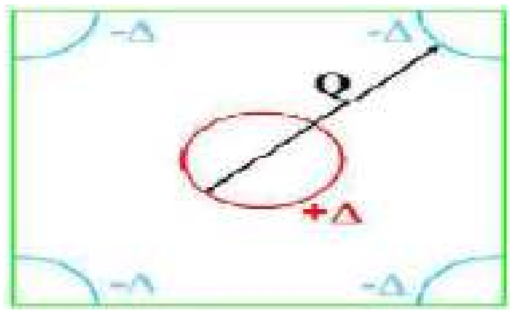


Fig. 2.9 Sketch of an idealized Fermi surface of undoped FePn/Ch.

Experimental work on the Fermiology of the FePn/Ch, with the hole pocket (red) at the Γ point (0,0) with energy gap +Δ, the electron pockets (blue) at the corner M (called 'X' in some notation points (π π) with energy gap -Δ, and the spin density wave momentum wave vector Q spanning the two nested pockets.

The pairing symmetry contain signiffcant information on pairing mechanism, Nuclear magnetic resonance(NMR) measurements have been conducted on 1111 material LaFeAsO0:89F0:11[84] and PrFeAsO0:89F0:11, 122 material BaFe1:8Co0:2As2 [54]&11 structure FeSe0.5Te0.5[85]. State. As a result, s±-wave and d-wave are more probable according to NMR studies. Both d-wave and s±-wave has internal - phase shifts. The difference is if the $\pi-$ phase shift is direction-dependent or not. Superconducting loop to establish a π-phase shift in the order parameter. This supports a sign change in the gap structure against conventional s-wave. These phase-sensitive experiments show strong evidence of the sign-reversed s-wave symmetry.

Another phase-sensitive measurement using scanning tunneling microscopy on the 11 structure Fe (Se, Te) to image the quasi-particle scattering interference patterns in the superconducting state was reported [55]. By observing the magnetic-field dependence of the quasiparticle scattering strength, Hanaguri et al. Found the sign of the gap is reversed between the holes and the electron pockets, favoring s± wave. The magnetic resonance mode is observed in 1111 material , more in 122 materials [56], and in 111 systems. The observation of magnetic resonance mode points to asign-reversed gap structure.ARPES reported the observation of three dimensional gaps. The calculated Fermi surfaces of undoped LaFeAsO [88] have two electron cylinders around the tetragonal M point, plus two hole cylinders and a hole pocket around the the point. Similar results for the Fermiology of LaFePO - the first reported superconducting (Tc≈5 K) iron pnictide[57] Calculation of the Fermiology for F (electron)-doped superconducting LaFeAsO1-xFx resulted in a somewhat simplified Fermi surface, with the hole pocket filled. Due to the nearness 0f magnetism spin-fluctuation mediated pairing (weak coupling) for wave vectors connecting the electron and hole cylinders, the so-called "**s±** pairing state, while rejecting the other possible spin fluctuation- induced order parameter, i.e. triplet pairing. Numerous authors have also discussed spin-fluctuation mediated pairing in the FePn/Ch, with some theories stating that the **"s±"**also known as " sign-reversing s-wave" or "extended s-wave".

The hole-like pocket and α hole like sheet are both centered at the Brillouin zone center Γ while the electron-like **γ** Fermi sheet is centered at the **M** point. Where the hole and electron pockets in the idealized sketch show perfect nesting).

Theories of the FePn / Ch superconductors are further split into subgroups depending on whether they involve strong or weak coupling of the magnetic excitations and whether the predicted pairing states are node less or have gaps. The predicted extended *s*-wave symmetry can be either node less or have nodes, depending on the interplay between intra band & interband interactions. This 3D variation is seen even in the parent $BaFe_2As_2$ but is accentuated around both the Brillouin zone hole the center and electron M corner pockets in the doped compound. This 3D Character in $BaFe_2As_2$ and its derivatives is consistent with ARPES work on the other 122's.

Early ARPES work on LaFePO found reasonable agreement with LDA calculations and the usual five Fermi sheets, with hole pockets centered at the point based on dyz and dyz Fe orbital's for the inner pocket and based on Fed3z_2-r_2 states hybridized with P orbital and La orbital's for the outer pocket) and electron pockets at the M point.

Most of the ARPES experiments with FeSCs have shown fully opened *s*-wave gaps with some degree of anisotropy around the FSs, this is consistent with the -wave gap scenario. This probe itself, however, cannot tell the sign-changing nature of the -gap function. On the other hand, the interesting and challenging issue is that even when the ARPES experiments measured isotropic full gaps, various other experimental probes—NMR, SH, thermal conductivity, penetration depth, etc have shown strong nodal-gap features in the SC state with basically the same compounds for which the ARPES experiments saw full *s*-wave gaps. Although the pairing mechanism of Fe-based superconductors (FeSCs) has not yet been settled.

The vast majority of experiments support the existence of spin-single sign-changing *s*-wave SC gaps on multi-bands (s±-wave state). This multi-band s±-wave state is a very unique gap state and displays numerous unexpected novel SC properties, such as a strong reduction of the coherence peak, non-trivial impurity effects, nodal-gap-like nuclear magnetic resonance signals and thermal conductivity. Large amount of experiments are consistent with s-wave symmetry, which can be fully gaped or nodal s± wave therefore the observation of in-plane nodes does not clash with this symmetry type.

Chapter 3

3.1 Application of Superconductors

The recent discovery of iron-based superconductors has provoked eagerness for extensive research on these materials because they form the second high-temperature superconductor family after the copper oxide superconductors and imparts an expectation for materials with a higher transition temperature. It has also been clarified that they have exceptionally unusual physical properties such as unconventional pairing mechanism and superconducting properties preferable for application with high upper critical field and small anisotropy. The development of an iron-based superconductor that Hosono's research group reported three years ago is a remarkable achievement, producing a superconductor with a maximum transition temperature of 56K, although it is below the highest recorded transition temperature of a copper oxide-based superconductor, iron-based superconductors have a large upper critical field of 50- 100T,along with a small anisotropy compared to copper oxide-based superconductors, it is highly anticipated that wire applications involving magnets that generate large magnetic fields exceeding those of metal-based superconducting wires will emerge[66]. Currently, the Tc of an iron-based superconductor is lower compared to a copper oxide based superconductor. Thus, a Y-based copper oxide thin film operating at a Tc greater than 90 K exhibits greater critical current density values when compared at the same temperature [67]. However, the characteristics of Fe-based superconductors, including their small anisotropy, high tolerance for magnetic field, large critical angle are now apparent, with these results implying the great potential for superconducting wires/tapes applications, in particular, wires that are able to generate greater magnetic fields than their metal-based counterparts at low temperatures. Iron based superconductor Josephson devices Scientists and engineers now developing a SIS (superconductor-insulator superconductor) tunneling Josephson junctions using newly discovered iron-based superconductors that is the basic component of superconducting devices With the development of high-Tc SQUID (superconducting quantum interference device) magnetometers that operates at temperatures higher than conventional, this research aims at applications involving ultra-sensitive biomagnetic measurement such as magnetocephalography & magnetocardiography.Fe-based high temperature superconducting devices are expected to operate at high temperatures, speeds and frequencies incomparable with conventional devices.

With conventional copper oxide high-temperature superconducting, devices are considered to be infeasible unless the interfaces are controlled, but at ethnology for creating junctions hasn't been established iron-based high-temperature superconductors have excellent lattice matching with Si and III-V-group semiconductors. Zero resistance and high current density have a major impact on electric power transmission and also enable much smaller or more powerful magnets for motors, generators, energy storage, medical equipment and industrial separations. at high frequencies and extremely low signal dispersion are key aspects in microwave components, communications technology and several military applications. Low resistance at higher frequencies also reduces substantially the challenges inherent to miniaturization brought about by resistive, or I_2R, heating. The high sensitivity of superconductors to magnetic field provides a unique sensing capability, in many cases 1000x superior to today's best conventional measurement technology. Magnetic fi exclusion is important in multi-layer electronic component miniaturization, provides a mechanism for magnetic levitation and enables magnetic field containment of charged particles.

Superconductivity is widely regarded as one of the great scientific discoveries of 20th Century. This miraculous property causes certain materials, at low temperatures, to lose all resistance to the flow of electricity. This state of "losslessness" enables a range of innovative technology applications. At the dawn of the 21st century, superconductivity forms the basis for new commercial products that are transforming our economy and daily life.

Current Applications

Magnetic Resonance Imaging, Nuclear Magnetic Resonance (NMR), High-energy physics accelerators and Plasma fusion reactors. Industrial magnetic separation of kaolin clay, The major applications of superconductivity in the medical diagnostic, science and industrial processing fields listed above all involve LTS materials and relatively high field magnets. Several smaller applications utilizing LTS materials have also been commercialized, e.g. research magnets and Magneto-Encephalography (MEG). The latter is based on Superconducting Quantum Interference Device (SQUID) technology which detects and measures the weak magnetic fields generated by the brain. The only substantive commercial products incorporating base HTS materials are electronic filters used in wireless stations.

Emerging Applications

Superconductor-based products are extremely environmentally friendly compared to their conventional counterparts. They generate no greenhouse gases and are cooled by non-flammable Liquid nitrogen (nitrogen comprises 80% of our atmosphere) as opposed to conventional oil coolants that are both flammable and toxic. They are also typically at least 50% smaller and lighter than equivalent conventional units which translate into economic incentives. These benefits have given rise to the ongoing development of many new applications in the following sectors: Applications in Electric Power, HTS wire, HTS power cables, HTS Transformers for Wind energy, energy storage ,Transportations, Revolution in ship design, Magnetically levitated Trains, Radiation free imaging, Applications of MRI, Ultera-low field ,Magnetic resonance imaging (ULF-MRI),Magneto encephalography(MEG),Magnetic source imaging (MSI),In high energy physics Space exploration, Future NMR,application in wireless communication ,all Digital revivers ,in sensors, Radar and other areas of research, Continuous Monitoring capabilities and cooling Utility science,[67].

Technology Development

The basic technology for very large and small-scale applications is in many respects well developed, based on considerable industrial experience in cryogenic distillation, as well as the years of experience of many manufacturers of small-scale cryocoolers. However, there is a need for ongoing research and development to meet the large-scale refrigeration needs, cost targets and rigorous reliability requirements for the full range of HTS application opportunities.

4. Result and discussion on magnetization measurement

4.1 Recent Studies on Iron based superconductor

In this Chapter, we will discuss the progress of study of Iron based superconductors as mentioned earlier the superconductivity of the 1111-type materials was first discovered in LaFePO [59]. With a relatively low Tc of 4 K; this Tc could be enhanced to 7 K by fluorine doping at the oxygen sites, this produces more electron carriers in the crystal lattice. This report was not widely noted until a break through appeared in February 2008, when the same research group announced a similar superconductor of F-doped LaFeAsO1-xFx, with reaching 26 K when x is around 0.11and 0.89 respectively. The undoped parent compound, LaFeAsO, was investigated but showed no superconductivity at low temperature. This relatively high Tc of 26 K, the iron-containing composition, and the layered crystal structure became immediate topics of interest and research. By replacing the La atoms with other rare-earth elements and modulating the structural parameters, new superconductors were discovered and Tc was quickly enhance xFx, CeFeAsO1-xFx, PrFeAsO1- xFx, and NdFeAsO1-xFx to above50 K[60]. The succeeding investigation has seen a doubling of the highest onset Tc of the 1111-type superconductors up to 55{57 K}. Apart from the 1111-type, other structural types of iron-based superconductors were also synthesized, these iron-based pnictide superconductors have been named the second class of the high-Tc family after cuprate superconductors.

4.2 Magnetization measurement

4.2.1 Motivations

In Ln1111 family of superconductors different approaches were applied to understand the mechanism and to push Tc. Typical example that shows the enhancement of sc are electron doping, hole doping and by applying pressure for example, applying 4GPa in LaAsFeO0.89F0.11 (43K) [61]. On the other hand the suppression of Tc by hole doping was reported by Mn substitution on Fe site [62]. The suppression effect of Mn atoms at low temperature gets attention due to its poisoning effect even at small amount of doping (x=0.2%)[63].

4.2.2 Methodology

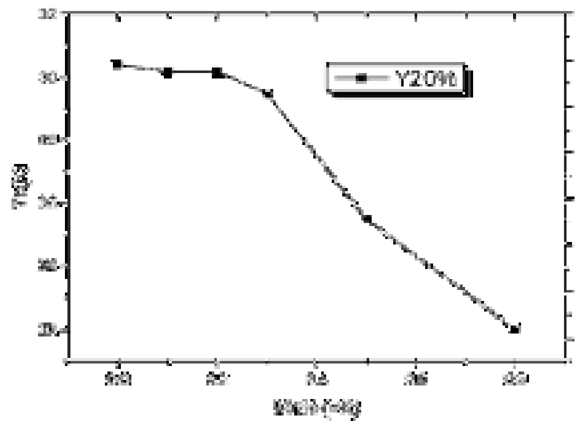
So far there was a few reports on the computation of Y and Mn impurities when both doped on same compounds. That means the increment of Tc via lattice shrinkage in the presence of Y impurities and the poisoning effect of Mn atoms was not mentioned.

In this work we report on Mn and Y doped La1111 poly crystalline sample from data obtained by magnetization measurement using VSM-SQUID. We took the data from Solid state research center IFW Dresden Germany. We focused on a series of $La_{1-x}Y_xFe_{1-y}Mn_yAsO_{0.86}F_{0.11}$ sample.

Polycrystalline samples of $La_{1-x}Y_xFe_{1-y}Mn_yAsO_{1-z}F_z$ were prepared from mixtures of LaAs, YAs, Fe_2O_3, FeF_3, Fe and Mn at nominal molar ratios as described in detail in Ref 64. All the ingredients were milled, mixed and pressed into pellets under Ar atmosphere. The samples were heated in an evacuated silica tube at 940 °C for 8 h and at 1150° C for 48 h. The annealed pellets were grind and polished and characterized with wavelength-dispersive X-ray spectroscopy (WDX). We took magnetization measurement data on polycrystalline sample that were prepared based on the aforementioned techniques. The measurements were taken using superconducting quantum interference device magnetometer (7T-SQUID) from Quantum Design. Data were taken in the temperature range 1.8-40k applying 10Oe in zero-filed-cooled (ZFC) and in field-cooled (FC) states.

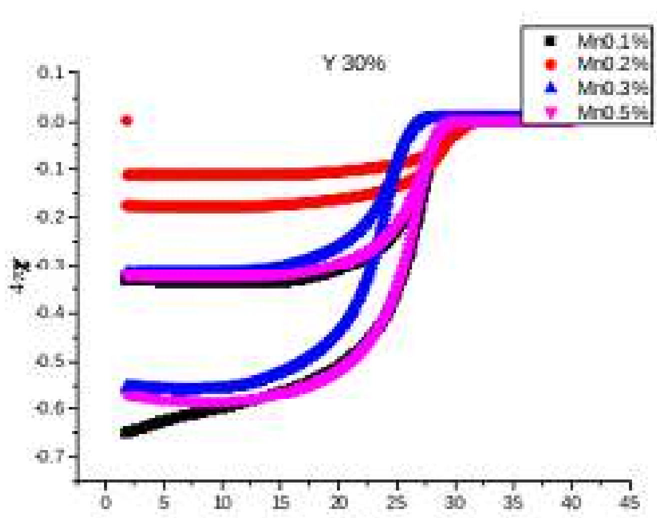
4.2.3. RESULT AND DISCUSSION Th

e superconducting critical temperature was determined from zfc/fc susceptibility measurement. Its value was decided using the data of the diamagnetic susceptibility figure (3a) shows Tc versus Mn content for 20% Yttrium doping sample. The value of Tc decreases as the concentration of Mn increases.



Mn(20%)

Figure 3a: Tc vs Manganese content for 20% Yttrium doping.



X=Mn (30%)

In Figure 3b, 30%Y doping samples for different Mn content(x= 0, 0.1, 0.2, 0.3, 0.5, 0.8%) is shown.

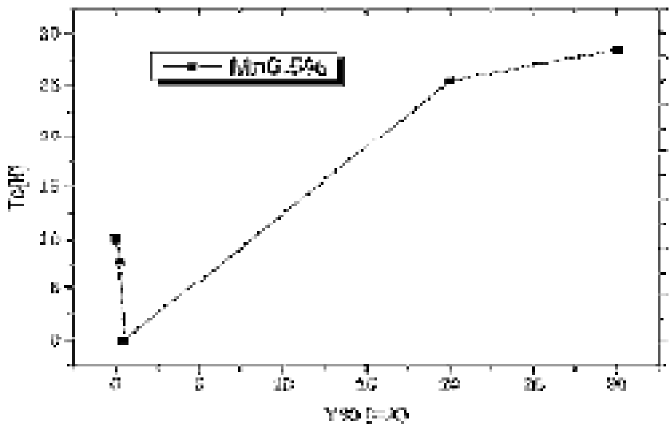


Figure 3c shows that Tc increases up on doping 20% Yttrium

In the absence of Mn, Y doping induces superconductivity, for example, for 30%y Tc=33k. But in the absence of Y, Mn doping suppress superconductivity, for example, for 0.5%Mn Tc=12.9k and for 1%Mn superconductivity completely suppressed. These results are in agreement with the already reported properties of Y and Mn doping on La1111 [65]. These result shows that superconducting mechanism cannot be understood without the knowledge of the interplay of superconductivity and Magnetism.

5. Summary

The discovery of superconductivity in systems not just containing iron, but in systems where the Magnetic behavior of iron appears to play a dominant role in the superconducting properties. Electron-phonon coupling is not sufficient to explain superconductivity in the whole family of iron-based superconductors based on the experiment done for the F-doped LaFeAsO compounds; The interplay of magnetism and superconductivity strongly suggests that magnetic fluctuations are involved either directly or indirectly in the Cooper pairing in the Iron Based Superconductors. Magnetism/magnetic fluctuations being linked with the superconducting pairing mechanism in the FePn/Ch materials. These results are in agreement with the already reported properties of Y and Mn doping on La1111 [69]. These result shows that superconducting mechanism cannot be understood without the knowledge of the interplay of superconductivity and Magnetism.

In the context of magnetism, pairing could arise from fluctuations emanating from a quantum critical point of three players coulomb repulsion, spin fluctuation and phonon coupling may favor high-Tc superconductivity in these materials. Many theoretical approaches found that strong antiferromagnetic correlation (spin fluctuation) triggers s± pairing next to the antiferromagnetism. The match between spin fluctuation structure and Fermiology might drive superconductivity in at least some of these materials. Therefore, antiferromagnetic spin fluctuations could possibly be the major mediating glue in the iron-based superconductors. In general, the superconductivity has been suggested to arise from a magnetic coupling between electron and hole pockets at the Fermi Surface [70]. Such a pairing interaction mediated by magnetic excitations (spin waves) can lead to a multiband superconductivity with a sign reversal between the electron pocket and the hole pocket, represented by the s wave symmetry.

In this paper, we have reviewed generic SC properties of the s±-wave pairing state and critically examined them in comparison with the available experiments on FeSC compounds. The generic SC properties of the s±-wave Pairing states are generating various nodal-gap-likes SC features in different experimental probe. Therefore, cross-checking with different probes is important to confirm the presence or absence of gap-nodes in the gap function.

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