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High-T_c Superconductors Based on FeAs Compounds

铁砷化合物高温超导体

（影印版）

〔俄〕伊久莫夫（Y. Izyumov）
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著

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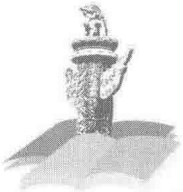

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序　言

物理学是研究物质、能量以及它们之间相互作用的科学。她不仅是化学、生命、材料、信息、能源和环境等相关学科的基础，同时还是许多新兴学科和交叉学科的前沿。在科技发展日新月异和国际竞争日趋激烈的今天，物理学不仅囿于基础科学和技术应用研究的范畴，而且在社会发展与人类进步的历史进程中发挥着越来越关键的作用。

我们欣喜地看到，改革开放三十多年来，随着中国政治、经济、教育、文化等领域各项事业的持续稳定发展，我国物理学取得了跨越式的进步，做出了很多为世界瞩目的研究成果。今日的中国物理正在经历一个历史上少有的黄金时代。

在我国物理学科快速发展的背景下，近年来物理学相关书籍也呈现百花齐放的良好态势，在知识传承、学术交流、人才培养等方面发挥着无可替代的作用。从另一方面看，尽管国内各出版社相继推出了一些质量很高的物理教材和图书，但系统总结物理学各门类知识和发展，深入浅出地介绍其与现代科学技术之间的渊源，并针对不同层次的读者提供有价值的教材和研究参考，仍是我国科学传播与出版界面临的一个极富挑战性的课题。

为有力推动我国物理学研究、加快相关学科的建设与发展，特别是展现近年来中国物理学者的研究水平和成果，北京大学出版社在国家出版基金的支持下推出了“中外物理学精品书系”，试图对以上难题进行大胆的尝试和探索。该书系编委会集结了数十位来自内地和香港顶尖高校及科研院所的知名专家学者。他们都是目前该领域十分活跃的专家，确保了整套丛书的权威性和前瞻性。

这套书系内容丰富，涵盖面广，可读性强，其中既有对我国传统物理学发展的梳理和总结，也有对正在蓬勃发展的物理学前沿的全面展示；既引进和介绍了世界物理学研究的发展动态，也面向国际主流领域传播中国物理的优秀专著。可以说，“中外物理学精品书系”力图完整呈现近现代世界和中国物理

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科学发展的全貌，是一部目前国内为数不多的兼具学术价值和阅读乐趣的经典物理丛书。

“中外物理学精品书系”另一个突出特点是，在把西方物理的精华要义“请进来”的同时，也将我国近现代物理的优秀成果“送出去”。物理学科在世界范围内的重要性不言而喻，引进和翻译世界物理的经典著作和前沿动态，可以满足当前国内物理教学和科研工作的迫切需求。另一方面，改革开放几十年来，我国的物理学研究取得了长足发展，一大批具有较高学术价值的著作相继问世。这套丛书首次将一些中国物理学者的优秀论著以英文版的形式直接推向国际相关研究的主流领域，使世界对中国物理学的过去和现状有更多的深入了解，不仅充分展示出中国物理学研究和积累的“硬实力”，也向世界主动传播我国科技文化领域不断创新的“软实力”，对全面提升中国科学、教育和文化领域的国际形象起到重要的促进作用。

值得一提的是，“中外物理学精品书系”还对中国近现代物理学科的经典著作进行了全面收录。20 世纪以来，中国物理界诞生了很多经典作品，但当时大都分散出版，如今很多代表性的作品已经淹没在浩瀚的图书海洋中，读者们对这些论著也都是“只闻其声，未见其真”。该书系的编者们在这方面下了很大工夫，对中国物理学科不同时期、不同分支的经典著作进行了系统的整理和收录。这项工作具有非常重要的学术意义和社会价值，不仅可以很好地保护和传承我国物理学的经典文献，充分发挥其应有的传世育人的作用，更能使广大物理学人和青年学子切身体会我国物理学研究的发展脉络和优良传统，真正领悟到老一辈科学家严谨求实、追求卓越、博大精深的治学之美。

温家宝总理在 2006 年中国科学技术大会上指出，“加强基础研究是提升国家创新能力、积累智力资本的重要途径，是我国跻身世界科技强国的必要条件”。中国的发展在于创新，而基础研究正是一切创新的根本和源泉。我相信，这套“中外物理学精品书系”的出版，不仅可以使所有热爱和研究物理学的人们从中获取思维的启迪、智力的挑战和阅读的乐趣，也将进一步推动其他相关基础科学更好更快地发展，为我国今后的科技创新和社会进步做出应有的贡献。

“中外物理学精品书系”编委会 主任

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王恩哥

2010 年 5 月于燕园

Preface

In the course of a year or slightly more that passed since the discovery of a new class of high-temperature superconductors (HTSCs) in FeAs-based compounds [1], the world's community of physicists, chemists and technologists achieved a substantial progress in understanding the mechanisms and details of this superconductivity. The intensity of researches coming about is comparable only to that which accompanied the discovery of HTSCs in cuprates. However, the present scientific context is markedly different from that having existed twenty years back. In those times, the researchers moved on while blindly palpating the terrain. At present, they can rely on a rich accumulated experience of work with complex compounds; novel experimental methods and numerical calculation schemes have emerged; computational resources became by far much more powerful, and, last but not least, the physical ideas elaborated in the studies of cuprates could have been immediately adapted for the study of new HTSC compounds.

An unprecedentedly fast advance of researches on the FeAs compounds was helped by an instantaneous propagation of knowledge via electronic data archives. A markedly international character of studies is noteworthy; as a rule, the articles on FeAs systems are published by joint teams of distant lands and laboratories that boosts a rapid augmentation of knowledge about the properties of systems under study and thinking over the wealth of experimental data. During last years (2008–2010), more than few thousand publications within this domain have appeared. This means that every day brought about, on an average, 2–3 new papers deposited in electronic archives.

If the epic of HTSC study in cuprates demanded years for arriving at some understanding of these materials' nature, with respect to new class of materials one year was sufficient as a due time to make a primary overview of the results obtained. Within half a year after the discovery of HTSC in FeAs compounds, first three reviews appeared in the *Physics – Uspekhi* [2–4]. In the beginning of 2009, a special issues of *Physica C* [5] and *New Journal of Physics* [6] appeared with review articles by leading scientists on the basics of the physics of the FeAs compounds, which also summarized the bulk of results accumulated within a year.

This book seems to be the world's first monograph on the physics of FeAs systems. It outlines in a systematic way the results of researches done in the global scientific community throughout the whole period since the end of February

2008, as the high-temperature superconductivity has been discovered in a LaOFeAs system.

The first three chapters cover experimental investigations of all classes of the FeAs compounds in which superconducting state has been discovered. The fourth chapter is devoted to theory models of these compounds and to the discussion, on this basis, of experimental results. Differently from the reviews published in [5, 6], which specifically addressed various aspects of the physics of FeAs systems in some detail, we attempted here to cover, within a unique concept, the whole bulk of experimental and theoretical material on these systems by now available. The authors' hope is that the book be of use for a broad fold of readers: those who already immediately work in this problem and who would wish to enter it.

Russia
August 2010

Yu. A. Izyumov
E.Z. Kurmaev

Acronyms

1111	compounds of type LaOFeAs
122	compounds of type $BaFe_2As_2$
111	compounds of type LiFeAs
11	compounds of type FeSe
LDA	Local Density Approximation
LSDA	Local Spin Density Approximation
DMFT	Dynamical Mean Field Theory
LDA + DMFT	joint LDA and $DMFT$ computational scheme
RPA	Random-Phase Approximation
FLEX	Fluctuation Exchange Interaction
Folded BZ	Folded BZ
Unfolded BZ	Unfolded BZ
SDW	Spin Density Wave
CDW	Charge Density Wave
NMR	Nuclear Magnetic Resonance
STS	Scanning Tunneling Microscopy
PCAR	Point-Contact Andreev Reflection
PES	Photoelectron spectroscopy
ARPES	Angle Resolved Photoelectron Spectroscopy
RXES	Resonant X-Ray Emission Spectroscopy
ZBC	Zero-Bias conductance
HTSC	High Temperature Superconductivity
OP	Order Parameter
GF	Green Function
BCS	Bardin–Cooper–Schrieffer's theory

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Chapter 1
Introduction

The first report of superconductivity in LaOFeAs appeared in 2006 [1]; however, the transition temperature was low, $T_c = 3.5$ K. Similarly, LaONiP have shown $T_c = 4.5$ K [7]. The breakthrough occurred in February 2008, as Kamihara et al. reported a superconductivity with $T_c = 26$ K in fluorine-doped compound $LaO_{1-x}F_x$FeAs [8]. Immediately afterwards several Chinese groups, by substituting lanthanum with other rare-earth elements, achieved much higher T_c values, namely, 41 K in $CeO_{1-x}F_x$FeAs [9], 52 K in $PrO_{1-x}F_x$FeAs [10] and reached 55 K in $SmO_{1-x}F_x$FeAs [11].

The pristine (undoped) compounds are antiferromagnetic (AFM) metals, in which the magnetic ordering comes about simultaneously with structural phase transition at the Neél temperature $T_N \approx 140$ K (in LaOFeAs) from tetragonal to orthorhombic phase. On substituting oxygen with fluorine, T_N rapidly falls down as the F concentration increases, and at $x \simeq 0.1$ the long-range magnetic ordering disappears, and a superconducting state sets on. A typical phase diagram of this type of compounds is shown in Fig. 1.1 in the (T, x) plane [12].

The situation so far resembles the HTSC in cuprates, e.g., $(La_{1-x}Sr_x)_2CuO_4$ exhibits a similar phase diagram. The superconductivity appears there in compounds of the type La_2CuO_4, which are also AFM under stoichiometry, in the course of lanthanum being substituted by strontium. In both systems, the doping brings along charge carriers (electrons or holes) that suppresses the AFM ordering and creates conditions for forming the Cooper pairs. This analogy supported a suggestion that the high-T_c superconductivity in newly discovered FeAs-based systems is influenced by the system's closeness to a magnetic phase transition, so that high T_c values are due to the carriers pairing mechanism via spin fluctuations.

An analogy between FeAs systems and cuprates becomes more apparent if we compare their crystal structures. The FeAs-based systems are built by stapling of the FeAs planes, intermediated by the LaO layers, similarly to how in cuprates the stacked CuO_2 planes are separated by the La- or Y-Ba layers. By force of their layered structure, both types of systems are strongly anisotropic, and electronic states therein are quasi two-dimensional.

Closely following the *Re*OFeAs compounds (with *Re* being a rare-earth element), the compounds of the type AFe_2As_2, (A = Ba,Sr,Ca) emerged, whose peculiarity is that a repeated unit in them contains a doubled FeAs plane, similarly to

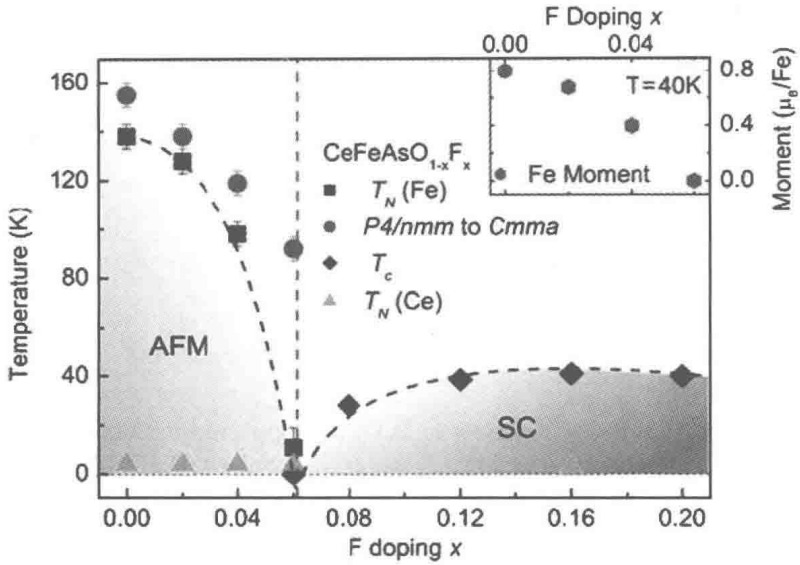

Fig. 1.1 Phase diagram in the (T, x) plane for the $CeO_{1-x}F_xFeAs$ compound

doubled layers in cuprates $YBa_2Cu_3O_6$. In doped AFe_2As_2, the superconductivity was immediately found with $T_c = 38$ K [13]. Further on, another class of FeAs-based systems has been discovered, the LiFeAs compound in which the FeAs planes are separated by the layers of lithium. It is remarkable that in this compound superconductivity with $T_c = 18$ K appears without any doping [14, 15].

A similar property is revealed by yet another structural type, namely, FeSe, FeS and FeTe, which are quite resembling the compounds of the FeAs group. These novel compounds are built from iron–chalcogen planes, in which, like in the FeAs compounds, the iron atoms form a squared lattice, each atom being surrounded by an octahedron of chalcogens. Here, no intermediary layers are present. In one such compound, FeSe, under pressure of $\sim$1.5 GPa a superconductic transition with $T_c = 27$ K has been detected [16].

Therefore as of now we are aware of three classes of compounds build of the FeAs layers: these are LaOFeAs, AFe_2As_2, LiFeAs and moreover a similar structure type of FeSe in which the superconductivity with high T_c was detected. Physical properties of these compounds have many similarities and are dominated by the influence of a common planar structural element. More precise analysis of physical properties confirms this suggestion.

Calculations on electron–phonon coupling in these compounds have shown [17, 18] that the standard electron–phonon coupling mechanism cannot account for such high T_c values.

A similarity in physical properties of the FeAs-compounds with those of high-temperature superconducting cuprates puts forward a question about a role of electron correlations in these new materials. It is known that in the materials on

the basis of transition-metal and rare-earth elements, such correlations do often play a primary role – see, e.g., a monograph by Fulde [19]. Another important question is that concerning the role of degenerate 3d orbitals of the Fe ions in the formation of electronic structure near the Fermi level in the FeAs-compounds, and about the spin state of the Fe ions in the compound [20]. Both these important questions will be addressed in the book from both experimental and theoretical viewpoints.

Chapter 2
Compounds of the ReOFeAs Type

2.1 Crystallochemistry and Basic Physical Properties of Doped Compounds

2.1.1 Crystal Structure

The highest values of T_c have been achieved in the row of *Re*OFeAs doped compounds, where *Re* stands for a rare-earth element (Table 2.1). All these compounds possess, at room temperature, a tetragonal structure with the $P4/nmm$ space group. Their crystal structure is formed by repeated FeAs layers, interlaced by the LaO layers. The FeAs layer is, in fact, created by three closely situated atomic planes: the middle one is a quadratic lattice of Fe atoms, sandwiched between two quadratic lattices of As, so that each atom of iron is surrounded by a tetrahedron of arsenic atoms. In other words, the FeAs layer is, in fact, formed by $FeAs_4$ complexes. The FeAs and LaO layers are separated by 1.8 Å.

The crystal structure of LaOFeAs is shown in Fig. 2.1. Lattice parameters for the *Re*OFeAs compounds are given in Table 2.1. As is seen, the tetragonal unit cell is strongly elongated, which explains a strong anisotropy of all its properties and a quasi-bidimensional nature of electronic states. The closest to each Fe atom are those of As, which underway to the next Fe neighbours, so that the electron transfer processes over the Fe sublattice are mediated by the Fe-As hybridization, and the exchange interaction between Fe atoms is of indirect character via the As atoms.

Crystallochemical properties of LaOFeAs compounds are determined by the configuration of the outer electron shells: Fe($4s4p3d$), As($4s4p$), La($6s5d4f$), O($2s2p$). The formal valences of ions are as follows: $La^{3+}O^{2-}Fe^{2+}As^{3-}$.

2.1.2 Electron Doping

On substituting an oxygen atom by fluorine, an extra electron goes into the FeAs layer; such situation is commonly referred to as electron doping. A substitution of lanthanum by, say, strontium, the LaO layer would lack one electron, which can be

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