ARTICLE IN PRESS

COMREN:3224

C. R. Physique ●●● (●●●●) ●●●–●●●

Contents lists available at ScienceDirect

Comptes Rendus Physique

www.sciencedirect.com

Iron-based superconductors / Supraconducteurs à base de fer

The phase diagrams of iron-based superconductors: Theory and experiments

Les diagrammes de phases des supraconducteurs à base de fer : la théorie et les expériences

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ARTICLE INFO

Article history:
Available online xxxx

Keywords:
Iron-based superconductors
Phase diagrams
Structural transformations
Superconductivity
Magnetism
Nematicity

Mots-clés :
Supraconducteurs à base de fer
Diagrammes de phase
Transformations structurels
Supraconductivité
Magnétisme
Phase nématique

ABSTRACT

Phase diagrams play a primary role in the understanding of materials properties. For iron-based superconductors (Fe-SC), the correct definition of their phase diagrams is crucial because of the close interplay between their crystallochemical and magnetic properties, on one side, and the possible coexistence of magnetism and superconductivity, on the other.

The two most difficult issues for understanding the Fe-SC phase diagrams are: 1) the origin of the structural transformation taking place during cooling and its relationship with magnetism; 2) the correct description of the region where a crossover between the magnetic and superconducting electronic ground states takes place. Hence a proper and accurate definition of the structural, magnetic and electronic phase boundaries provides an extremely powerful tool for material scientists.

For this reason, an exact definition of the thermodynamic phase fields characterizing the different structural and physical properties involved is needed, although it is not easy to obtain in many cases. Moreover, physical properties can often be strongly dependent on the occurrence of micro-structural and other local-scale features (lattice micro-strain, chemical fluctuations, domain walls, grain boundaries, defects), which, as a rule, are not described in a structural phase diagram.

In this review, we critically summarize the results for the most studied 11-, 122- and 1111-type compound systems, providing a correlation between experimental evidence and theory.

RÉSUMÉ

Les diagrammes de phase jouent un rôle de première importance dans la compréhension des propriétés des matériaux. En ce qui concerne les supraconducteurs à base de fer (Fe-SC), la définition correcte de leurs diagrammes de phase est cruciale à cause de l'intime interaction entre leurs propriétés cristallochimiques et magnétiques, d'une part, et la possible coexistence de magnétisme et de supraconductivité, d'autre part.

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http://dx.doi.org/10.1016/j.crhy.2015.06.001
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Please cite this article in press as: A. Martinelli et al., The phase diagrams of iron-based superconductors: Theory and experiments, C. R. Physique (2015), http://dx.doi.org/10.1016/j.crhy.2015.06.001

Les deux difficultés principales pour la compréhension des diagrammes de phase Fe-SC sont : 1) l'origine de la transformation structurelle ayant lieu pendant le refroidissement et sa relation avec le magnétisme ; 2) la description correcte de la région où survient un recouvrement entre les états fondamentaux électroniques, magnétiques et supraconducteur électronique survient. De ce fait, une définition appropriée et précise des frontières des phases structurelle, magnétique et électronique fournit un outil extrêmement puissant pour les scientifiques du domaine des matériaux.

Pour cette raison, une définition exacte des champs de phases thermodynamiques caractérisant les différentes propriétés structurelles et physiques impliquées est nécessaire, bien qu'elle ne soit pas aisée à obtenir dans de nombreux cas. De plus, les propriétés physiques peuvent souvent dépendre fortement de la survenue de caractéristiques micro-structurelles ou autres à l'échelle locale (micro-contraintes dans le réseau, fluctuations chimiques, parois de domaines, joints de grains, défauts), qui, d'ordinaire, ne sont pas décrites dans un diagramme de phases structurelles.

Dans cette revue, nous résumons de manière critique les résultats obtenus pour les systèmes composites le plus étudiés de types 11, 122 et 1111, qui établissent une corrélation entre les preuves expérimentales et la théorie.

1. Overview

The fascinating physics distinguishing the class of materials referred to as iron-based superconductors (Fe-SC) emerges from the delicate and tangled interplay between magnetism, superconductivity and crystallochemistry. The understanding of the normal state properties is a fundamental step in the development of a theory of superconductivity in Fe-SC. Despite the outstanding attention paid to these systems, it is not yet clear if a universal phase diagram can be established.

Pnictides (typically 122- and 1111-type systems) display quite similar structural and magnetic phase relationships. The chalcogenides (11-type systems) are rather different; in particular, the pseudo-binary system β-FeSe$_{1-x}$–β-Fe$_{1+y}$Te is the only relevant system among the Fe-chalcogenides and will be treated in detail below. A schematic phase diagram is drawn in Fig. 1, highlighting the features shared by most of these systems.

1.1. Structural transformations

As a rule, the undoped parent compound undergoes a structural transformation upon cooling at the temperature T_s, followed by a magnetic transition at T_m, where $T_m < T_s$. For the 122- and 1111-type compounds, a translation-equivalent (*translationengleiche*) structural transition of index 2 changes the structure from tetragonal to orthorhombic. The unit cell of the low-temperature orthorhombic phase is rotated by 45° in the *xy* plane with respect to that of the high-temperature tetragonal one, and the edges of the basal cell are a factor of $\sqrt{2}$ larger in the orthorhombic structure.

So far, two main scenarios have been proposed to explain the occurrence of the transformation from tetragonal to orthorhombic in the 122- and 1111-type compounds: 1) orbital ordering drives the structural transition and induces magnetic anisotropy, thus triggering the magnetic transition [1–3]; 2) magnetic fluctuations drive the structural transition and induce orbital ordering [4].

The structural transformation temperature T_s can be reliably ascertained by diffractometric analysis carried out as a function of temperature; in particular for 122- and 1111-type compounds a selective Bragg peak splitting marks the symmetry breaking (Fig. 2). Conversely, no anomaly can be detected on crossing T_s by optical measurements [5,6], since no displacive optical mode is involved [7]. For this reason in this review we usually refer to the structural transformations temperatures T_s obtained by diffraction, whenever not specified. Otherwise it is indicated when data stems from other trustworthy methods, such as specific heat measurements or NMR analysis.

In this review these kinds of data are used to draw phase boundaries in phase diagrams. Remarkably the thermal dependence of the resistivity often exhibits discontinuities that are commonly related to the structural transition; actually such discontinuities mark a change of the electronic properties, rather than a real structural change, that in some cases can become extremely reduced. Hence these kinds of data are not considered in this review, since they cannot be considered a reliable probe for detecting structural transformations.

1.2. Magnetism

When dealing with magnetic ordering in 1111- and 122-type compounds, confusion can arise when comparing works referring to the parent tetragonal phase with those analyzing the distorted orthorhombic structure. In fact, due to the aforementioned rotation undergone by the unit cell after the structural transformation, the in-plane magnetic wave-vector is (1,0) or (½, ½) when referred to the orthorhombic or the tetragonal structure (Fig. 3), respectively (for a detailed discussion,

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