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ACADEMY TRANSACTIONS NOTE

Oxygen deficiency structure in iron-based high temperature superconductor $GdFeAsO_{1-\delta}$

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Abstract

Oxygen deficiency in the iron-based HTSC GdFeAsO $_{1-\delta}$ seems to create a parallelogram shaped Fe^{2+}-ion/oxygen deficiency pattern in the Fe_2O_2 plane in *c*-direction. These two-dimensional nanostructures form superconducting current channels which are separated by $h = 0.828$ nm. The doping distance in direction of the super-current shows a strong correlation to the transition temperature.
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1. Introduction

Very recently, a new family of high temperature superconductors (HTSC) – consisting of fluorine-doped iron-based layered $LnO_{1-\Delta}F_{\Delta}FeAs$ with lanthanide elements Ln = La, Gd, Ce, Pr, Nd, Sm – have been discovered ([1–4] and references therein) with critical transition temperatures T_c between 26 and 54 K. These superconductors have a tetragonal layered structure and a two-dimensional superconducting plane.

Several research groups [2,5] have succeeded in synthesising iron-based HTSCs with oxygen deficiency instead of F-doping, e.g. $GdFeAsO_{1-\delta}$. This material has been well studied showing a transition temperature above 50 K at an optimum deficiency level of $\delta = 0.15$. In this paper, we will show that the correlation between the spacing (x) of Fe^{2+}-ion/oxygen deficiency positions in the Fe_2O_2 plane and T_c, as described by Eq. (1) for cuprates and F-doped iron-based HTSCs [3,6,7], applies also to $GdFeAsO_{1-\delta}$ (GAFO) for $n = 1$.

$$(2x)^2 \cdot n^{-2/3} \cdot 2M_{\text{eff}} \cdot \pi k T_c = h^2 \qquad (1)$$

2. Electronic and geometrical structure

The crystal unit cell structure of GAFO consists of 2 · [GdFeAsO] and has a tetragonal layered structure with the space group P4/nmm (Fig. 1). The atoms Gd^{3+}+Fe^{2+} provide five electrons to As^{3-}+O^{2-}, creating a metallic behaviour with a uniform potential pattern throughout the crystal. Superconductivity

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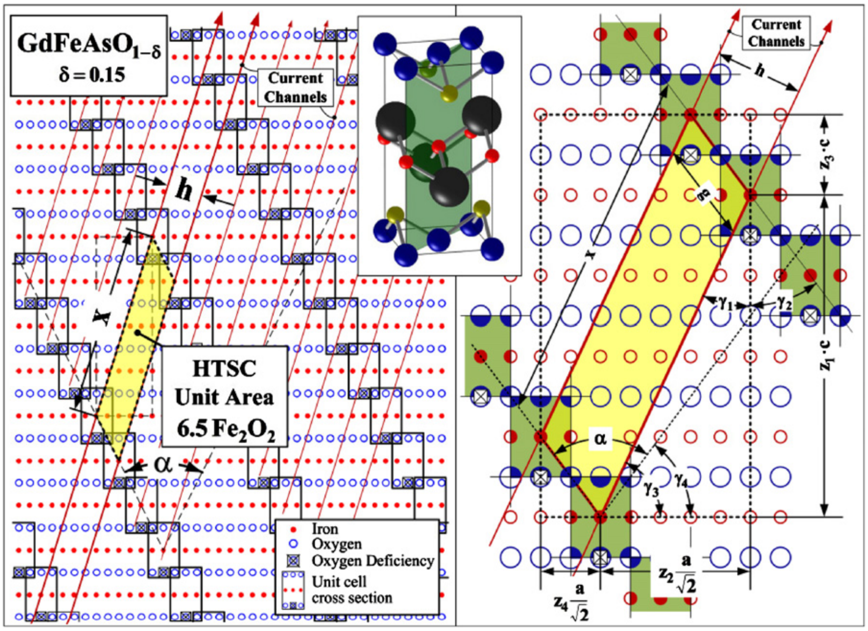

Fig. 1. (a) Superconducting Fe_2O_2 plane of $GdFeAsO_{1-\delta}$ showing the oxygen deficiency distribution and the superconducting current channels. (b) Illustration to determine the current carrying periodicity x by the parallelogram shaped HTSC unit area.

is achieved by doping using $2F^{1-}$-ions at O^{2-}-ion sites or through oxygen deficiency. The electronic arrangement in the unit cell with a missing O-atom is Gd^{3+}+Fe^{2+}+As^{3-} creating a periodic potential disorder with two free electrons in this unit cell. This is similar to $YBa_2Cu_3O_{7-\delta}$ with two free electrons at the oxygen deficiency position [6] and a super-current flow in the CuO_2 plane. For the F-doped Fe-based HTSCs it has been suggested that the super-current flows in c-direction [3]. We will assume the same situation for the oxygen deficiency case. This is supported by electronic structure calculations showing the same results for fluorine doping and oxygen deficiency [4]. Assuming a regular oxygen deficiency distribution in the Fe_2O_2 plane, the doping δ can be transformed into distances x and g for the missing O-atoms. Using the same nomenclature as in previous papers [3,6,7], $(\Sigma)^{-1}$ is the doping density and Σ represents the HTSC unit area A_{SC} with a doped element at each corner. Fig. 1 shows crystals sliced through the diagonal plane in c-direction. The optimum doping $\delta = (\Sigma)^{-1} = 0.15$ leads to $\Sigma = 6.67 \approx 6.5$ because the Fe_2O_2 unit area contains two O-atoms (Fig. 1b) and therefore the Fe_2O_2 unit area can be split into two halves and the HTSC unit area is made of integrals of $\frac{1}{2}Fe_2O_2$ unit areas. Because of the fact that the Fe_2O_2 unit area is rectangular with an area of $A = a\sqrt{2} \cdot c$, the super-current is anisotropic and probably only flows in a straight line from Fe–O to Fe–O and within an angle α. This results in A_{SC} having the form of a parallelogram with

$$A_{SC} = x \cdot h = \Sigma \cdot a\sqrt{2} \cdot c \quad (2)$$

Within the Fe_2O_2 superconducting plane the doping distances x and g are given by Pythagoras formula

$$x^2 = z_1^2 \cdot c^2 + z_2^2 \cdot (a/\sqrt{2})^2 \quad (3)$$

$$g^2 = z_3^2 \cdot c^2 + z_4^2 \cdot (a/\sqrt{2})^2 \quad (4)$$

The superconducting unit area can also be calculated by

$$A_{SC} = (z_1 + z_3) \cdot c \cdot (z_2 + z_4) \cdot (a/\sqrt{2}) - z_1 \cdot z_2 \cdot c \cdot (a/\sqrt{2}) - z_3 \cdot z_4 \cdot c \cdot (a/\sqrt{2}) \quad (5)$$

as illustrated in Fig. 1b leading to

$$z_1 \cdot z_4 + z_2 \cdot z_3 = 2 \cdot \Sigma \quad (6)$$

with $z_i \in \mathbb{N}$. The requirements that

(a) the super-current flows along two neighbouring doped unit cells where the closest doped half Fe_2O_2 unit cell must lay within the angle range α and
(b) no super-current flows in the Fe–Fe direction within the angle range $2\gamma_4$

Table 1
Structural data of superconducting $GdFeAsO_{1-\delta}$ with an deficiency value of $\delta = 0.15$.

T_c (K)	Crystal structure (nm)	Atomic doping	HTSC unit area	$(2x)^2 \times 10^{-18}$ (m^2)
Exp. 52.9 ± 0.6	$a = 0.389$ $c = 0.838$	$\delta = 0.15$	$z_1(c) = 4$; $z_2(a/\sqrt{2}) = 5$ $x = 3.62\,nm$	52.5
Calc. 52.9	Tetragonal	$A_{SC} = 6.5 \cdot Fe_2O_2$	$z_3(c) = 1$; $z_4(a/\sqrt{2}) = 2$ $g = 1.00\,nm$; $h = 0.828\,nm$	

lead to the following inequalities:

$$(z_1 \cdot c)/(z_2 \cdot a/\sqrt{2}) > c/a\sqrt{2} \rightarrow 2z_1 > z_2 \quad (7)$$

$$(z_3 \cdot c)/(z_4 \cdot a/\sqrt{2}) \leqslant c/a\sqrt{2} \rightarrow 2z_3 \leqslant z_4 \quad (8)$$

For GAFO, Eq. (6) results in $2 \cdot \Sigma = 13$ with the consequence that $z \neq 0$ and only a few combinations of $z \leqslant 12$ are possible. A calculation with a simple computer program using Eq. (6) and inequalities (7) and (8) leads to a one-to-one correspondence with $z_1 = 4$, $z_2 = 5$, $z_3 = 1$ and $z_4 = 2$ as illustrated in Fig. 1a and b. The above results show that GAFO works with a superconducting unit area of $A_{SC} = 6.5\ Fe_2O_2$ and the supercurrent flows in current channels as illustrated in Fig. 1 with a periodicity distance x given by Eq. (3) resulting to $x = 3.62\,nm$. The parallel current channels are separated by $h = 0.828\,nm$ (Table 1).

3. Discussions

Oxygen deficiency doping with $\delta = 0.15$ creates a disorder pattern with $x = 3.62\,nm$ and $g = 1.00\,nm$ and forms a parallelogram with a superconducting unit area of $A_{SC} = 6.5\ Fe_2O_2$. According to Eq. (1) with one superconducting plane per unit cell ($n = 1$) and $M_{eff} = 2m_e$ this leads to a transition temperature of T_c (calc.) $= 52.9\,K$. This value compares well with the experimental value of $52.9 \pm 0.6\,K$ [2] and matches the correlation curve in [7]. This result supports the suggestion that Fe_2O_2 represents the superconducting plane [3].

The separation (d) of neighbouring superconducting Fe_2O_2 planes is given by $d = a\sqrt{2}$ so that the superconducting unit volume $V_{SC} = A_{SC} \cdot a\sqrt{2} = (6.5 \times 0.461 \times 0.550)\,nm^3$ results in a superconducting carrier density N_{SC} with an effective mass of $M_{eff} = 2m_e$ of $N_{SC} = (V_{SC})^{-1} = 6.07 \times 10^{20}\,cm^{-3}$.

With the correlation described by Eq. (1) and the assumption that $2x = \lambda_{DB}$, the resonance effect between the de Broglie wavelength and the doping structure would require a maximum (de Broglie) velocity of the superconducting pair of $v_{DB} \approx 2.5 \times 10^6\,cm\,s^{-1}$. This would result in a maximum current density at $T = 0\,K$ for superconducting $GdFeAsO_{1-\delta}$ of $j(\max) \approx 5 \times 10^8\,A\,cm^{-2}$ according to

$$j(\max) \approx 2N_{SC} \cdot e \cdot v_{DB} \quad (9)$$

It appears that the oxygen deficiency in FeAs HTSCs has the same effect for the superconducting process as in Y123, except that the HTSC unit area is not square as for the symmetrical CuO_2 cuprate unit cells, but it has the size of a parallelogram.

The quality of the correlation depends strongly on the accuracy of the doping density δ. Measurements with other rare-earth elements like Ce, La, Nd, Pr and Sm have been done, but the actual deficiency value δ could not be determined precisely from polycrystalline samples [5].

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