Dependence of critical temperature on carrier density in $NdFeAsO_{1-y}$ using BCS theory

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This study addresses the influence of the carrier density on the critical temperature of layered superconductors by using the real dependence of density of states on energy in the framework of ordinary Bardeen-Cooper-Schrieffer (BCS) model. It is shown that such a model is in good agreement to obtain experimental data for new $NdFeAsO_{1-y}$ superconductors.

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1. Introduction

A new Fe-based era in the research of high-temperature superconductivity was initiated in [1], where the authors discovered superconductivity in LaOFeP compound with the critical temperature, T_c=4K. After which the transition temperature has reached the 26 K for the compound of $LaO_{1-x}F_xFeAs$ [2]. Additionally, a series of oxypnictides LaOMPn, where (M=Mn,Fe,Co,Ni) and (Pn=P,As,Sb) were synthesized, which has gained a lot of attention from researchers. By the end of 2008, the superconducting transition temperature T_c reached a saturation value of 56K in SmO_{1-x} F_xFeAs [3]. Furthermore, the authors found that the $BaFe_2As_2$ non-oxyde compound with antiferromagnetic ordering of Fe spins also becomes superconducting at T_c=38K under partial substitution of Ba by K [4]. Partial substitution of Co for Fe suppresses antiferromagnetic ordering and leads to the electron-type conductance with T_c=23K [5]. Superconductivity was also observed in Fe-based compounds of type 111 (LiFeAs [6] and NaFeAs [7]). Another type of Fe-based superconductor is the 011 type compounds (FeSe with critical temperature T_c=8K [8]). As a rule, superconducted Fe-based compounds have a layered tetragonal structure, which consist of alternating two-dimensional layers of FeAs, FeP or Fe_2As_2 and doping elements (see [9, 10]). These iron-containing layers are likely to be responsible for superconductivity.

Until now, several series of Fe-based superconductors have been found [11] possessing a layered crystal structure similar to that of the high-T_c cuprates. In similarity to cuprates, superconductivity appears while antiferromagnetism is suppessed by hole (or electron) doping or by application of external pressure. However, significant discrepancies have been observed between the Fe-based superconductors and cuprate superconductors. For example, d-wave superconductivity was realized in cuprate compounds, but an s±-type order parameters has been proposed for Fe-based superconductors [12]. Another peculiarity of superconducting state in Fe-based compounds is related with multiband character of state [13,14]. One of the widely investigated Fe-based superconductor is the $NdFeAsO_{1-y}$. The effect of oxygen deficiency on the critical temperature in $NdFeAsO_{1-y}$ was experimentally investigated in [15] which revealed that T_c increased abruptly to a maximum with slight oxygen vacancies. Similar behaviour was obtained for other compounds of 1111 class FeAs based superconductors [16,17].

Despite of large number of work devoted to oxypnictides, many open issues still remain in theoretical understanding of origin superconductivity in this compounds. Multiband Eliashberg theory with antiferromagnetic spin fluctuatuations was considered in [18]. Four-band Eliashberg model was applied for the study of thermodynamic properties of optimally doped $Ba_{1-x}K_xFe_2As_2$ [19]. Firstly multiband BCS theory for oxypnictides was suggested in studies [20], [21]. In the presented work, the generalization of single-band BCS theory was conducted, taking into account quasi-two-dimensional character of $NdFeAsO_{1-y}$ compound. As shown in this works, the presence of real dependence of density of states near Fermi energy gives nonlinear dependence of critical temperature on carrier density. Since the standart single-band BCS approach has turned to be constant of density of states. In this paper the analytical result for $T_c(n)$ dependence using quasi-two-dimensional energy spectrum of carriers are obtained. Firstly, it is derived from BCS equations for with energy dependent of density of states. Finally, the results of calculations with the available experimental data for $NdFeAsO_{1-y}$ are compared.

2. Basic equations

In the case of quasi-two-dimensional superconductors, one can write the BCS equation to calculate the critical

temperature with real dependence of density of states as shown below:

$$1=\int_{-\pi}^{\pi}\frac{d(p_z d)}{2\pi}\int_0^{\infty}\frac{d^2p}{(2\pi)^3}\frac{\tanh\frac{(\xi^2(p-p',p_z-p_z')+\Delta^2(p-p',p_z-p_z'))^{172}}{2T}}{(\xi^2(p-p',p_z-p_z')+\Delta^2(p-p',p_z-p_z'))^{172}}V \quad (1)$$

where V- is the electron pairing potential. In Eq. (1) for simplicity we neglected the effects of anisotropy in planes and Columb repulsion between electrons. Equation (1) should be solved with the equation for the chemical potential $\mu(n)$ at critical temperature, which is illustrated as follow:

$$\int N(\mu+\xi)d\xi = n, \quad (2)$$

where N(μ+ξ) is the density of states. Energy spectrum for quasi-two-dimensional superconductors shifted from chemical potential $\mu(n)$, given by the equation

$$\xi(p,p_z)=\frac{p^2}{2m}+2t(1-\cos p_z d)-\mu, \quad (3)$$

where d is the distance between planes, m mass of electrons in planes, t tunnelling integral between planes. Similar energy spectrum was used for study of physical properties of different quasi-two-dimensional superconductors [22-26]. Tunnelling integral must depend on the ratio a/d as t=F(a/d), where a is the thickness of conducting layer, d is the characteristic distance of the order of unit cell size in the superconducting layers. The F(a/d) function rapidly decreases when the distance increases. In principle, it is possible, to obtain an explicit expression for this function providing that the electron density distribution inside the superconducting layers is known. According to [27], the density of states for systems with energy spectrum (3) can be presented as:

$$N(\xi)=\frac{m}{d\hbar^2\pi^2}z(\xi), \quad (4a)$$

where

$$z(\xi)=\begin{cases}\pi, \text{ if } \xi>4t\\ \arccos(1-\frac{\xi}{2t}), \text{ if } \xi<4t\end{cases}. \quad (4b)$$

Relation between carrier density n and chemical potential μ under fixed temperature is determined by the following equation:

$$n=\frac{mT}{2\pi^2}\frac{\mu-2t}{T}+\frac{1}{\pi}\int_{-\pi}^{\pi}dz\ln(1+\exp(\frac{2t(1-\cos z)-\mu}{T})\cdot \quad (5)$$

For the generated electron gas, we can carry out the integration in Eq. (5) analytically. For $\mu>4t$, Eq. (5) can be simplified to given expression:

$$\frac{\mu}{2t}=1+\frac{n}{n_0}, \quad (6)$$

where $n_0=(4mt)/(\pi d\hbar^2)$. In the case $\mu<4t$, we have the following expression for the chemical potential

$$\frac{\mu}{2t}=1-\cos(z_0(n)), \quad (7)$$

where $z_0(n)$ can be defined by the solution of the equation

$$\frac{n}{n_0}=\frac{\sin z_0 - z_0\cos z_0}{\pi} \quad (8)$$

Equations (6-8) give us non-appearance form of the $\mu(n)$ function. It is obvious that in all cases chemical potential μ increases by increasing the carrier density n. Using asymptotical expression for the density of states (4), and using condition BCS $\omega_0<<\mu$ (ω_0 is the typical boson frequency of electron-boson based superconductor and for oxypnictides, it is about 20 meV [14]), we can get the following equation for the critical temperature T_c for the case of $\mu<4t$:

$$T_c=T_{c0}\exp(\frac{1}{\lambda}(1-\frac{4t}{\mu(n)})), \quad (9)$$

where $\lambda=m/(d\hbar^2\pi)$,V is the electron-boson coupling constant. For the case $\mu>4t$, the critical temperature is given as:

$$T_c=T_{c0}, \quad (10)$$

where T_{c0} is the critical temperature for the two-dimensional superconductors. It can also be realized from the last equation that once μ increases, the critical temperature T_c also increases. It is clear that the small chemical potential critical temperature T_c is extremely sensitive to changes in the carrier density and we take this as an indication that the model is also capable of a qualitative description of oxygen deficiency effects in new superconductors $NdFeAsO_{1-y}$. If the chemical potential is greater than $4t$ changes, the carrier density does not change as indicated by the Eq. (10).

3. Discussion

The measurements show that for the $NdFeAsO_{1-y}$, the chemical potential is about μ=1.78 eV at y=0.1 and μ=2 eV at y=0.15 [17], [28]. Tunnelling integral between the planes is t=0.448 eV and the distance between planes is d=0.3943 nm [9],[29]. The estimated value of electron-boson coupling constant is λ=0.643. It means that the BCS approach can be used in calculations of critical temperature of $NdFeAsO_{1-y}$. Relation between y and carrier density n considered as $n=0.85y$. Result of calculations using above presented parameters and Eqs.(6-9) are presented in Fig. 1 as open cycles. In calculations, we estimated the value of $T_{c0}\simeq$55K. Experimental data for the critical temperature in $NdFeAsO_{1-y}$ superconductor was taken from [15] and denoted as full cycles. As can be seen there is an agreement between the presented theory and experimental data. Similar results were also observed experimentally for other 1111 class compounds which are $LaNiAsO_{1-x}F_x$ [28] and $CeFeAsO_{1-x}F_x$ [29]. Above presented calculations can also be applied to these

compounds by properly choosing the fitting parameters of the corresponding theory.

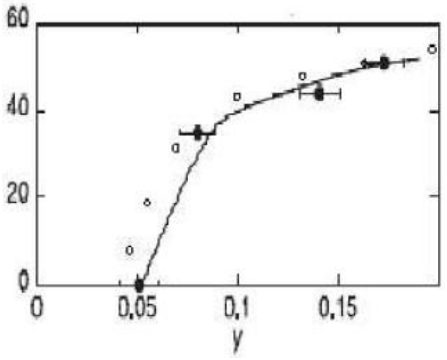

Fig. 1. Influence of oxygen deficite on the critical temperature in $NdFeAsO_{1-y}$ compound (full cicles experimental data [15], open cicles theoretical calculations in this study).

Another interesting conclusion is followed from Eq. (9). Critical temperature T_c is more sensitive to the carrier density for superconductors having weak electron-boson coupling (λ<1) (see Eq.(9)). Increasing of electron-boson coupling constant λ leads to decrease the influence of doping effects on critical temperature. As well known that [30] for high electron-boson coupling parameters (λ>1) for the calculations of $T_c(n)$ we need system of Eliashberg equations. According to [18] a simple Eliashberg three-band model, with antiferromagnetic spin-fluctuation electron couplings obtained the values of gaps and the critical temperatures. As previously mentioned in this work, a moderate strong-coupling regime is important in numerical simulations of Eliashberg equations. In contrast to [18], above presented theory is simple, but it allows to get analytical calculations. According to the single-band Eliashberg theory, the inclusion of carrier density effects on critical temperature needs the third integral equation. For the case of multiband superconductors, the system of Eliashberg equations becomes more complicated. For this purpose we also should add equations for the carrier density in different bands and equation for the conservation of number of particles in many band systems. From this point of view, the proposed calculations seem attractive and useful for applications in weak-coupling limit.

Thus, the special feature of Fermi surface model for quasi-two-dimensional systems allows to study the influence of the carrier density on the critical temperature for layered superconductors. It is shown that the saturation effects in T_c with increasing carrier density n are qualitative in agreement with experimental observation in compound $NdFeAsO_{1-y}$.

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References

[1] Y. Kamihara, H. Hiramatsu, M. Nirano, R. Kawamura, H. Yanagi, T. Kamiya, H. Hosono, J. Am. Chem. Soc., **128**, 10012 (2006).
[2] Y. Kamihara, T. Watanabe, M. Nirano, H. Hosono, J. Am. Chem. Soc., **130**, 3296 (2008).
[3] Z-A Ren, W. Lu, J. Yang, W. Yi, et al, Chin. Phys. Lett. **25**, 2215 (2008).
[4] M. Rotter, M. Tegel, D. Johrendt, Phys. Rev. Lett. **101**, 107006 (2008).
[5] R. Prozorov, N. Ni, M. A. Tanatar, et al Phys Rev **B78**, 224506 (2008).
[6] X. C. Wang, Q. Q. Liu, Y. X. Lv et al, Solid State Commun. **148**, 538 (2008).
[7] C. V. Chu, B. Lorentz, Physica C, **469**, 385 (2009).
[8] F-C. Hu, J-Y Luo, K-W Yeh et al, Proc. Natl. Acad. Sci. USA **105**, 14262 (2008).
[9] L. I. Ivanovskii, Uspekhi Fiz. Nauk, **178**, 1273 (2008).
[10] S. V. Sadovski, Uspekhi Fiz. Nauk, **178**, 1243 (2008).
[11] Z. A. Ren, Z. X. Zhao, Adv. Mater. **21**, 4584 (2009).
[12] T. Hanaguri, S. Niitaka, K. Kuroki, H. Takagi, Science **328**, 474 (2010).
[13] V. M. Pudalov et al Uspekhi Fiz. Nauk, **178**, 1273 (2008).
[14] L. Benfanto, et al, Physical Review **B80**, 214522 (2009).
[15] C. Lee, A. Iyo, H. Eisaki, et al J. Phys. Soc. Japan **77**, 083704 (2008).
[16] L. Zheng et al, Physica Review B **78**, 060504 (2008).
[17] Y. Izyumov, E. Kurmaev, Springer Series in Material Sciences, 278 (2010).
[18] G. A. Ummarino, Phys. Rev. B **83**, 092508 (2011).
[19] L. Benfato, E. Cappelluti, C. Castellani, Phys. Rev. B **80**, 214522 (2009).
[20] V. Barzykin, L. P. Gorkov, JETP Lett. **88**, 131 (2008).
[21] O. V. Dolgov, I. I. Mazin, D. Parker, et al, Phys Rev **B79**, 060502 (2008).
[22] I. Askerzade, Unconventional superconductors: anisotropy and multiband effects, Springer-Verlag, 177p. (2012).
[23] E. P. Nakhmedov, O. A. Saçlı, I. N. Askerzade, J. Phys. Cond. Mat. **5**, 1099 (1993).
[24] I. N. Askerzade, Modern Phys. Lett. **B17**, 11 (2003).
[25] I. N. Askerzade, J. Korean Phys. Society, **45**, 475 (2004).
[26] I. N. Askerzade, Physics Uspekhi, **52**, 977 (2009).
[27] R. C. Fivas, Nuovo Cimento **B63**, 10 (1969).
[28] E. Z. Kurmaev, R. G. Wilks, A. Moewes, et al Physical Review B,**78**, 220503(R) (2008).
[29] G. F. Chen, et al, Phys. Rev. Lett. 100, 247002 (2008).
[30] J. P. Carbotte, Rev. Mod. Phys. **62**, 1027 (1990).

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