Impurity Doping Effect in High T_c Superconductors

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Abstract

It has been observed that impurity doping and/or ion-beam-induced damage in high T_c superconductors cause a metal-insulator transition and thereby suppress the critical temperature. Based on our recent theory of the weak localization effect on superconductivity, we examine the variation of T_c with increasing of impurity concentration (x) in $\mathrm{La_{1.85}Sr_{0.15}Cu_{1-x}A_xO_4}$ systems, where A = Fe, Co, Ni, Zn, or Ga. We find that the doping impurity decreases the scattering matrix elements for electron-electron attractions, such as $V_{nn'} = -V[1 - \frac{2}{\pi k_F \ell} ln(L/\ell)]$, where L and ℓ are the inelastic and elastic mean free paths, respectively. Using the mean free path ℓ determined from resistivity data, we find good agreements between our calculated values for T_c and experimental data except for Ni-doped samples, where Ni impurities may enhance the pairing interaction.

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Although impurity scattering may provide a clue to understanding the superconducting mechanism of high T_c superconductors, its effect is not well understood yet.[1−3] In strongly correlated systems such as high T_c superconductors, impurity potentials are significantly renormalized by strong electron-electron interactions.[4] In particular, (unitarity) resonant impurity scattering seems to be important. Using the marginal Fermi liquid theory, Kotlier and Varma[4] showed that scattering by ordinary impurities is close to the unitarity limit. Recently, it was argued that very low concentrations of impurities in non-Fermi-liquid systems lead to a vanishing of density of states at the chemical potential and infinite resistivity for $T \to 0$.[5] In a one-channel Luttinger liquid with repulsive interactions, Kane and Fisher[6] showed that electrons are completely reflected even by the smallest scatterer as if it were effectively infinite. Hirschfeld and Goldenfeld[7] considered the effect of resonant scattering on the penetration depth of a d-wave superconductor. Poilblanc, Scalapino and Hanke[8] showed by an exact diagonalization technique for small clusters that strong correlations give rise to resonant scattering due to local defects in the $t-J$ model. In addition, Ziegler and his coworkers[9] introduced a simple static approximation to the effective impurity potential which reproduces resonant scattering for both two-dimensional $t-J$ and Hubbard models. Nevertheless, the impuirty effect on the transition tempearture of high T_c superconductors remains to be unsettled, because the effect of resonant scattering on the superconducting temperature is not much different from that of Born scattering.[3,10]

We note that experimental results show consistently that impurity doping and ion-beam-induced damage give rise to a metal-insulator transition and thereby suppress T_c.[11−15] Recently, we studied the weak localization effect on low T_c superconductors,[16] and found that for two-dimensional systems weak localization decreases effective interactions, similarly to conductivity. Here we use the same theoretical approach to investigate the impurity doping effect on the superconducting temperature for $La_{1.85}Sr_{0.15}CuO_4$ with Cu replaced with 3d transition elements or Ga. The effect of strong correlation is taken into account by the simple renormalization of the impurity potential.[9] The mean free path ℓ is determined from resistivity data. We find good agreements between our theoretical calculations and experimental data except for Ni-doped samples. In Ni-doped case, the suppression of T_c is much slower than the theory predicts, implying that Ni may enhance the pairing interaction.

Let us consider a simple pairing potential, $V(|\mathbf{r}_1 - \mathbf{r}_2|)$, between electrons of a pair. The matrix elements of $V(r)$ for the plane wave states are

$$\begin{aligned} V_{\vec{k}\vec{k}'} &= \int\int d\mathbf{r}_1 d\mathbf{r}_2 e^{-i\vec{k}'\cdot(\mathbf{r}_1-\mathbf{r}_2)} V(|\mathbf{r}_1-\mathbf{r}_2|) e^{i\vec{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)} \\ &\cong V_o + V_1 \hat{k}\cdot\hat{k}' + \frac{V_2}{2}[3(\hat{k}\cdot\hat{k}')^2 - 1] + \cdots . \end{aligned} \tag{1}$$

For a s-wave pairing, $V_{\vec{k}\vec{k}'}$ is assumed to be a constant $V_0 < 0$, whereas for a d-wave pairing, $V_{\vec{k}\vec{k}'}$ depends on the unit vectors $\hat{k}$ and $\hat{k}'$, such as

$$V_{\vec{k}\vec{k}'} = \frac{V_2}{2}[3(\hat{k}\cdot\hat{k}')^2 - 1]. \tag{2}$$

In the presence of impurities, the pairing interaction between scattered basis pairs $(\psi_n, \psi_{\bar{n}})$ and $(\psi_{n'}, \psi_{\bar{n}'})$ is given by[17]

$$V_{nn'} = \int\int d\mathbf{r}_1 d\mathbf{r}_2 \psi^*_{n'}(\mathbf{r}_1)\psi^*_{\bar{n}'}(\mathbf{r}_2) V(|\mathbf{r}_1-\mathbf{r}_2|)\psi_{\bar{n}}(\mathbf{r}_2)\psi_n(\mathbf{r}_1), \tag{3}$$

where $\psi_{\bar{n}}$ denotes the time-reversed partner of ψ_n. The metal-insulator transition driven by the impurity doping may be understood by the localization of wave function.[18,19] In high T_c superconductors, resistivity data showed that correlation enhances significantly the strength of impurity potential. Kaveh and Mott[19] derived the weakly localized scattered states in the form of power-law and extended wave functions for two-dimensional systems,

$$\psi_n(\mathbf{r}) = A_2 e^{i\vec{k}\cdot\mathbf{r}} + B_2 \frac{e^{ikr}}{r}, \tag{4}$$

$$A_2^2 = 1 - 2\pi B_2^2 ln(L/\ell), \quad B_2^2 = \frac{1}{\pi^2 k_F \ell}, \tag{5}$$

where ℓ and L are the elastic and inelastic mean free paths, respectively. We can calculate $V_{nn'}$ by substituting Eq. (4) into Eq. (3). Since the Cooper pairs in a BCS condensate form bound states, only the power-law wave functions within the BCS coherence length are relevant.[20] Thus, the Cooper pair wave functions basically consist of the plane waves with reduced amplitudes. The resulting matrix elements are[21,22]

$$V_{nn'} = V_{\vec{k}\vec{k}'}[1 - \frac{2}{\pi k_F \ell} ln(L/\ell)], \tag{6}$$

for both the s- and d-wave pairings. In the d-wave pairing, Eq. (6) does not include the effect of impurity scattering in the Borm limit. Then, the effective coupling constant λ_{eff} becomes

$$\lambda_{eff} = \lambda[1 - \frac{2}{\pi k_F \ell} ln(L/\ell)], \tag{7}$$

which satisfies the modified BCS T_c equation,

$$T_c = 1.13\epsilon_c exp(-1/\lambda_{eff}). \tag{8}$$

Xiao and his coworkers[11] conducted a systematic study on the effect of Cu-site doping in $La_{1.85}Sr_{0.15}CuO_4$ polycrystals and determined the relation between T_c and dopant level for Fe-, Co-, Ni-, Zn-, Ga-, and Al-impurities. Cieplak and his coworkers[12] also measured resistances for the same materials with different impurities (Fe, Co, Ni, Zn, and Ga) down to 50 mK and found the metal-insulator transitions produced by impurities. Here we use Eq. (8) to calculate T_c as a function of dopant concentration, assuming that the cutoff energy $\epsilon_c = 450$K and the Fermi wave vector $k_F = 0.2\text{Å}^{-1}$. In this case, λ is chosen to give $T_{co} = 37$K without impurities. The inelastic mean free path is obtained from disordered two-dimensional systems, which is employed for all the systems considered here, with the $1/\sqrt{lnT}$ dependence removed, i.e, $L = 500\text{Å}/\sqrt{\text{T}}$.[18] Because of the Sr doping, the elastic mean free path is estimated to be about 50Å without Cu-site doping.[13] Then the total elastic mean free path ℓ_{tot} (in unit of Å) is

$$\frac{1}{\ell_{tot}} = \frac{1}{50} + \frac{1}{\ell_{imp}}, \tag{9}$$

where ℓ_{imp} is the mean free path caused by impurity doping for Cu. For two-dimensional layered systems such as high T_c superconductors, the mean free path ℓ_{imp} can be obtained from the Drude formula, $k_F\ell = h/R_\Box e^2$, where $R_\Box$ is the sheet resistance, defined as $R_\Box = \rho/d$. In this case, d is the interlayer distance (6.5 Å in the LSCO system)[23] and ρ is resistivity. ¿From experimental data by Cieplak et al.,[12] the resistivities of Ga-, Zn-, Fe-, Co-, and Ni-doped systems can be fitted such as $\rho_{Ga} = 198.41 \times c$, $\rho_{Zn} = 147.11 \times c + 40$, $\rho_{Fe} = 227.4 \times c + 33.7$, $\rho_{Co} = 190.67 \times c$, and $\rho_{Ni} = 164.35 \times c + 12$, respectively, where c denotes the concentration of dopants.

The superconducting transition temperatures are plotted as a function of dopant concentration and compared with experiments in Figs. 1 and 2. For nonmagnetic (Ga and Zn) and magnetic (Fe and Co) impurities, the agreements between theory and experiment are satisfactory, considering the simple approximation of strong correlation effect. It is clearly seen that the impurity doping gives rise to a metal-insulator transition and suppresses T_c. We find that only the strength of (effective) impurity potential is important and the effect of nonmagnetic impurities on destroying superconductivity is similar to magnetic impurities, which agrees well with experiments. Although the Zn and Ga atoms have filled d-shells whereas the Fe, Co, and Ni atoms have unfilled d-shells, it appears that the variation of T_c with impurity doping does not depend significantly on the valence states of impurities. We find that the initial drops of T_c for all the samples are larger than the theory predicts.

Fig. 3 shows the variation of T_c for Ni-doped samples. We find a large deviation between the theoretical and experimental curves. Although the origin of the discrepancy is not clear, it seems that Ni may enhance the pairing interaction. It is interesting to note that a Ni impurity in $YBa_2Cu_3O_{7-x}$ has an unpaired spin of $S = \frac{1}{2}$ rahter than $S = 1$, as expected for Ni^{2+}.[24] It is also possible that Ni-doped samples may develop some inhomogeneous granular structures[25] or stripe phases[26] and their superconducting phases may persist for very high impurity concentrations. However, x-ray diffraction measurements in Ni-doped single-crystals $YBa_2Cu_3O_{7-x}$ did not support this idea.[27]

In the underdoped regime, experiments showed that impurity scattering produces a large residual resistivity close to (or even larger than) the unitarity limit and the metal-insulator transition occurs almost simultaneously when T_c drops to zero.[13,14] Consequently, our theory which considered the optimum doping regime is also applicable for the underdoped regime. As the hole density increases from the optimum doping, T_c drops to zero more quickly before the metal-insulator transition is reached. This behavior may be related to the dimensional crossover from two-dimension to three-dimension. Nevertheless, our theory may explain the decrease of T_c in moderately overdoped samples. Recently, Suryanarayanan and his coworkers[28] found the recovery of superconductivity in $Y_{1-x}Ca_xSrBaCu_{2.6}Al_{0.4}O_{6+z}$ when Y is substituted by Ca. This result may be understood if we consider the importance of the metal-insulator transition caused by impurity doping. Since Ca increases the hole density in the Cu-O planes, the mobility edge is shifted with respect to the Fermi energy, so that the system becomes metallic and superconducting. The transition between the insulating and superconducting phases was also explored in thin films such as $DyBa_2Cu_3O_7$,[29] $Nd_{2-x}Ce_xCuO_4$,[30] and $YBa_2Cu_3O_7$,[31] where the two-dimensional localization is the main reason for the suppression of superconductivity and the critical sheet resistance lies in the range of 6 to 8 kΩ. In $YBa_2Cu_3O_{7-x}/PrBa_2Cu_3O_{7-x}$ superlattices,[32,33] the decrease of T_c in isolated $YBa_2Cu_3O_{7-x}$ layers with increasing sheet resistance is on the scale of $\hbar/e^2$, as observed for ordinary superconductors.[32] This behavior may also be explained in terms of our theory.

In conclusion, we have studied the impurity doping effect on the superconducting temperatures of $La_{1.85}Sr_{0.15}Cu_{1-x}A_xO_4$ systems (A=Fe, Co, Ni, Zn, and Ga) based on our recent theory of weak localization effect on superconductors. The strong correlation effect is taken into account by a simple renormalization of the effective impurity potential. The calculated values for T_c are in good agreement with experiments, while in Ni-doped samples the agreement was poor, implying that Ni may enhance the pairing interaction.

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Figure Captions

Fig. 1 Variation of T_c with dopant concentration for $La_{1.85}Sr_{0.15}Cu_{1-x}A_xO_4$ (A=Ga and Zn). Experimental data are from Ref. 11.

Fig. 2 Variation of T_c with magnetic dopant content for $La_{1.85}Sr_{0.15}Cu_{1-x}A_xO_4$ (A=Fe and Co). Experimental data are from Ref. 11.

Fig. 3 Variation of T_c with Ni concentration for $La_{1.85}Sr_{0.15}Cu_{1-x}Ni_xO_4$. Experimental data are from Ref. 11.