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Oxygen deficiency dependence of transition temperature in (Sm, Er) $Ba_2Cu_3O_{7-\delta}$ superconductors

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Abstract. We have investigated the effects of oxygen deficiency (δ) on the transition temperature (T_c) of (Sm, Er)$Ba_2Cu_3O_{7-\delta}$ superconductors by incorporating the effects of the two dimensional (2D) acoustic phonons and plasmons in the framework of strong coupling theory. The proposed approach for yttrium cuprates properly takes care of the double CuO_2 plane in a unit cell and has been found earlier to be successful in describing the pairing mechanism as well as the variation of T_c with δ in $YBa_2Cu_3O_{7-\delta}$ system. The coupling strength (λ), the screening parameter (μ^*) and the two dimensional acoustic phonon (plasmon) energy $\hbar\omega_-(\omega_+)$ as a function of oxygen deficiency is worked out. Finally, the transition temperature is evaluated and is found to be consistent with the earlier experimental data on yttrium cuprates. Thus, coupled phonon–plasmon mechanism is adequate to understand the nature of pairing mechanism and oxygen deficiency dependence of transition temperature in 90 K (Sm, Er)$Ba_2Cu_3O_{7-\delta}$ superconductors.

Keywords. Oxygen deficiency; transition temperature; coupling strength; screening parameter; yttrium cuprates.

1. Introduction

The discovery of superconductivity in yttrium based cuprates $YBa_2Cu_3O_{7-\delta}$ (Wu *et al* 1987) stimulated the research activities of various groups in this field. Chemical substitutions of Yb, Sm and Er on Y site have been systematically studied by Kerkels *et al* (1992) who reported the variation of superconducting transition temperature (T_c) with oxygen deficiency (δ). These compounds possess layered structure and for the lower values of $\delta(\sim 0{\cdot}0)$ the phase is orthorhombic and becomes superconducting at low temperatures. For high values of $\delta(\sim 1{\cdot}0)$, the phase is tetragonal and nonsuperconducting at all temperatures. We now understand the pairing mechanism in yttrium cuprates with two conducting CuO_2 layers sandwiched in between the insulating layers of a unit cell. The developed approach properly incorporates the excitations developed in CuO_2 layer and succeeds in revealing the oxygen deficiency dependence of transition temperature (T_c) for Y(Yb)$Ba_2Cu_3O_{7-\delta}$ superconductors (Singh *et al* 1996).

Motivated by the success of our earlier approach and with the availability of experimental data on (Sm, Er)$Ba_2Cu_3O_{7-\delta}$, we now, probably for the first time, understand the anomalous behaviour of oxygen deficiency (δ) dependence of T_c in yttrium cuprate superconductors. Thus, the main aim of the present investigation is to employ the coupled phonon–plasmon mechanism to analyse the oxygen deficiency (δ) dependence of T_c in (Sm, Er)$Ba_2Cu_3O_{7-\delta}$ superconductors. We have achieved considerable success in understanding the pairing mechanism and observed δ dependence of T_c in yttrium cuprate superconductors with $T_c = 91$ K ($\delta \cong 0{\cdot}0$) and 90 K ($\delta \cong 0{\cdot}0$) for

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Sm and Er doped systems respectively. The essential formalism of interaction potential is given in § 2. The computed results and their discussions along with conclusions are presented in § 3.

2. Essential formalism

Previously, we have shown that coupled 2D acoustic phonon plasmon approach in yttrium cuprates with two CuO_2 plane in a unit cell play a significant role in describing the pairing mechanism as well as superconducting transition temperature using the following effective potential (Singh *et al* 1996)

$$V(q, q_z, \omega) = \frac{2\pi e^2}{q\varepsilon_0} \frac{S(q, q_z)}{\varepsilon(q, q_z, \omega)}, \tag{1}$$

with $S(q, q_z)$ as the structure factor and is

$$S(q, q_z) = \frac{\sinh(qd)}{\cosh(qd) - \cos(q_z d)}. \tag{2}$$

Here, d is the distance between consecutive CuO_2 planes in a unit cell, q_z the wave vector in the 'z' direction. The longitudinal dielectric response function $\varepsilon(q, q_z, \omega)$ for two planes in a unit cell is

$$\varepsilon(q, q_z, \omega) = 1 + 2P(q, \omega) S(q, q_z) + P^2(q, \omega) S(q, q_z) S'(q), \tag{3}$$

with

$$S'(q) = \frac{\cosh(qd) - \cosh(qd')}{\sinh(qd)}, \tag{4}$$

and

$$d' = 2d_1 - d \text{ with } d_1 = d/3.$$

Cuprates are highly anisotropic in their physical properties. Restricting ourselves in the a-b plane conduction, we average (1) to obtain

$$V(q, \omega) = \frac{d}{2\pi} \int_{-\pi/d}^{+\pi/d} V(q, q_z, \omega)\, dq_z, \tag{5}$$

$$= \frac{4\pi e^2}{q\varepsilon_0} \frac{[1 + P(q, \omega) S'(q) + R(q, \omega)] \sinh(qd)}{[|D^2(q, \omega) - 1|]^{1/2}}, \tag{6}$$

with

$$R(q, \omega) = \frac{\sinh(q(d - d_1)) + D(q, \omega) \sinh(qd_1)}{\sinh(qd)}, \tag{7}$$

and

$$D(q, \omega) = \cosh(qd) + 2P(q, \omega) \sinh(qd) + P^2(q, \omega) \sinh(qd) S'(q). \tag{8}$$

Zero's of the modified dielectric response function $D(q,\omega)$ will yield the frequencies of the coupled 2D acoustic plasmon and phonon modes. The resonant frequencies are described by

$$2\omega_\pm^2 = [\alpha\omega_{pl}^2 + \alpha\omega_{pi}^2 + \$^2] + [(\alpha\omega_{pl}^2 + \alpha\omega_{pi}^2 + \$^2)^2 - 4\alpha\omega_{pi}^2 \$^2]^{1/2}. \tag{9}$$

Here, ω_{pl} (ω_{pi}) is the usual electron (ion) plasmon energy and $\alpha = qd$. $\$^2$ is $q^2 V_F^2/2$.
Simplification of above yields

$$\omega_+^2 \cong \alpha\omega_{pl}^2 + \$^2, \tag{10}$$

where, we use an approximation that $\omega_{pl} \gg \omega_{pi}$. Since electron–plasmon energy is higher at least by three orders of magnitude than of ion–plasmon energy.

Also, the low frequency $\omega_-(q)$ is

$$\omega_-^2 \cong \alpha\omega_{pi}^2[1 + \alpha\omega_{pl}^2/\$^2]^{-1}. \tag{11}$$

Here, $\omega_{pi}^2 \ll \$^2$ and hence $\omega_{pl}^2/\$^2 \cong 1$.

Using the above approach, we have derived the following expressions for the screening parameter (μ) and the coupling strength (λ) from the interaction potential following the strong coupling theory (Elishberg 1960) as

$$\mu = \frac{2\pi e^2 d N(0)}{\varepsilon_0} \text{Ln}\left[\frac{2+K}{K}\right], \tag{12}$$

and

$$\lambda = \frac{\omega_-^2}{2a_B K_F^2 C}. \tag{13}$$

The renormalized screening parameter (μ^*) is expressed as

$$\mu^* = \mu[1 + \mu \,\text{Ln}\,(E_F/\hbar\omega_-)]^{-1}. \tag{14}$$

In yttrium cuprates, the Fermi energy (E_F) is comparable to the 2D acoustic phonon energy ($\hbar\omega_-$), so the screening parameter (μ) is renormalized with $\hbar\omega_-$ only. However, 2D acoustic plasmon energy is at least three orders of magnitude higher than Fermi energy, so it is not appropriate to renormalize the Coulomb screening parameter (μ) with respect to $\hbar\omega_+(q)$.

We first attempt to evaluate the superconducting transition temperature (T_c) by considering the low energy 2D acoustic phonons alone as (Ruvalds 1987)

$$T_c^{ph} = 0{\cdot}7\omega_- \exp\left[-\frac{1+\lambda}{\lambda-\mu^*}\right]. \tag{15}$$

Finally, we consider the simultaneous presence of both 2D acoustic phonons and plasmons and the total T_c is (Kresin 1987)

$$T_c = T_c^{ph}\left[\frac{\hbar\omega_+}{T_c^{ph}}\right]^h, \tag{16}$$

with

$$h = \frac{\lambda_{pl}}{\lambda + \lambda_{pl}}. \tag{17}$$

Here, λ_{pl} denotes the electron–plasmon coupling strength. The results thus obtained have been discussed below.

3. Results and discussion

We have computed the model parameters as coupling strength between electrons and phonons (λ), modified screening parameter (μ^*) and the 2D acoustic phonon (plasmon) frequency [$\hbar\omega_-$ ($\hbar\omega_+$)] at different δ values using the expressions (13), (14) and (11) for (Sm, Er)$Ba_2Cu_3O_{7-\delta}$ superconductors in the range $0{\cdot}0 \leqslant \delta \leqslant 0{\cdot}6$. For this purpose we have used the value of $\varepsilon_0 = 4{\cdot}5$ (Bozovic 1990) for yttrium cuprates systems. The effective mass is evaluated from the electronic specific heat coefficient (γ) values 1·55 m_e for $SmBa_2Cu_3O_{7-\delta}$ superconductor (Molokac *et al* 1990). For $ErBa_2Cu_3O_{7-\delta}$ system, we use $m^* = 1{\cdot}6\, m_e$, although no experimental data on γ is available. The mass of CuO_2 unit cell is 12·77 amu. The charge carrier density and ionic density are evaluated from the lattice parameters for the optimized pairing condition (Varshney and Singh 1995). Taking '*a*' = 3·855 (3·815) Å, '*b*' = 3·899 (3·884) Å and '*c*' = 11·721 (11·659) Å for Sm(Er) systems, respectively (Tarascan *et al* 1987), to obtain $n_c = 2{\cdot}416 \times 10^{14}\,\mathrm{cm}^{-2}$ and $n_i = 6{\cdot}77 \times 10^{14}\,\mathrm{cm}^{-2}$ at $\delta = 0{\cdot}0$. We make them oxygen deficient dependence as

$$n_{c(i)}(\delta) = n_{c(i)}(\delta = 0{\cdot}0)[\exp - (\delta/\delta_c)^2]. \tag{18}$$

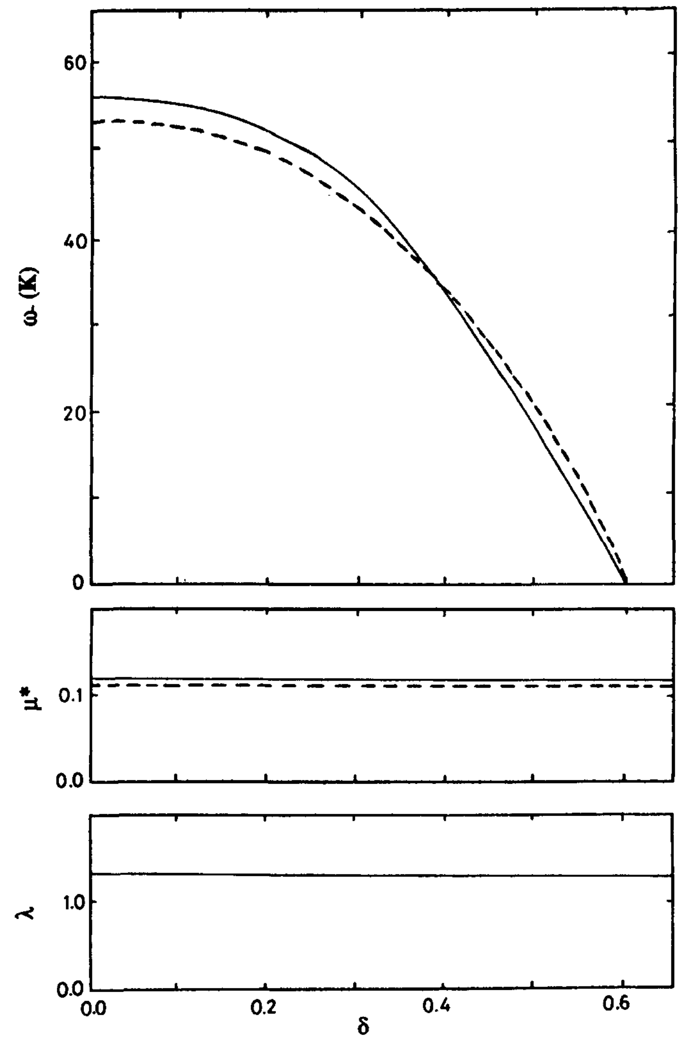

Figure 1. Variation of ω_-(K), μ^* and λ with δ in Sm(Er)$Ba_2Cu_3O_{7-\delta}$ superconductor represented by full line (dashed line), respectively.

Here, we choose $\delta_c = 0{\cdot}4$ and $Z = -2$.

The model parameters (λ and μ^*) and 2D acoustic phonon energy ($\hbar\omega_-$) have been obtained from (11), (13) and (14) and are plotted as a function of δ in figure 1 for Sm(Er)$Ba_2Cu_3O_{7-\delta}$ superconductors, respectively. It is noted that the values of coupling parameter (λ) as well as screening parameter (μ^*) remains constant in the range $0{\cdot}0 \leqslant \delta \leqslant 0{\cdot}6$. The value of $\lambda > 1{\cdot}0$, indicates that they have been obtained from the strong coupling mechanism. The 2D acoustic phonon energy ($\hbar\omega_-$) is estimated as 48(45) meV for Sm(Er), respectively. The 2D acoustic phonon energy $\hbar\omega_-(q)$ decreases with the increased value of δ. Using the above, we have estimated the transition temperature due to phonon mechanism from (15) and is 55 (53) K for Sm(Er) systems. It is inferred that T_c obtained from the phonon mechanism alone does not produce high T_c values. Incorporating the 2D acoustic plasmons by taking $\lambda_{pl} = 0{\cdot}1$ and estimating $\hbar\omega_+(q) = 3\,\text{eV}$ from (10), we find that T_c enhanced to 94 K (92 K) is consistent with the earlier reported data (Kerkels *et al* 1992). Hence, there is an enhancement of 70% on T_c values as obtained from phonon mechanism for these superconductors. Figures 2 and 3 depict the oxygen deficiency dependence of T_c. It is noticed that with the increase of δ the T_c drops linearly and is nearly zero for $\delta \cong 0{\cdot}6$. We find that the proposed theory successfully predicts the first plateau that is observed in the range $0{\cdot}0 > \delta < 0{\cdot}3$ but fails to show the second plateau in the range $0{\cdot}3 < \delta < 0{\cdot}5$.

Finally, it may be concluded that the coupled phonon–plasmon mechanism based on the strong coupling theory, is capable of predicting the observed oxygen deficiency (δ) dependence of transition temperature in Y 123 superconductors. We believe that the major contribution to T_c in yttrium cuprate superconductors is from plasmon

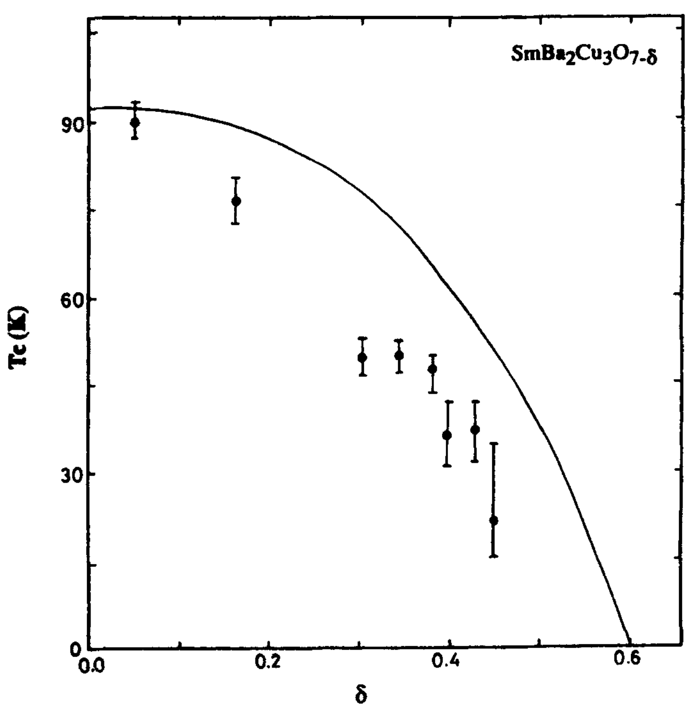

Figure 2. Variation of T_c with δ in $SmBa_2Cu_3O_{7-\delta}$ superconductors. Experimental data (ɸ) are taken from Kerkels *et al* (1992).

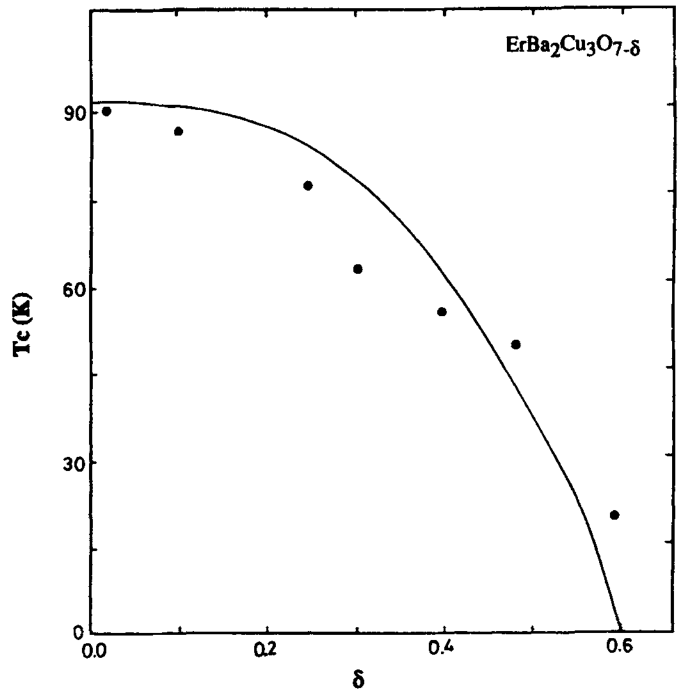

Figure 3. Variation of T_c with δ in $ErBa_2Cu_3O_{7-\delta}$ superconductors. Experimental data (●) are taken from Kerkels *et al* (1992).

mechanism. The appropriateness of the above approach is due to the proper care of layered structure and the use of experimental observations on lattice parameter and the specific heat measurement data.

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References

Bozovic I 1990 *Phys. Rev.* **B42** 1969
Elishberg G M 1960 *Sov. Phys. (JETP)* **11** 696
Kerkels T, Zou H, Ven Tendeloo G, Wagener D, Buchgeister M, Hosseini S M and Herzog P 1992 *Physica* **C196** 363
Kresin V Z 1987 *Phys. Rev.* **B35** 3116
Molokac S, Flachbart K, Bischof J and Belling A 1990 *Physica* **B165–166** 1205
Ruvalds J 1987 *Phys. Rev.* **B35** 8869
Singh R K, Varshney Dinesh and Khaskalam A K 1996 *Bull. Mater. Sci.* **19** 737
Tarascan J M, Mckinon W R, Grene L H, Hull G W and Vogel E M 1987 *Phys. Rev.* **B36** 226
Varshney Dinesh and Singh R K 1995 *Phys. Rev.* **B52** 7629
Wu M K *et al* 1987 *Phys. Rev. Lett.* **58** 908