

IN-PLANE OXYGEN BREATHING AS MECHANISM OF SUPERCONDUCTIVITY IN CUPRATE HIGH T_c MATERIALS

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ABSTRACT

The electron-phonon coupling constant in cuprate high temperature superconductors has been determined by acoustic method. A direct proportional relation between the electron-phonon coupling constant in the Van Hove scenario (which is 10-100 times smaller than the conventional BCS-type) and the transition temperature is observed. Our results show the importance of interplay between the Debye frequency and electron-phonon coupling in the two dimensional system and their variations have combined effect in governing the transition temperature. The electron-phonon coupling constant λ_{vH} in this scenario is in the range of 0.02 – 0.05, consistent with Cooper pair formation by in-plane oxygen breathing.

INTRODUCTION

The origin of high temperature superconductivity in the cuprates continues to be a major topic in materials research since the discovery of this class of superconductors. A number of experimental[1] and theoretical[2] results point towards the important role of phonons in the mechanism of these cuprate and should be considered in the microscopic theory. The CuO_2 planes have been established to play a major role in this family of superconductors. In the conventional picture, a high superconducting transition temperature would require a strong electron-phonon coupling for the formation of electron pair involved in the charge transport. In this research however, we observe an interesting effect. By combining the two dimensional nature of the structure together with electron-phonon coupling mechanism, we found that the electron-phonon coupling is 10-100 times smaller than the conventional superconductors which is rather unusual for such a high transition temperature. This is observed in all the samples studied which cover a broad range of materials and transition temperatures. The phonon mode that couples the electrons which leads to high temperature superconductivity is also discussed in this paper.

The electron-phonon coupling constant of various cuprate high temperature superconductors has been determined from sound velocity measurements. Sound velocity can give information about the elastic property and also the characteristic phonons frequency, as well as the acoustic Debye temperature, θ_D of the material.

According to the Bardeen-Cooper-Schrieffer (BCS) theory, in the weak coupling limit the transition temperature T_c and θ_D can be related using the equation $T_c = 1.13\theta_D e^{-1/\lambda}$ where $\lambda \equiv \lambda(\omega) = N(0)V$ is the electron-phonon coupling constant, ω is the phonon frequency, $N(0)$ is the density of states at Fermi level and V is the scattering matrix. For a two dimensional system the density of states can exhibit a singularity near the Fermi level[3]. In this scenario, λ in the weak coupling limit can be replaced by $\sqrt{\lambda}$ [5]. Consequently, according to Getino et al.[6], T_c can be written as $T_c = 2.72T_F e^{(-1/\sqrt{\lambda})}$ where $T_F = \frac{E_F}{k_B}$ (E_F is the Fermi energy) with $T_F = 10\theta_D$ for high T_c materials in the weak coupling limit.

EXPERIMENTAL DETAILS

The samples in this study were prepared via solid-state reaction using high-purity (>99.9%) metal oxides and carbonates. Samples of about 12.5 mm diameter and about 2 mm thickness were sintered in air at various temperatures followed by annealing in oxygen and various gases.

The sound velocity was measured using a Matec 7700 system which utilizes the pulse-echo-overlap technique. The samples were bonded to a transducer using Nonaq stopcock grease. The ultrasonic waves were propagated along the direction of pressing using *X*-cut (longitudinal) or *Y*-cut (shear) quartz transducers at 5 – 10 MHz. The sound velocity measurements were performed in an Oxford Instruments liquid nitrogen cryostat model DN 1711. The absolute longitudinal and shear velocities were evaluated at 80 K.

The temperature-dependent electrical resistance measurements were carried out using the four-point probe technique with silver-paint contacts. Powder XRD analyses with $\text{CuK}\alpha$ radiation using Siemens D5000 diffractometer were used to confirm that the samples are single phased.

The sound velocity in an ideal void-free material can be estimated from the measured velocity using the relation, $v_l = v_m \sqrt{\frac{\rho_{th}}{\rho}}$, where v_l is the void free velocity, ρ_{th} is the theoretical density and v_m is the measured velocity. The Debye temperature, θ_D can be estimated by using the standard formula, $\theta_D = \left(\frac{h}{k}\right) \left(\frac{3N}{4\pi V}\right)^{1/3} v_m$, where $\frac{3}{v_m^3} = \frac{1}{v_l^3} + \frac{2}{v_s^3}$, h is the Planck constant, k is the Boltzmann constant, N is the number of mass point, V is the atomic volume and v_m is the mean velocity.

RESULTS AND DISCUSSION

Table 1: Transition temperature T_c (K), Debye temperature θ_D (K) and Van Hove electron-phonon coupling λ_{VH} constant of various cuprate superconductors.

Sample	T_c (K)	θ_D (K)	λ_{VH}
EuBa ₂ Cu ₃ O _{6.98}	90	457	0.041
ErBa ₂ Cu ₃ O _{6.9}	94	375	0.046
(Er _{0.9} Pr _{0.1})Ba ₂ Cu ₃ O _{6.9}	89	387	0.044
(Er _{0.8} Pr _{0.2})Ba ₂ Cu ₃ O _{6.9}	77	428	0.040
ErBa ₂ Cu _{2.99} Zn _{0.01} O _{6.9}	86	398	0.043
ErBa ₂ Cu _{2.95} Zn _{0.05} O _{6.9}	78	388	0.042
ErBa ₂ Cu ₃ O _{6.3}	NS	351	-
GdBaSrCu ₃ O _{7-□}	87	385	0.044
GdBaSr(Cu _{2.99} Zn _{0.01})O _{7-δ}	84	420	0.041
GdBaSr(Cu _{2.97} Zn _{0.03})O _{7-δ}	82	449	0.040
GdBaSr(Cu _{2.94} Zn _{0.06})O _{7-δ}	73	440	0.038
GdBaSr(Cu _{2.9} Zn _{0.1})O _{7-δ}	NS	452	-
DyBaSrCu ₃ O _{7-δ}	82	464	0.039
(Dy _{0.9} Pr _{0.1})BaSrCu ₃ O _{7-δ}	75	400	0.040
(Dy _{0.8} Pr _{0.2})BaSrCu ₃ O _{7-δ}	59	374	0.038
(Dy _{0.6} Pr _{0.4})BaSrCu ₃ O _{7-δ}	28	402	0.028
(Dy _{0.3} Pr _{0.7})BaSrCu ₃ O _{7-δ}	NS	434	-
Tl ₂ Ba ₂ Ca ₂ Cu ₃ O ₁₀	123	268	0.060
Pr ₂ CuO ₄	NS	408	-
Pr _{2-x} Ce _x CuO ₄	21	406	0.025

NS: non-superconducting

The Debye temperature and electron-phonon coupling constant in the Van Hove scenario are shown in Table 1. The uncertainty in θ_D and λ_{VH} is about 2.5 % of the absolute value, and the uncertainty in the transition temperature is ± 1 K. There is no clear indication of linear relation between T_c and θ_D when comparing between samples. For example the $Tl_2Ba_2Ca_2Cu_3O_{10}$ with the highest T_c of 123 K showed the lowest θ_D of 268 K. However, when comparing samples of same composition except for the oxygen contents, for example $ErBa_2Cu_3O_{6.9}$ and $ErBa_2Cu_3O_{6.3}$, the superconducting sample ($O_{6.9}$) showed a higher θ_D . Higher oxygen content (higher T_c) gives a higher Debye temperature. The suppression of superconductivity in the reduced oxygen samples is due to the reduction of the carrier concentration in the materials. Although a direct proportional relation between T_c and θ_D cannot be made among samples of different chemical formulae, proportional relation are observed in samples with similar chemical formula except for the oxygen content.

The calculated electron-phonon coupling constant using the Van Hove scenario, λ_{VH} is between 0.025 – 0.060. The Van Hove coupling constant is proportional to the transition temperature of the samples studied. The coupling constant is much closer to the value found in the Bi based and $RBa_2Cu_3O_{7-\delta}$ superconductors (λ is centered at around 0.04) from Raman scattering data[7-9].

According to the conventional theory two factors govern the electron-phonon coupling. Usually the coupling constant is determined by the density of states given as $\lambda = N(0)V$, with V reasonably constant. In the doped HTSC, this can be interpreted as the variation in the density of states near the Fermi level. The Van Hove singularity moves closer or further away from the Fermi level depending on doping. The coupling constant in the BCS-McMillan scheme can also be related to the characteristic phonon frequency ω ,

with $\lambda \sim \frac{C}{M\langle\omega\rangle}$, where C is a constant and M the ionic mass. In this case an elastically

softer material will have a stronger electron-phonon coupling. The two expressions for λ however are related because materials with high density of states are elastically softer[10]. However, in the cuprate HTSC, a decrease in the electron-phonon coupling constant does not necessarily results in lower T_c . The corresponding changes in the characteristic phonons frequency may instigate suppression of the transition temperature and vice-versa. The variation in the characteristic phonons (Debye) frequency and the electron-phonon coupling constant has combined effect on T_c .

We now discuss the phonon mode that can be responsible in forming the electron pairs. The main physics in these materials lies in the CuO_2 planes, where interplanar coupling is weak. The important phonon modes in the plane are related to oxygen vibrations which are the breathing (in plane vibrations) and buckling modes (out of plane vibrations). For each mode there can be a diagonal and non-diagonal electron-phonon interaction. The electron-phonon coupling constant for the breathing mode is $\lambda = 0.02$ [11]. The non-diagonal electron-phonon interaction of the breathing mode has been shown to have attractive interaction leading to pair formation.

The electron phonon coupling constant in this scenario is very small, which is surprising considering the high transition temperature. However, from our acoustic results on a

broad range of cuprates and various reports, we show that this is sufficient and essential for the formation of Cooper pairs. The density of states diverges near the Fermi level and even very weak electron-phonon interactions can result in an unexpectedly large effect. Our results also show that the non-diagonal electron-phonon interaction of the breathing mode is important for the pair formation in these high temperature cuprate superconductors. This may provide further insights into the mechanism of superconductivity in the cuprates.

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