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# Specific heat jump in anisotropic $YBa_2Cu_30_{7-\delta}$ superconductor

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Using the exotic pairing model, the jump in the specific heat $\Delta C/T_c$ in $YBa_2Cu_30_{7-\delta}$, for both breathing mode and buckling mode has been calculated. Its value was compared with the experimental values and it has been found that the specific heat jump in superconductor and the density of states were one fifth of the earlier reported values. This is indicative of the small fraction of carriers close to the Fermi level, which are paired and exotic pairing due to anharmonic perturbation of the apical oxygen ions leads to a lowering of $\Delta C/T_c$.

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## 1 Introduction

$YBa_2Cu_3O_{7-\delta}$, $0\leq \delta \leq 0.1$, is a superconductor that has perovskite-like orthorhombic structure. It is made up of two corrugated $CuO_2$ planes separated by a layer of Yttrium atoms and intercalated with two BaO layers and one CuO layer. It is assumed that this compound is moderately anisotropic with anisotropy parameter[1] of 5. Superconductivity of this material and hence the transition temperature is strongly dependent on the content and ordering of oxygen deficiencies.Although there is no clear theory for the microscopic understanding of high-$T_c$ superconductivity, it is believed that the existence of several equivalent positions of oxygen atoms causes a strong anharmonic perturbation, which can increase the electron-phonon coupling[2,3] leading to increase in transition temperature $T_c$.

Important properties of a superconducting material include the specific heat discontinuity $\Delta C$ at $T_c$ due to the second-order transition of the normal state to superconducting state and the electronic specific heat coefficient $\gamma$. This specific heat coefficient is proportional to the density of electronic states of the Fermi surface and is one of the three parameters (others being the effective attraction coupling constant and the energy shell around the Fermi surface) which specify the interactions of the electrons and thus, determine $T_c$. Understanding of these electronic properties may lead to a clue to high $T_c$ mechanism.

Exotic pairing is assumed[3] to be contributing to the high value of the transition temperatures in $YBa_2Cu_3O_{7-\delta}$. Specifically it was found that anharmonic perturbation of phonons with quadratic temperature dependence significantly increases the transition temperature. Furthermore[4], the shape of the specific heat graph was found to be typical of the superconducting state and gave support to the exotic pairing, due to anharmonic perturbation, as contributing to the electron-phonon coupling. The graph was found to consist of two sections. First, an exponential term for $0\leq T \leq 0.7T_c$, which is indicative of an existence of the energy gap in the electronic energy levels. Secondly, a linear term for $0.7T_c<T<T_c$.

Therefore, the properties of the specific heat discontinuities and specific heat coefficient and their dependence on $T_c$ may be essential to the understanding of the nature of superconductivity in high $T_c$ ceramic oxides. In normal metals, the low temperature behaviour of the specific heat is $C_V = aT + bT^3$, where $bT^3$ term is associated with the Debye vibrations of lattice. At very low temperatures, the linear term $aT$ dominates, and this term arises from the kinetic energy of the heat motions of the electron gas. In the superconducting state, the phonon specific heat $C_{ph} \propto T^3$ and the electron specific heat $C_{es} \propto e^{-\Delta/T}$ and this vanishes exponentially in the limit of very low temperatures. Thus, the specific heat $C_s$ in the superconducting state is $C_s = [3\gamma T^3/T_c^2]$. The electronic contribution to specific heat varies exponentially and approaches zero at very low temperatures. As a rule at very low temperature, phonon contribution will be negligible in the superconducting state, and the specific heat will be due to electronic motion. We should get the known value of $C_{es}/C_{en}$ as $C_{es}/C_{en}$ =2.43 at $T=T_c$ where $C_{es}$ is electronic specific heat in the superconducting state and $C_{en}$ is the electron contribution in the normal state. In this paper, the specific heat coefficient and the step in the specific heat capacity are calculated together with related parameters.

## 2 Theory

In the normal state the specific heat is composed of the lattice contribution and the electronic contribution and is given by:

$$C_n = c_1 T + c_2 T^3 \qquad ...(1)$$

At very low temperatures lattice contribution and the electronic contribution are negligible and the expression is reduced to:

$$C_n = \gamma T \qquad ...(2)$$

where γ is the specific heat coefficient (Sommerfeld gamma).

In the superconducting state

$$C_s = \frac{3\gamma T^3}{T_c^2}, \quad 0.7T_c<T<T_c$$

The specific heat can be assumed to have the form $C_s \propto \exp\frac{-\Delta}{kT}$ because of the existence of an energy gap in the temperature range $0 \le T \le 0.7T_c$.

$$C_s \propto \exp\frac{-\Delta}{kT}, \; 0<T<0.7T_c \qquad ...(3)$$

where Δ represents the gap in the allowed energy states and $k$ is the Boltzmann constant. The jump in the specific heat capacity[5] at the transition temperature is given by

$$\Delta C = C_s - C_n = T\Delta\frac{\partial S}{\partial T} = -T\Delta\frac{\partial^2 G}{\partial T^2} \qquad ...(4)$$

where $G$ is the Gibbs free energy density and $S$ is the entropy.

## 3 Results

The value of the specific heat coefficient has been calculated with the aid of the specific heat data[3] using Eq. (3).

### (a) Breathing mode

Kirui[3] worked out the value of the specific heat for this mode as:

$$C= e^{-1160/T}(1.06372\times0^{-21} + 1.834\times10^{-24}T - 8.3868\times10^{-27}T^2 - 2.892\times10^{-29}T^3) \qquad ...(5)$$

The specific heat at the critical temperature ($C_{max}$) was calculated and found to be $5.38\times10^{-24}$JK$^{-1}$. Hence, the transition temperature ($T_c$) has been easily worked out to be 258.5K. A graph of specific heat ($C$) against temperature cubed ($T^3$) for $220<T<233$ is obviously a straight line whose gradient is $4\times10^{-31}$JK$^{-4}$. Using Eq. (3), $\gamma = 8.91\times10^{-27}$ JK$^{-2}$ = 5.36 JK$^{-2}$mol$^{-1}$. Since the electronic specific heat is related to the free carriers in the $CuO_2$ plane and there are three *Cu* atoms in $YBa_2Cu3O_{7-\delta}$, then:

$$\gamma = 1.79\left(\frac{mJ}{K^2.g-at}\right) \qquad ...(6)$$

Hence, the density of states[6] is given by :

$$v(0)\left(\frac{\text{states}}{eV.\text{atom}}\right) = 0.414\gamma\left(\frac{mJ}{K^2.g-at}\right) = 0.74\left(\frac{\text{states}}{eV.\text{Cu atom}}\right) \qquad ...(7)$$

At the transition temperature ($T_c$), the specific heat in the normal state ($C_n$) is:

$$C_n = \gamma T_c = 2.30\times10^{-24}\text{JK}^{-1} \qquad ...(8)$$

Hence, at the phase transition temperature $T_c$, the specific heat jump is given by:

$$\frac{\Delta C}{T_C} = \frac{C_S - C_N}{T_C} = 1.19\times10^{-26}\text{JK}^{-2} = 7.164\text{mJK}^{-2}/\text{mol} \qquad ...(9)$$

and

$$\frac{\Delta c}{\gamma T_c} = 1.33 \qquad ...(10)$$

**(b) Buckling mode**

Again, from Ref. (3), the specific heat under this mode has been derived as:

$$C = e^{-580/T}(4.2514\times10^{-21} + 1.466\times10^{-23}T - 2.697\times10^{-25}T^2 - 1.86\times10^{-27}T^3) \quad \ldots(11)$$

Again, the transition temperature($T_c$) has been computed to be 96.8K while the specific heat at critical temperature ($C_{max}$) is found to be $3.64\times10^{-24}$JK$^{-1}$. Thus, the graph of $C$ versus $T^3$ is again linear and similarly,we have calculated the value of $\gamma$ to be $1.87\times10^{-26}$JK$^{-2}$ = 11.28mJK$^{-2}$/mol.

For Cu atom

$$\gamma = 3.76\left(\frac{mJ}{K^2.g-at}\right) \Rightarrow \nu(0) = 1.56\frac{\text{state}}{eV.\text{Cu atom}} \quad \ldots(12)$$

At the critical temperature, the specific heat in the normal state is:

$$C_n = \gamma T_c = 1.81\times10^{-24}\text{JK}^{-1} \quad \ldots(13)$$

Thus

$$\frac{C_s - C_n}{T_c} = 1.89\times10^{-26}\ \text{JK}^{-2} = 11.38\ \text{mJK}^{-2}/\text{mol and}$$

$$\frac{\Delta C}{C_n} = 1.01$$

If $\Delta C = C_s - C_n$ then $\frac{\Delta C}{C_n} = 1.01 = \frac{C_s - C_n}{C_n} = \frac{C_s}{C_n} - 1$

The ratio of the two values of the specific heat $C_s/C_n$ is then equivalent to 2.01 which is close to that of $C_{es}/C_{en}$ ($\cong$ 2.43).

## 4 Discussion

Specific heat is defined as the heat capacity of a mole of $YBa_2Cu_3O_{7-\delta}$, which fills a volume of $1.05\times10^{-4}$m$^3$. The jump at the transition temperature signifies the electronic contribution. According to the exotic pairing model[3], the electronic specific heat of the superconductor decreases exponentially at temperatures $T<T_c$ and vanishes at $T<<T_c$ indicating that there is no residual specific heat. Therefore, it is concluded that this model describes an ideal superconductor that has no impurities.

In the breathing mode, the density of states is 0.74 (states/eV.Cu atom) and the specific heat jump is $\Delta C/T_c$ = 7.16 mJ/mol K$^2$ while the buckling mode, the density of state is 1.56 (states/eV Cu atom) and the specific heat jump is $\Delta C/T_c$ = 11.38 mJ/molK$^2$. These values are about one fifth of the reported values[7,8]. The small value of the specific heat discontinuity indicates that in the type of pairing model assumed, the density of the electronic states of the Fermi level for this compound is low which means that only a very small fraction of carriers close to the Fermi level are paired. It is argued, therefore, that the formation of exotic pairs, due to the anharmonic perturbation is due to a small number of free carriers in the $CuO_2$ plane.

It has been pointed out[9] that the quasi particle excitation spectrum has two branches depending on the spin orientation. At the transition, it is only the spin-up Fermi surface that open up the superconducting gap and this reduces the specific heat jump from the BCS value of 1.43. It is possible then that $YBa_2Cu_3O_{7-\delta}$ oxide compounds are neither the weakly coupled BCS superconductors nor the strongly coupled BCS superconductors but some exotic superconductors. In conclusion, we have established that the exotic pairing due to strong anharmonic perturbation of the apical oxygen ions leads to a high transition temperature of $YBa_2Cu_3O_{7-\delta}$, a small number of electron pairs as carriers and a reduced specific heat jump at the transition to superconducting state.

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