

Variation of Isotope Coefficient with Number of CuO_2 Layers in High T_C Superconductors

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Abstract

In this paper, an effort has been made to study the isotope coefficient in high T_C Superconductors by using the variation of isotopic coefficient with the number of CuO_2 layers and the variation of isotope coefficients on transition temperature T_C . The Hamiltonian for CuO_2 layers using BCS type model and extra term of interlayer interaction between CuO_2 layers has been considered. Expressions for isotope effect (α) and transition temperature (T_C) are obtained and numerically calculated for experimental values by using Green's function technique.

Keywords: Isotope effect; CuO_2 layers; Isotope coefficient; High T_C superconductors

Introduction

After the discovery of high T_C cuprate superconductors in 1986 [1] at 35 K, the field is buzzing with research activities. Efforts to increase the transition temperature are currently going on. Till now the highest reached T_C under pressure is 164 K in $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+\delta}$ [2]. These cuprates have unconventional properties both in normal and superconducting state [3,4]. Till date there is no consensus on the origin of pairing mechanism. It is now widely suggested that spin fluctuation driven pairing mechanism provides a good agreement between theory and experiments [5]. However, there are several experimental observations which clearly indicate that this purely electronic picture is incomplete and lattice effects have to be taken into account [6-8]. Isotope shift of T_C is regarded as the defining signature of superconducting pairing resulting from phonons. In high T_C superconductors, a small isotope effect is found [9-11]. Suppression of this effect is not explained within conventional BCS theory which predicts that the critical temperature T_C and isotope mass M are related by $T_C \propto M^{-\alpha}$ where $\alpha=0.5$ for all elements. To explain the small isotope effect in high T_C compounds, many mechanisms including resonance valence bond [12], excitons [13], Plasmon's [14] and antiferromagnetic spin fluctuation mediated pairing are proposed [15]. Daemen and Overhauser [16] found that the existence of a short-range attraction in addition to the conventional phonon pairing interaction suppresses the isotope effect significantly at high temperatures. Here we present the variation of isotope coefficients with number of CuO_2 layers and the variation of isotope coefficients on transition temperature T_C [17-22]. As the trilayer material has highest (T_C) in these cuprates but it has very small isotope coefficient (α). Clearly the argument that a mechanism other than an electron phonon interaction dominates the superconductivity based only on a small (α) in a cuprate with relatively high (T_C) is inappropriate. The observed CuO_2 layer dependence of the isotope effect indicates that the interlayer coupling between the adjacent CuO_2 planes is necessary for superconductivity in layered cuprates [23-26]. For monolayer materials having lower (T_C) the interlayer coupling plays a less important role and (T_C) can be mainly controlled by the phonon coupling yielding a larger size of isotope coefficient with increasing the number of CuO_2 layers in a unit cell, the interlayer coupling begins to play an important role in enhancing (T_C) and the isotope effect is expected to be small.

Formulation

The model Hamiltonian for our system can be described as

$$H = H_{\text{intra}} + H_{\text{inter}}$$

$$H_{\text{intra}} = \sum_{k\sigma} E_k a_{k\sigma}^+ a_{k\sigma} - V \sum_{mkk'} a_{mk\uparrow}^+ a_{m-k\downarrow}^+ a_{m-k\downarrow} a_{mk'\uparrow}$$

$$H_{\text{inter}} = -W \sum_{mkk'} a_{mk\uparrow}^+ a_{n-k\downarrow} a_{mk'\uparrow}$$

$$H = \sum_{k\sigma} E_k a_{k\sigma}^+ a_{k\sigma} - V \sum_{mkk'} a_{mk\uparrow}^+ a_{m-k\downarrow}^+ a_{m-k\downarrow} a_{mk'\uparrow} - W \sum_{mkk'} a_{mk\uparrow}^+ a_{n-k\downarrow}^+ a_{n-k\downarrow} a_{mk'\uparrow} \quad (1)$$

Where $a_{k\sigma}^+$, $a_{k\sigma}$ denote the fermions creation and annihilation operator respectively, k is the wave vector and σ is spin index for fermions.

In our present analysis we use a Green's function, defining as

$$G_{mkk'}^{\uparrow\uparrow} = \langle \langle a_{mk\uparrow}^+, a_{nk'\uparrow}^+ \rangle \rangle \quad (2)$$

Equation of motion is written as

$$\omega G_{mkk'}^{\uparrow\uparrow} = \frac{1}{2\pi} + \langle \langle [a_{mk\uparrow}^+, H], a_{nk'\uparrow}^+ \rangle \rangle$$

Evaluating the commutator $[a_{m-k\downarrow}^+, H]$ using the Hamiltonian (1) we get

$$[a_{mk\uparrow}^+, H] = E_k a_{mk\uparrow}^+ - \sum_k (V) a_{m-k\downarrow}^+ a_{m-k\downarrow} a_{mk'\uparrow} - \sum_{nk'} (W) a_{n-k\downarrow}^+ a_{n-k\downarrow} a_{mk'\uparrow}$$

And writing the equation of motion as

$$\omega G_{mkk'}^{\uparrow\uparrow} = \frac{1}{2\pi} + \langle \langle [a_{mk\uparrow}^+, H], a_{nk'\uparrow}^+ \rangle \rangle \quad (3)$$

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Putting the value of commutator $[a_{mk\uparrow}, H]$ in equation (3) we get

$$\omega G_{mnkk}^{\uparrow\uparrow} = \frac{1}{2\pi} \left\langle \left\langle E_k a_{mk\uparrow}, a_{nk}^{\uparrow} \right\rangle \right\rangle - \sum_k V \left\langle \left\langle a_{m-k\downarrow}, a_{m-k\downarrow}, a_{mk\uparrow}, a_{nk}^{\uparrow} \right\rangle \right\rangle - \sum_k W \left\langle \left\langle a_{n-k\downarrow}, a_{n-k\downarrow}, a_{mk\uparrow}, a_{nk}^{\uparrow} \right\rangle \right\rangle$$

$$\text{Or } (\omega - E_k) G_{mnkk}^{\uparrow\uparrow} = \frac{1}{2\pi} \left[\Delta V + \sum_n \Delta W \right] G_{mnkk}^{\uparrow\uparrow} \quad (4)$$

Now we introduce the order parameter Δ such as

$$\Delta_{rr} = \sum_k V_{rr}(kq) \langle C_{rk\uparrow}^+ C_{r-k\downarrow}^+ \rangle, \quad \Delta_{rj} = \sum_k V_{rj}(kq) \langle C_{jk\uparrow}^+ C_{j-k\downarrow}^+ \rangle$$

Where $G_{mnkk}^{\downarrow\uparrow}$ is another Green's function which may be written as

$$G_{mnkk}^{\downarrow\uparrow} = \left\langle \left\langle a_{m-k\downarrow}^+, a_{nk\uparrow}^+ \right\rangle \right\rangle \quad (5)$$

This Green's function may also be written in terms of equation of motion as

$$\omega G_{mnkk}^{\downarrow\uparrow} = \left\langle \left\langle [a_{m-k\downarrow}^+, H]; a_{nk\uparrow}^+ \right\rangle \right\rangle \quad (6)$$

Evaluating the commutator $[a_{m-k\downarrow}^+, H]$ using the Hamiltonian

$$a_{m-k\downarrow}^+, H = \left[a_{m-k\downarrow}^+, \sum_{k\sigma} E_k a_{m\sigma}^+ a_{m\sigma} - V \sum_{mkk'} a_{m-k\downarrow}^+ a_{m-k\downarrow} a_{mk\uparrow} - W \sum_{mkk'} a_{m-k\downarrow}^+ a_{n-k\downarrow} a_{mk\uparrow} \right]$$

Putting the commutator $E_{(-k)} = E_k$ from (7) in equation (6) we get

$$\omega G_{mnkk}^{\downarrow\uparrow} = -E_k \left\langle \left\langle a_{m-k\downarrow}^+, a_{nk\uparrow}^+ \right\rangle \right\rangle - V \sum_{mkk'} \left\langle \left\langle a_{m-k\downarrow}^+, a_{m-k\downarrow} \right\rangle \right\rangle \left\langle \left\langle a_{mk\uparrow}, a_{nk\uparrow} \right\rangle \right\rangle - W \sum_{mkk'} \left\langle \left\langle a_{m-k\downarrow}^+, a_{n-k\downarrow} \right\rangle \right\rangle \left\langle \left\langle a_{mk\uparrow}, a_{nk\uparrow} \right\rangle \right\rangle$$

But from the law of conservation of energy

$$E_{(-k)} = E_k$$

$$(\omega + E_k) G_{mnkk}^{\downarrow\uparrow} = - \left[\Delta V + \sum_n \Delta W \right] G_{mnkk}^{\downarrow\uparrow} \quad (8)$$

In equation (4) we finally obtained the equation

$$(\omega - E_k) G_{mnkk}^{\uparrow\uparrow} = \frac{1}{2\pi} \left[\Delta V + \sum_n \Delta W \right] G_{mnkk}^{\downarrow\uparrow} \quad (9)$$

Multiply $(\omega + E_k)$ in equation (9) and putting the value of $(\omega - E_k) G_{mnkk}^{\downarrow\uparrow}$ from equation (8) then we get the Green's function $G_{mnkk}^{\uparrow\uparrow}$ as

$$(\omega^2 - E_k^2) G_{mnkk}^{\uparrow\uparrow} = \frac{1}{2\pi} (\omega + E_k) \left[\Delta V + \sum_n \Delta W \right] (\omega + E_k) G_{mnkk}^{\downarrow\uparrow} \quad (10)$$

Multiplying by $(\omega + E_k)$ in the equation (8) and putting the value of $(\omega - E_k) G_{mnkk}^{\downarrow\uparrow}$ from equation (9) we get the Green's function as

$$G_{mnkk}^{\uparrow\uparrow} = \frac{\omega + E_k}{2\pi \left[(\omega^2 - E_k^2) + \left(\Delta V + \sum_n \Delta W \right) \left(\Delta V + \sum_n \Delta W \right) \right]}$$

$$(\omega^2 - E_k^2) G_{mnkk}^{\downarrow\uparrow} = - \left[\Delta V + \sum_n \Delta W \right] (\omega - E_k) G_{mnkk}^{\uparrow\uparrow}$$

We know from equation (9)

$$G_{mnkk}^{\downarrow\uparrow} = - \frac{\left(\Delta V + \sum_n \Delta W \right)}{2\pi \left[\omega^2 - E_k^2 - \left(\Delta V + \sum_n \Delta W \right)^2 \right]} \quad (11)$$

Using the Green's function, we can obtain the expression for order

parameter Δ_{mn} and correlation parameter γ the order parameter Δ_{mn} may be written as

$$\Delta_{mn} = \sum_{k'} V \langle a_{mk\uparrow}^+ a_{m-k\downarrow}^+ \rangle \quad (12)$$

Correlation function $\langle a_{mk\uparrow}^+ a_{m-k\downarrow}^+ \rangle$ is related to Green's function $G_{mnkk}^{\downarrow\uparrow}$ as

$$\langle a_{mk\uparrow}^+ a_{m-k\downarrow}^+ \rangle = - \frac{1}{i} \int_{-\infty}^{\infty} \frac{G_{mnkk}^{\downarrow\uparrow}(\omega + i\epsilon) - G_{mnkk}^{\downarrow\uparrow}(\omega - i\epsilon)}{e^{\omega/kT} - \eta} d\omega \quad (13)$$

Where $\eta = -1$ for fermions, $K =$ Boltzmann constant and $T =$ Temperature

Green's function $G_{mnkk}^{\downarrow\uparrow}(\omega + i\epsilon)$ and $G_{mnkk}^{\downarrow\uparrow}(\omega - i\epsilon)$ may be expressed as

$$G_{mnkk}^{\downarrow\uparrow}(\omega + i\epsilon) = \frac{- \left(\Delta V + \sum_n \Delta W \right)}{2\pi \left[(\omega + i\epsilon)^2 - E_k^2 - \left(\Delta V + \sum_n \Delta W \right)^2 \right]} \quad (14)$$

$$\therefore \xi_q^2 = E_k^2 + \left(\Delta V + \sum_n \Delta W \right)^2$$

$$G_{mnkk}^{\downarrow\uparrow}(\omega + i\epsilon) = - \frac{\left(\Delta V + \sum_n \Delta W \right)}{4\pi \xi_q} \left\{ \frac{(\omega - \xi_q)}{(\omega - \xi_q)^2 - \epsilon^2} - i\pi \delta(\omega - \xi_q) - \frac{(\omega + \xi_q)}{(\omega - \xi_q)^2 - \epsilon^2} + i\pi \delta(\omega + \xi_q) \right\} \quad (15)$$

$$G_{mnkk}^{\downarrow\uparrow}(\omega - i\epsilon) = \frac{- \left(\Delta V + \sum_n \Delta W \right)}{2\pi \left[(\omega - i\epsilon)^2 - E_k^2 - \left(\Delta V + \sum_n \Delta W \right)^2 \right]} \quad (16)$$

$$\therefore \xi_q^2 = E_k^2 + \left(\Delta V + \sum_n \Delta W \right)^2$$

$$G_{mnkk}^{\downarrow\uparrow}(\omega - i\epsilon) = \frac{- \left(\Delta V + \sum_n \Delta W \right)}{2\pi \left[(\omega - i\epsilon)^2 - \xi_q^2 \right]}$$

$$G_{mnkk}^{\downarrow\uparrow}(\omega - i\epsilon) = - \frac{\left(\Delta V + \sum_n \Delta W \right)}{4\pi \xi_q} \left\{ \frac{(\omega - \xi_q)}{(\omega - \xi_q)^2 + \epsilon^2} + i\pi \delta(\omega - \xi_q) - \frac{(\omega - \xi_q)}{(\omega - \xi_q)^2 + \epsilon^2} + i\pi \delta(\omega - \xi_q) \right\} \quad (17)$$

Substitute both the Green's function $G_{mnkk}^{\downarrow\uparrow}(\omega + i\epsilon)$ and $G_{mnkk}^{\downarrow\uparrow}(\omega - i\epsilon)$ from equation (13) and then after

solving we get correlation function.

$$G_{mnkk}^{\downarrow\uparrow}(\omega + i\epsilon) - G_{mnkk}^{\downarrow\uparrow}(\omega - i\epsilon) = - \frac{\left(\Delta V + \sum_n \Delta W \right)}{4\pi \xi_q} \left(2i\pi \delta(\omega - \xi_q) - 2i\pi \delta(\omega + \xi_q) \right) \quad (18)$$

$$\therefore \langle a_{mk\uparrow}^+ a_{m-k\downarrow}^+ \rangle = - \frac{1}{i} \int_{-\infty}^{\infty} \frac{G_{mnkk}^{\downarrow\uparrow}(\omega + i\epsilon) - G_{mnkk}^{\downarrow\uparrow}(\omega - i\epsilon)}{e^{\omega/kT} - \eta} d\omega$$

Where $\eta = -1$

$$\langle a_{mk\uparrow}^+ a_{m-k\downarrow}^+ \rangle = - \frac{1}{i} \int_{-\infty}^{\infty} \frac{\left(\Delta V + \sum_n \Delta W \right)}{4\pi \xi_q} \left(\frac{2i\pi \delta(\omega - \xi_q) - 2i\pi \delta(\omega + \xi_q)}{e^{\omega/kT} - \eta} \right) d\omega$$

$$\langle a_{mk\uparrow}^+ a_{m-k\downarrow}^+ \rangle = - \frac{1}{i} \int_{-\infty}^{\infty} \frac{\left(\Delta V + \sum_n \Delta W \right)}{4\pi \xi_q} \left(\frac{2i\pi \delta(\omega - \xi_q) - 2i\pi \delta(\omega + \xi_q)}{e^{\omega/kT} - \eta} \right) d\omega = \frac{\left(\Delta V + \sum_n \Delta W \right)}{\xi_q} \left[\frac{1}{e^{1/kT} + 1} - \frac{1}{e^{1/kT} + 1} \right]$$

Put $x = \frac{\xi_q}{kT}$

$$\langle a_{mk,\uparrow}^+ a_{m-k,\downarrow}^+ \rangle = \frac{\left(\Delta V + \sum_n \Delta_n W \right)}{2\xi_q} \left[\frac{1}{e^x + 1} - \frac{1}{e^{-x} + 1} \right] \quad (19)$$

$$\therefore \frac{1}{e^x + 1} - \frac{1}{e^{-x} + 1} = \frac{e^{-x/2} + e^{x/2}}{e^{-x/2} + e^{x/2}} = \tanh \frac{x}{2} = \tanh \frac{\xi_q}{2kT}$$

(19) we get

$$\langle a_{mk,\uparrow}^+ a_{m-k,\downarrow}^+ \rangle = \frac{\left(\Delta V + \sum_n \Delta_n W \right)}{\xi_q} \left(\tanh \frac{\xi_q}{2kT} \right) = \frac{\Delta V + \sum_n \Delta_n W}{\sqrt{E_q^2 + \left(\Delta V + \sum_n \Delta_n W \right)^2}} \tanh \sqrt{E_q^2 + \left(\Delta V + \sum_n \Delta_n W \right)^2} \quad (20)$$

Then we can obtain the expression of order parameter Δ_{ir} by substituting correlation function in equation (12)

$$\Delta_{ir} = \sum_{k'} V_{ir}(k'_q) \langle c_{ik',\uparrow}^+ c_{i-k',\downarrow}^+ \rangle = \sum_{k'} V_{ir}(k'_q) \langle a_{mk,\uparrow}^+ a_{m-k,\downarrow}^+ \rangle$$

$$\Delta_{mn} = \sum_{k'} V_{ir}(k'_q) \frac{\Delta V + \sum_n \Delta_n W}{\sqrt{E_q^2 + \left(\Delta V + \sum_n \Delta_n W \right)^2}} \tanh \sqrt{E_q^2 + \left(\Delta V + \sum_n \Delta_n W \right)^2} \quad (21)$$

Converting summation over K into integration with cut-off energy $\hbar\omega_D$ from the Fermi level we get

$$\Delta_{mn} = N_s \int_0^{\hbar\omega_D} V_{ir}(k'_q) \frac{\left(\Delta V + \sum_n \Delta_n W \right)}{\sqrt{E_q^2 + \left(\Delta V + \sum_n \Delta_n W \right)^2}} \tanh \sqrt{E_q^2 + \left(\Delta V + \sum_n \Delta_n W \right)^2} dE_q \quad (21)$$

$$\therefore \frac{1}{N_0 V} = \int_0^{\hbar\omega_D} \frac{1}{\sqrt{E_q^2 + \left(\Delta V + \sum_n \Delta_n W \right)^2}} \tanh \sqrt{E_q^2 + \left(\Delta V + \sum_n \Delta_n W \right)^2} dE_q \quad (22)$$

At $T = T_C, \Delta = 0$

$$\frac{1}{N_0 V} = \frac{1}{2K_B T_C} \int_0^{\hbar\omega_D} \frac{1}{\left(\frac{E_q}{2K_B T_C} \right)} \tanh \frac{E_q}{2K_B T_C} dE_q \quad (23)$$

$$\therefore \frac{1}{N_0 V} = \frac{1}{2K_B T_C} \int_0^{\frac{\hbar\omega_D}{2K_B T_C}} \frac{1}{x} \tanh x (2K_B T_C) dx$$

$$\text{Or } \frac{\hbar\omega_D}{2K_B T_C} e^{0.8185} = \exp \frac{1}{N_0 V}$$

$$\therefore T_C = (1.13072) \frac{\hbar\omega_D}{2K_B} \exp \frac{1}{N_0 V} \quad (24)$$

The Isotope effect coefficient is

$$\alpha = -\frac{d \ln T_C}{d \ln M} \quad (25)$$

Using equation (29) and (30) we get

$$\alpha = \frac{d}{d \ln M} \left[\log(1.13072) \frac{\hbar\omega_D}{K_B} + \log e^{-\frac{1}{N_0 V}} \right] \quad (26)$$

$$\text{Put } T_C \propto M^{-\frac{1}{2}}, \text{ or } T_C = KM^{-\frac{1}{2}}$$

$$\therefore \alpha = -\frac{d}{4d \log V} [2 \log V] - \frac{d}{4d(\log V)} \left(\frac{1}{N_0 V} \right) \quad (27)$$

Differentiating we get

$$\frac{1}{N_0 V} = (2(1 + 2\alpha)) \quad (28)$$

Now from equation (24) we get

$$T_C = 1.13072 \frac{\hbar\omega_D}{K_B} \exp(-2(2\alpha + 1)) \quad (29)$$

By solving equation (33), we get α as

$$\alpha = \frac{1}{4N_0 V \left(1 + \frac{D}{N_0} \right)} - \frac{1}{2} \quad (30)$$

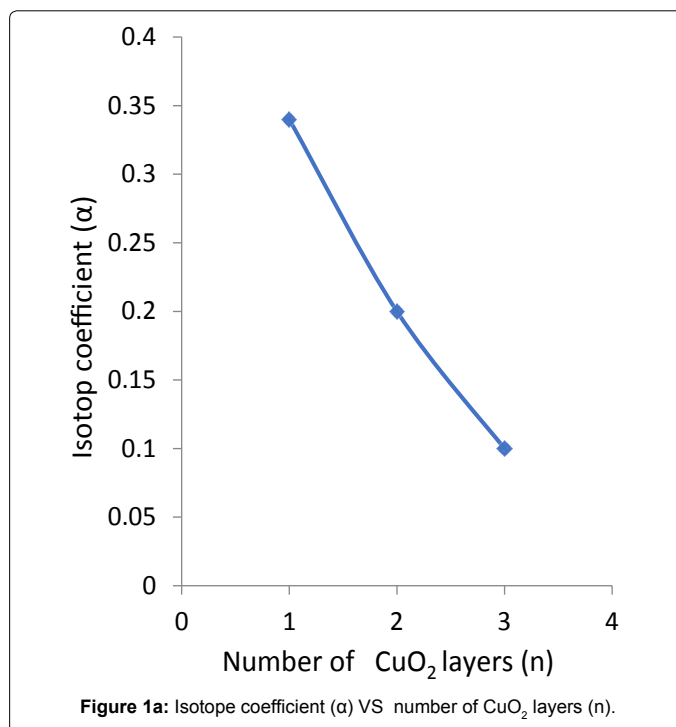
The values of α and T_C are calculated from equation (29) and (30) respectively for various values of different CuO₂ layers (Table 1).

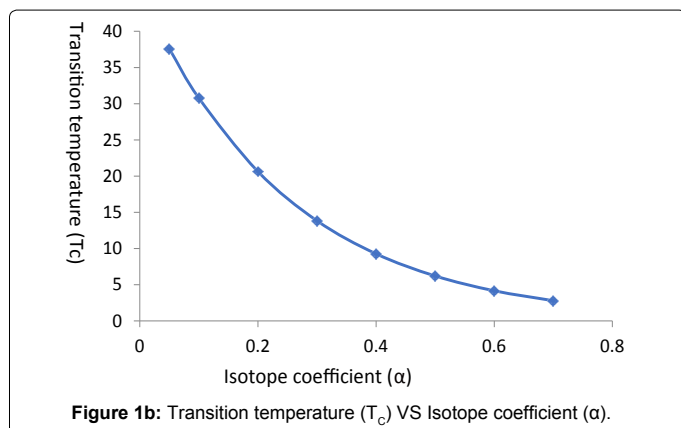
Results and Discussion

The numerical analysis of equation (29) and (30) have been calculated for different CuO₂ layers taking $\frac{D}{N_0} = 0.2$ (for $n=1$) and $\frac{D}{N_0} = 0.6$ (for $n=3$). Figure 1a is plotted between isotope coefficient (α) and number of CuO₂ layers (n) per unit cell. Figure shows that as increasing number of CuO₂ layers per unit cell, isotope coefficient (α) linearly decreases. For $n=1$, the value of (α) is 0.34 and it decreases continuously with number of CuO₂ layers. At $n=3$, isotope coefficient (α) is 0.1317 which is very low. This systematic reduction of isotope coefficient with increasing CuO₂ layers indicates that isotope effect can be negligible for multi-layer cuprates. This result is good agreement with experimental result made by Chen et al. Figure 1b is plotted between transition temperature (T_C) and isotope coefficient. The curve shows that as increasing (α), the transition temperature exponentially decreases so for lower isotope coefficient T_C will be maximum and T_C decreases for higher values of (α). So we can say that as increasing number of CuO₂ layers, (α) decreases and the transition temperature increases. This result also supported by Chakravarty et al.

Conclusion

First of all Hamiltonian for CuO₂ layers using BCS type model





S No	α	T_c
1	0.05	37.586
2	0.1	30.772
3	0.2	20.627
4	0.3	13.827
5	0.4	9.268
6	0.5	6.212
7	0.6	4.164
8	0.7	2.791

Table 1: Table for values of (α) and (T_c).

and extra term of interlayer interaction between CuO_2 layers has been considered, using this equation expression for isotope effect (α) and transition temperature (T_c). Expression obtained is numerically solved using Green's function technique and then the value of isotope effect (α) and transition temperature (T_c) is calculated. The graph is plotted between isotopic coefficient and number of CuO_2 layers. The second graph is plotted between isotope effect (α) and transition temperature (T_c). Then conclusion is drawn comparing with available experimental result. The tri layer material has highest (T_c) in these cuprates but it has very small isotope coefficient (α). Clearly the argument that a mechanism other than an electron-phonon interaction dominates the superconductivity based only on a small (α) in a cuprate with relatively high (T_c) is inappropriate. The observed CuO_2 layer dependence of the isotope effect indicates that the interlayer coupling between the adjacent CuO_2 planes is necessary for superconductivity in layered cuprates. For monolayer materials having lower (T_c) the interlayer coupling plays a less important role and (T_c) can be mainly controlled by the phonon coupling yielding a larger size of isotope coefficient with increasing the number of CuO_2 layers in a unit cell, the interlayer coupling begins to play an important role in enhancing (T_c) and the isotope effect is expected to be small.

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