

On the Isotope-Like Effect for High- T_c Superconductors in the Scenario of 2-Phonon Exchange Mechanism for Pairing

G. P. Malik^{1,2}

¹Present Address: B-208 Sushant Lok 1, Gurgaon, Haryana, India

²Formerly: Theory Group, School of Environmental Sciences, Jawaharlal Nehru University, New Delhi, India

Email: gulshanpmalik@yahoo.com, malik@mail.jnu.ac.in

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Abstract

By generalizing the isotope effect for elemental superconductors (SCs) to the case of pairing in the 2-phonon exchange mechanism for composite SCs, we give here an explanation of the well-known increase in the critical temperature (T_c) of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ from 95 K to 110 K and of $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$ from 105 to 115 - 125 K when Bi and Sr in these are replaced by Tl and Ba, respectively. On this basis, we also give the estimated T_c s of some hypothetical SCs, assuming that they may be fabricated by substitutions similar to $\text{Bi} \rightarrow \text{Tl}$ and $\text{Sr} \rightarrow \text{Ba}$.

Keywords

Isotope-Like Effect, 2-Phonon Exchange Mechanism, Bi- and Tl-Based High- T_c SCs, Suggestions for New Substitutions for Further Enhancement of T_c of the Bi-Based SCs

1. Introduction

In this note we deal with an explanation of why the replacements of Bi and Sr in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ and $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$ by Tl and Ba, respectively, lead to an increase in the critical temperature T_c of the former from 95 K to 110 K and of the latter from 105 to 115 - 125 K. This is an important undertaking because it has the potential to act as a general guide about substituting one or the other element in a composite superconductor (SC) in order to enhance its T_c .

Empirically, it has been shown [1] that greater the T_c of an SC, greater is its critical current density j_0 , for which, theoretically, an expression has been derived in terms of the following five parameters [2] [3]: Debye temperature θ , the

electronic specific heat constant γ , gram-atomic volume v_g , Fermi energy E_F and a dimensionless construct $y = (k\theta/P_0)\sqrt{2m^*/E_F}$ where k is the Boltzmann constant, P_0 the critical momentum of Cooper pairs and m^* the effective mass of an electron. Therefore, if theory could predict the values of these parameters after one or more substitutions are made in an SC, then we would have a handle on its j_0 and T_c . Since, as of now, theory cannot perform this task, we must resort to an approach that relies on a property or properties that can be unequivocally determined, regardless of the number of elements that are replaced by others. Such a property is the mass of the SC.

Above considerations lead us to recall the isotope effect

$$T_c \propto M^{-\alpha}, \quad (1)$$

where M is the average mass of ions of an *elemental* SC. While BCS theory gives the value of α as 0.5, values significantly different from this have also been found for some elements, e.g., Mo, Os, and Ru, which are characterized by $\alpha = 0.33$, 0.2, and 0, respectively. Hence, while (1) does not have the status of a *law*, it nonetheless helped in the formulation of BCS theory because it sheds light on the role of the ion lattice in the scenario of 1-phonon exchange mechanism (1 PEM) for pairing. Since the T_c s and gaps of all the SCs dealt with here have been explained in the framework of the generalized-BCS equations (GBCSEs) employing the 2-phonon exchange mechanism (2 PEM) [4], we take up in the next Section the task of generalizing (1) for this case. Applications of the generalized equation are addressed in Section 3, where also given are the estimated values of T_c s of some members of the families of SCs represented by $X_2Y_2CaCu_2O_8$ and $X_2Y_2Ca_2Cu_3O_{10}$ for different choices of X and Y. The final Section sums up our present study.

2. Isotope-Like Effect in the 2 PEM Scenario

GBCSE for the T_c of a composite SC in the 2 PEM scenario is [5]

$$\begin{aligned} & \text{Re} \left\{ \frac{\lambda_1}{2} \int_{-k\theta_1}^{k\theta_1} d\xi \frac{\sqrt{\xi + \mu} \tanh(\xi/2kT_c)}{\xi} + \frac{\lambda_2}{2} \int_{-k\theta_2}^{k\theta_2} d\xi \frac{\sqrt{\xi + \mu} \tanh(\xi/2kT_c)}{\xi} \right\} \\ & = \text{Re} \left\{ \left[\frac{3}{4} \int_{-\mu}^{k\theta_2} d\xi \sqrt{\xi + \mu} \{1 - \tanh(\xi/2kT_c)\} \right]^{1/3} \right\}, \end{aligned} \quad (2)$$

where chemical potential μ has been used interchangeably with E_F , θ_1 and θ_2 are the Debye temperatures and λ_1 and λ_2 the interaction parameters of the ion-species responsible for pairing, and the operator *Re* ensures that the integrals yield real values even when $\xi + \mu < 0$. When either of the λ s is zero and $\mu \gg k\theta_1$ (or $k\theta_2$), (2) reduces to the usual BCS equation for the T_c of an elemental SC in the 1 PEM scenario. Since T_c of an SC in the 2 PEM scenario is due to the cooperative effect of two kinds of ions, the following generalization of (1) suggests itself naturally

$$T_c = p(M_1M_2)^{-\alpha} \quad (3)$$

where p is the constant of proportionality and M_1 and M_2 are the masses of the ion-species that cause pairing. A discussion of (3) vis-à-vis (1) will be given below.

3. Applications of Equation (3)

3.1. $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$

Pairing in this SC may be caused by the cooperative effect of one or more of the following pairs of ions: Bi and Sr, Bi and Ca, and Sr and Ca. For each of these choices, guided by the values of α noted in Section 1, we calculate the value of p corresponding to $T_c = 95$ K, and $\alpha = 0.5, 0.4, 0.3, 0.2,$ and 0.1 . With $M_{\text{Bi}} = 208.98$, $M_{\text{Sr}} = 87.62$, and $M_{\text{Ca}} = 40.08$ (amu), we then obtain the results given in **Table 1**.

3.2. $\text{Tl}_2\text{Ba}_2\text{CaCu}_2\text{O}_8$

We calculate T_c ($\text{Tl}_2\text{Ba}_2\text{CaCu}_2\text{O}_8$) via (3) for each of the 15 $\{\alpha, p\}$ -values in **Table 1** by successively taking M_1M_2 as $M_{\text{Tl}}M_{\text{Ba}}$, $M_{\text{Tl}}M_{\text{Ca}}$, and $M_{\text{Ba}}M_{\text{Ca}}$. With $M_{\text{Tl}} = 204.39$ and $M_{\text{Ba}} = 137.33$ (amu), the resulting 45 values are given in **Table 2**.

It is seen from **Table 1** and **Table 2** that while $\alpha = 0.2$ and $p = 676.6$ correspond to T_c ($\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$) = 95 K in the 2PEM scenario involving predominantly the Bi and Sr ions, they lead to T_c ($\text{Tl}_2\text{Ba}_2\text{CaCu}_2\text{O}_8$) = 111.6 K when pairing is predominantly due to the Tl and Ca ions. Two other notable pairs of $\{\alpha, p\}$ -values in **Table 1** are $\{0.3, 1427.7\}$ and $\{0.1, 253.5\}$ which yield, respectively, values of T_c ($\text{Tl}_2\text{Ba}_2\text{CaCu}_2\text{O}_8$) as 107.8 and 107.1 K (pairing via the Ba and Ca ions in each case); both of these T_c s are also close to the experimental values of 110 K.

Since Bi and Tl belong to the same period and Sr and Ba to the same group of the periodic table, it seems interesting to investigate the effects of further similar substitutions in light of the above results. We assume that it is feasible to obtain the compounds noted below from the parent compound $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$.

For $\alpha = 0.2$ and $p = 676.6$ K amu^{2 α} , we obtain

- 1) T_c ($\text{Bi}_2\text{Mg}_2\text{CaCu}_2\text{O}_8$); via Bi + Mg) = 123 K = T_c ($\text{Tl}_2\text{Mg}_2\text{CaCu}_2\text{O}_8$); via Tl + Mg)
- 2) T_c (Bi_2 (or Tl_2) $\text{Mg}_2\text{CaCu}_2\text{O}_8$); via Bi + Mg) = 171 K

Table 1. The values of p obtained by solving (3) corresponding to $T_c = 95$ K, $\alpha = 0.5, 0.4, 0.3, 0.2,$ and 0.1 and different choices of ions responsible for pairing in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$.

α	p (Bi + Sr) (K amu ^{2α})	p (Bi + Ca) (K amu ^{2α})	p (Sr + Ca) (K amu ^{2α})
0.5	12855.2	8694.4	5629.7
0.4	4817.3	3523.2	2488.5
0.3	1805.2	1427.7	1100.0
0.2	676.5	578.5	486.2
0.1	253.5	234.4	214.9

Table 2. T_c ($Tl_2Ba_2CaCu_2O_8$) calculated via (3) for each pair of $\{\alpha, p\}$ values in **Table 1** for different combinations of ions in the 2 PEM scenario.

α	p	T_c (Tl + Ba)	T_c (Tl + Ca)	T_c (Ba + Ca)
		K	K	K
0.5	12855.2	76.7	142.0	173.3
	8694.4	51.9	96.1	117.2
	5629.7	33.6	62.2	75.9
$\alpha = 0.4$	4817.3	80.1	131.1	153.6
	3523.2	58.6	95.8	112.4
	2488.5	41.4	67.7	79.4
$\alpha = 0.3$	1805.2	83.6	120.9	136.2
	1427.7	66.1	95.6	107.8
	1100.0	50.9	73.7	83.0
$\alpha = 0.2$	676.5	87.2	111.6	120.8
	578.5	74.6	95.4	103.3
	486.2	62.7	62.7	86.8
$\alpha = 0.1$	253.5	91.0	103.0	107.1
	234.4	84.2	95.2	99.1
	214.9	77.2	87.3	90.8

3) T_c ($Bi_2Be_2CaCu_2O_8$); via Bi + Be) = 150 K = T_c ($Tl_2Be_2CaCu_2O_8$); via Tl + Be)

4) T_c (Bi_2 or (Tl_2) $Be_2CaCu_2O_8$); via Be + Ca) = 208 K

3.3. $Bi_2Sr_2Ca_2Cu_3O_{10}$ and $Tl_2Ba_2Ca_2Cu_3O_{10}$

Following the same procedure as above, we can find 15 $\{\alpha, p\}$ -values, each of them corresponding to T_c ($Bi_2Sr_2Ca_2Cu_3O_{10}$) = 105 K. Among these, the following four sets: {0.4, 3894.1; Bi + Ca}, {0.3, 1578.0; Bi + Ca}, {0.1, 280.2; Bi + Sr}, and {0.2, 747.7; Bi + Sr} also lead to T_c ($Tl_2Ba_2Ca_2Cu_3O_{10}$) in the range 115 - 125 K; the T_c -values corresponding to the first three due to the (Ba + Ca) ions are 124.2, 119.1, and 118.4 K, respectively, and the fourth value is 123.3 K due to the (Tl + Ca) ions.

Some typical T_c -values corresponding to $\{\alpha, p\} = \{0.4, 3894.1\}$ when Sr in $Bi_2Sr_2CaCu_3O_{10}$ is replaced by Mg and Be, respectively, are 248.2 (due to Mg + Ca) and 190.8 K (due to Bi + Be).

4. Discussion and Conclusion

It was noted above that BCS theory gives the value of α in (1) as 0.5. This follows from two relations: (a) $kT_c \cong 1.13\hbar\omega_c \exp\left(-1/\left[N(0)\right]V\right)$, where ω_c is Debye frequency of the ions, $N(0)$ the density of states at the Fermi surface, and V the net attraction between electrons bound as pairs, and (b) $\omega_c \propto M^{-1/2}$. It is hence

seen that $\alpha = 0.5$ only if $N(0)$ and V do not change when one isotope is replaced by another. This is a reasonable assumption for $N(0)$ because it is a purely electronic property; not so for V which is determined jointly by the ions and the electrons. It is not surprising therefore that $\alpha = 0.5$ holds only for a few so-called classic elemental SCs, e.g., Zn, Pb, and Hg and that most of the other SCs are characterized by a multitude of values—some of which were noted above. Since, unlike elemental SCs, we do not have an analytic expression for the T_c of a composite SC, we cannot derive for it a “blanket relation” such as $\alpha = 0.5$. The value of α for such SCs is expected to differ from family-to-family and we believe to have indicated how it may be tested; besides, in the best-case scenario, it may prove to be useful in the current endeavor to reach room temperature T_c s.

The applicability of the isotope effect via (1) has been investigated experimentally for the high- T_c SC $YBa_2Cu_3O_7$ by replacing up to 75% of its O-16 by O-18 [4]. Since this did not have any effect on the T_c , it was concluded that $\alpha = 0$ for this SC. We note in this context that scattering with the O ions is not the direct cause of pairing in any SC; what needs to be monitored is the change in T_c when one or more ions that are actually responsible for pairing are substituted. A remark about the vital role of CuO_2 planes in an SC is in order since greater their number, greater is the T_c of the SC. We believe that the dual role of these planes is (a) to meet the stoichiometric requirements for the stability of the SC when new ion layers are added to it to provide additional channels for pairing and (b) to provide additional sites for pairs to reside on.

To conclude, by appealing to an isotope-like effect, we have given here an explanation of the known increase in the T_c s of $Bi_2Sr_2CaCu_2O_8$ and $Bi_2Sr_2Ca_2Cu_3O_{10}$ when Bi and Sr in these are replaced by Tl and Ba, respectively. Based on this approach, we have given plausible values of T_c s of some hypothetical SCs that may be obtained from the parent SCs by one or more substitutions. Fabrication of these hypothetical SCs, e.g., $Tl_2Be_2CaCu_2O_8$ and ensuring that pairing in it occurs predominantly via the Be and the Ca ions (which lead to $T_c = 208$ K), is a problem that belongs to the realm of chemical engineering.

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