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ELECTRON-PHONON INTERACTION IN THE Ba(K)Pb(Bi)O_3 SYSTEM

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We have used the results of band structure calculations to evaluate the electron-phonon coupling and the superconducting transition temperature in the cubic perovskites Ba(K)Pb(Bi)O_3.

1. INTRODUCTION

The discovery of superconductivity[1] in $BaPb_{1-x}Bi_xO_3$ and in $Ba_{1-x}K_xBiO_3$ with maximum transition temperature T_c of 12K and 30K respectively has generated many investigations to explain the mechanism and understand the relationship between these systems and the other high T_c cuprate superconductors. The apparent absence of magnetic order and the large isotope effect in the cubic perovskites has led to a consensus that the pairing mechanism is the conventional electron-phonon interaction. We present here a quantitative evaluation of the parameters responsible for BCS superconductivity.

2. METHOD

We have performed band structure calculations of the cubic perovskites $BaPbO_3$, $BaBiO_3$ and $KBiO_3$ by the augmented plane wave (APW) method. Using the APW results we constructed tight-binding Hamiltonians by an accurate least-squares fit. We then used the coherent potential approximation to study disorder effects on $BaPb_{1-x}Bi_xO_3$ and $Ba_{1-x}K_xBiO_3$. Details of these calculations will be published elsewhere.[2] In this paper we report the evaluation of the electron-phonon coupling. Our approach is to evaluate the McMillan-Hopfield[3] parameter $\eta=\langle I^2\rangle N(E_F)$, where $N(E_F)$ is the density of states at the Fermi level and $\langle I^2\rangle$ is an electron-ion matrix element that we calculate from our band structure results in the rigid muffin-tin approximation (RMTA).[4] We then use the McMillan equation[3] to find the superconducting transition temperature, i.e.

$$T_c = \frac{\langle\omega\rangle}{1.45} \exp\left[-\frac{1.04(1+\lambda)}{\lambda-\mu^*-0.62\lambda\mu^*}\right]$$

where we set the Coulomb pseudopotential $\mu^*=0.1$ and the electron-phonon coupling $\lambda=\frac{1}{\langle\omega^2\rangle}\sum_i(\eta/M)_i$ since the average phonon frequency is not known for these materials we vary $\langle\omega\rangle$ from 200K to 500K.

3. RESULTS

In Fig. 1 we show our results of T_c v $\langle\omega\rangle$ and λ v $\langle\omega\rangle$ corresponding to the RMTA values[2] of η for the ideal cubic $BaBiO_3$ which has the strongest values of η from this family of perovskites. We note that both η and T_c decrease with increasing $\langle\omega\rangle$ and that for $\langle\omega\rangle$ close to 300K we obtain $\lambda\approx1$ and $T_c\approx20$K which is consistent with the experimental values for the $Ba_{1-x}K_xBiO_3$ system.[1]

Since it has been argued[5] that the RMTA seriously underestimates the value of η, we have arbitrarily raised η by a factor of 2. We have repeated our calculation and find that the variation of T_c and λ with $\langle\omega\rangle$ shows a maximum T_c of approximately 37K at $\langle\omega\rangle$=300K and a corresponding λ of 2.1 as is shown in Fig. 2.

So it appears that if the estimate[5] that the value of λ in these materials is indeed higher than the RMTA value, one would obtain T_c in the range of 30K in agreement with experiment.

As an aside we present in Table 1 the values

of η and T_c as a function of $<\omega>$ for values of η 1 to 5 times the RMTA value η_o. It is interesting to note that for the high values of η despite the very large values of λ, T_c doesn't exceed 60K. This observation should not be taken to mean that T_c has reached a limit within the BCS theory. There would still be higher η or $<\omega>$ which could raise T_c not to mention the possibility of lowering the value of μ^*.

In conclusion we find that the electron-phonon interaction is likely to dominate in the pairing of electrons in the cubic perovskites and, therefore, the BCS theory is probably valid for these materials.

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Table I. Variation of λ and T_c with $<\omega>$ for different values of η. η_o is the rigid muffin-tin value for $BaBiO_3$ where η_{Ba}=o, η_{Bi}=0.7eV/A^2 and η_o=2.7eV/A^2

	η_o		$2\eta_o$		$3\eta_o$		$4\eta_o$		$5\eta_o$	
$<\omega>$	λ	T_c	λ	T_c	λ	T_c	λ	T_c	λ	T_c
200	2.4	26	4.8	35	7.2	38	9.6	40	11.9	41
300	1.1	19	2.1	37	3.2	46	4.3	51	5.3	54
400	0.6	7.5	1.2	30	1.8	44	2.4	53	3.0	59
500	0.4	1.4	0.8	18	1.2	35	1.5	48	1.9	58

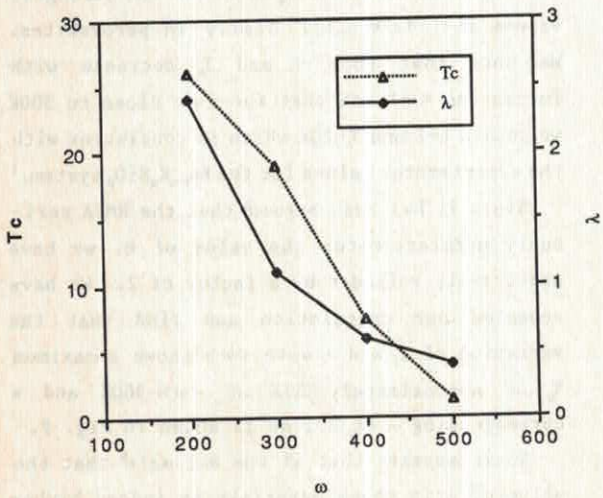

Fig. 1 Variation of T_c and λ for $\eta=\eta_o$.

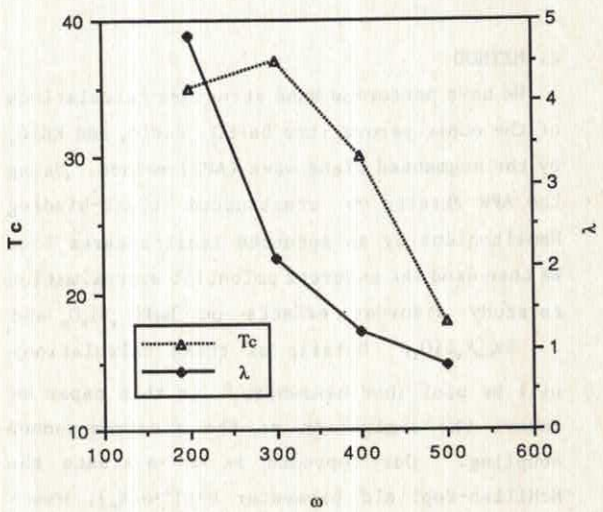

Fig. 2 Variation of T_c and λ for $\eta=2\eta_o$.