ELECTRON–PHONON INTERACTION IN THE Ba(K)Pb(Bi)O₄ 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)O₄.

1. INTRODUCTION

The discovery of superconductivity in BaPbₓBi₂O₅ and in BaₓKBiO₃ 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 BaPbO₄, BaBiO₃ and KBiO₃ 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 BaPbₓBi₂O₅ and BaₓKBiO₃. Details of these calculations will be published elsewhere. In this paper we report the evaluation of the electron-phonon coupling. Our approach is to evaluate the McMillan–Hopfield parameter $\eta = \langle T\rangle N(\varepsilon_F)$, where $N(\varepsilon_F)$ is the density of states at the Fermi level and $\langle T\rangle$ is an electron–ion matrix element that we calculate from our band structure results in the rigid muffin-tin approximation (RMTA). We then use the McMillan equation to find the superconducting transition temperature, i.e.

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

where we set the Coulomb pseudopotential $\mu^\ast = 0.1$ and the electron–phonon coupling $\lambda = \frac{1}{<\omega>} \sum_{\gamma} \frac{1}{n_B} (\eta/M\chi)$ since the average phonon frequency is not known for these materials we vary $<\omega>$ from 200K to 500K.

3. RESULTS

In Fig. 1 we show our results of $T_c$ vs $<\omega>$ and $\lambda$ vs $<\omega>$ corresponding to the RMTA values of $\eta$ for the ideal cubic BaBiO₄ which has the strongest values of $\eta$ from this family of perovskites. We note that both $\eta$ and $T_c$ decrease with increasing $<\omega>$ and that for $<\omega>$ close to 300K we obtain $\lambda = 1$ and $T_c = 20K$ which is consistent with the experimental values for the BaₓKBiO₃ system.

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

So it appears that if the estimate that the value of $\lambda$ 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

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of $\eta$ and $T_c$ as a function of $<\omega>$ for values of $\eta$ 1 to 5 times the RMTO value $\eta_0$. It is interesting to note that for the high values of $\eta$ despite the very large values of $\lambda$, $T_c$ 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 $\eta$ or $<\omega>$ which could raise $T_c$ not to mention the possibility of lowering the value of $\mu^*.$

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.

Table 1. Variation of $\lambda$ and $T_c$ with $<\omega>$ for different values of $\eta$. $\eta_0$ is the rigid muffin-tin value for BaBiO$_3$ where $\eta_{\text{RMT}}=0$, $\eta_{\text{RMT}}=0.7 \text{eV/Å}^2$ and $\eta_{\text{RMT}}=2.7 \text{eV/Å}^2$

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Fig. 1 Variation of $T_c$ and $\lambda$ for $\eta=\eta_0$.

Fig. 2 Variation of $T_c$ and $\lambda$ for $\eta=2\eta_0$.

REFERENCES


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