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Evaluation of the Electron–Phonon Interaction and Transition Temperature in the Oxide Superconductors

D. A. Papaconstantopoulos[1]

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The Allen-Dynes equation applicable to the oxide superconductors is studied, which shows that for moderate values of the electron-phonon coupling constant the superconducting transition temperature is found in the range of 100 K. This result is based on an approximate evaluation of large values of the McMillan-Hopfield parameter and evidence from frozen-phonon calculations that strong ionic character in the copper oxide superconductors invalidates the rigid muffin-tin approximation.

KEY WORDS: oxide superconductors; electron-phonon interaction.

Despite the abundance of publications advocating a variety of mechanisms to understand the high transition temperatures T_c in the oxide superconductors, electron-phonon interaction remains the primary candidate to explain the new phenomena.

In this paper we show that equations derived from the BCS theory can give values of T_c exceeding 100 K with reasonable values of the electron-phonon coupling constant λ. Allen and Dynes [1], starting from the Eliasberg [2] theory, derived the following equation:

$$T_c = f_1 f_2 \frac{\omega_{\log}}{1.2} \exp\left[-\frac{1.04(1+\lambda)}{1-\mu^*(1+0.62\lambda)}\right] \tag{1}$$

where $\omega_{\log}$ is a special average phonon frequency, μ^* is the so-called Coulomb pseudo+potential, λ is the electron-phonon coupling constant, and f_1, f_2 are dimensionless quantities that depend on $\omega_{\log}$, μ^*, and λ. The

[1]Complex Systems Theory Branch, Naval Research Laboratory, Washington, D.C. 20375-5000.

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strongest variation of T_c is due to the parameter λ which is defined as follows:

$$\lambda = \frac{1}{\langle \omega^2 \rangle} \sum_i \frac{\eta_i}{M_i} \tag{2}$$

with

$$\eta = N(E_F) I_i^2 \tag{3}$$

where $\langle \omega^2 \rangle$ is an average phonon frequency, M_i the mass of the ith atom, $N(E_F)$ the density of electronic states at the Fermi level, E_F, and I_i an electron–ion matrix element that, in the rigid muffin-tin approximation (RMTA) [3], is given by the expression

$$I_i^2 = \frac{E_F}{\pi^2 N^2(E_F)} \sum_l 2(l+1) \frac{N_l^i N_{l+1}^i}{N_l^{(1)i} N_{l+1}^{(1)i}} A_{l,l+1}^2 \tag{4}$$

with

$$A_{l,l+1} = \langle R_l | \frac{dV_i}{dr} | R_{l+1} \rangle \tag{5}$$

where R_l is the radial wavefunction of angular momentum l, dV_i/dr represents the change of the crystal potential during the displacement of the atom i, N_l^i are the site angular momentum densities of states at E_F, and $N_l^{(1)i}$ the single scatterer density of states [3].

For ordinary superconductors the matrix element I_i has been evaluated [4–6] accurately using the (RMTA) of Gaspari and Gyorffy [3] which consists of equating dV_i/dr to the gradient of the muffin-tin potential resulting from a self-consistent band structure calculation, that is, assuming a rigid displacement of the potential with the atom. In practice the integral of Eq. (4) becomes

$$A_{l,l+1} = \sin(\delta_l - \delta_{l+1}) \tag{6}$$

where δ_l is the scattering phase shift at E_F. Calculations for the oxide superconductors [7,8] using the RMTA resulted in small values of I_i that might account for $T_c = 30$ K but are inconsistent with the large values of η_i (referred to as the McMillan–Hopfield parameter) and λ needed to obtain the high T_c values of 90–125 K. However, calculations by the potential induced breathing model [9] and recent frozen phonon calculations [10], which are in good agreement with neutron and Raman scattering data, show strong ionic character in these systems which probably invalidates the applicability of the RMTA. At this writing we believe that the RMTA is even qualitatively wrong for these materials and find it possible that an accurate determination of I_i including noncubic corrections [11] and non-RMTA contributions may give values that are much higher than those obtained within the RMTA.

A few years ago Zdetsis *et al.* [12] proposed a theory that corrects for non-RMT effects in simple metals. This theory is based on the idea of adding a potential well to the MT potential with the correct asymptotic behavior of a screened Coulomb potential. This potential has the following form:

$$U_c(r) = U_0\{(r/r_{MT}) \exp[q_{TF}(r - r_{MT})] + 1\}^{-1} \tag{7}$$

where r_{MT} is the muffin-tin sphere radius and q_{TF} is the Thomas–Fermi wave vector. The addition of the potential $U_c(r)$ to the muffin potential $V(r)$ adds a new term to Eq. (6), i.e.,

$$A_{l,l+1} = \sin(\delta_l - \delta_{l+1}) + \int_0^\infty dr\, r^2 R_l \frac{dU_c}{dr} R_{l+1} \tag{8}$$

In the case of Cu this approach gave a value of η larger by almost a factor of 2 than the RMTA value [12]. Since the generalization of this theory to compounds is not straightforward, we have simply applied it to the Cu atom only, using the self-consistent potential of Cu in La_2CuO_4. The result is $\eta_{Cu} = 5.7$ eV/A^2 which is about a factor of 8 larger than the RMTA value [7]. Our expectation is that η for the oxygen sites will be even higher. (Note that the RMTA gives [7,8] $\eta_O \approx 3\eta_{Cu}$.) This is supported by the recent work of Jarlborg [13] who estimates large η from O modes in the $YBa_2Cu_3O_7$ compound.

Using the above evidence that large values of η may be a reality for the CuO superconductors, we proceed with the following analysis. We use Eq. (1) to calculate T_c as a function of λ for a range of η values that starts from the RMTA value and increases to ten times that value. For the evaluation of λ we use Eq. (2) for fixed values of the phonon frequency ω. For μ^* we use 0.1 and note that a factor of 2 reduction of μ^* increases T_c by about 20% while doubling of μ^* would reduce T_c by about 20% in the high-T_c temperature range. Finally, we point out that the prefactors f_1 and f_2 are close to unity for low and average T_c (less than 50 K), but f_2 approaches the value 1.25 for high T_c (~100 K). The results of this study are shown in Fig. 1 which plots T_c vs. λ for different values of ω. One can see from this figure that T_c of 94 K can be attained with λ values of 1.7, 2.4, and 4.4 for $\omega = 690$, 518, and 345 K respectively. The above values of λ that correspond to $T_c \approx 90$ K require values of η approximately 10 times larger than the RMTA values. Considering the ionic character of these materials and the above evaluation of η for the Cu site, we believe that such a large enhancement is possible.

An independent evaluation [14] of λ using the measured temperature derivative of the resistivity and the plasmon energy derived from band structure results in La_2CuO_4 gave $\lambda \approx 3$.

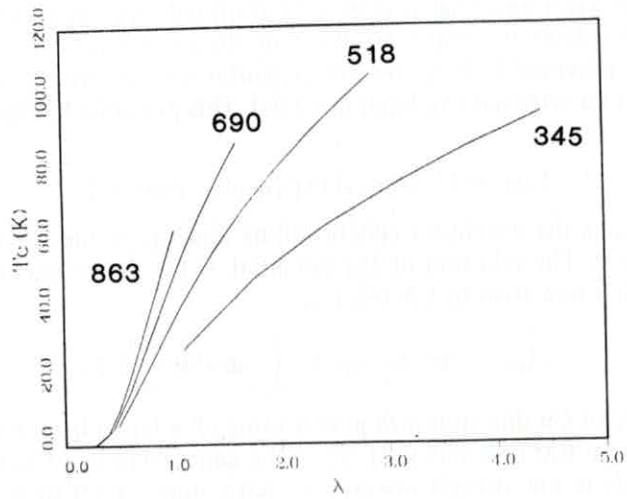

Fig. 1. Calculated superconducting temperature T_c versus the electron–phonon coupling constant λ for average phonon frequencies $\omega = 345$, 518, 690, and 863 K.

In summary, based on estimates of large values of the McMillan–Hopfield parameter η, we have shown that the Allen–Dynes equation would yield a T_c in the range of 100 K for reasonable vibrational frequencies and λ values.

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