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Defects, lattice instabilities, and isotope effects in (Y,Pr)Ba-Cu-O high-temperature superconductors

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The relationship between isotope effects and the micromorphology of $YBa_2Cu_3O_7$ and its alloys is discussed in the context of recent experiments.

The observation[1] of a nearly zero isotope effect in $YBa_2Cu_3O_7$ has led to much speculation concerning nonphonon superconductive mechanisms.[2] Recently I examined[3] a wide range of structural anomalies in $YBa_2Cu_3O_7$ for indications of lattice instabilities. The evidence showed that the micromorphology of $YBa_2Cu_3O_7$ is probably inhomogeneous, and that the inhomogeneities consisted not only of point defects, as in intermetallic compounds such as Nb_3Ge, but also of domain walls, as one typically finds in ferroelectric and ferroelastic oxides. Chemical trends in the vibrational spectra[4] of $Y_{1-y}Pr_yBa_2Cu_3O_7$ and $YBa_2Cu_3O_{7-x}$ are surprisingly parallel, especially as regards the disappearance with increasing x or y of a vibrational band near 55 meV as T_c decreases in both cases. This extra band shows little temperature dependence,[4] is nearly independent of wave vector $\mathbf{k}$, and is resolved[5] only over a narrow range of $\mathbf{k}$, as would be expected for a localized mode associated with a domain wall.

The parallel behavior in structural properties between $Y_{1-y}Pr_yBa_2Cu_3O_7$ and $YBa_2Cu_3O_{7-x}$ suggests that the former alloys are ideal for a controlled study of the isotope shift α ($T_c = \text{const}\, m_O^{-\alpha}$) as a function of T_c. The results[6] obtained by Franck, Jung, and Mohamed are reproduced in Fig. 1 for the reader's convenience. The general trend here is a reduction in α with increasing T_c. As illustrated in Fig. V.3 of the book,[2] this is the general trend that one would expect from "relaxation modes of a large number of internal coordinates which anharmonically stabilize a soft lattice (which would have been dynamically unstable without relaxation)."[7] The purpose of this paper is to make this general statement more explicit in the light of the data now available.[4-6]

The most popular model for anharmonic modes is the double-well model, and the isotope effect for this model in the medium- and strong-coupling limit of the Eliashberg equations has been solved numerically. The solutions clearly show[8] that $\alpha = 0$ is easily obtained by accident, depending on the values of the electron-phonon coupling constant λ and the Coulomb-repulsion parameter μ^*. Clearly values of λ and μ^* can be chosen which reproduce both T_c and α as shown in Fig. 1. The main point to notice, however, is that in all likelihood the micromorphology of $YBa_2Cu_3O_7$ is described by two building blocks, domain interiors (I) and domain walls (II), described by parameters λ_I, μ_I^* and λ_{II}, μ_{II}^*, respectively. On physical grounds we expect $\lambda_I > \lambda_{II}$ and $\mu_{II}^* > \mu_I^*$, because in stabilizing the lattice the domain walls presumably undergo Jahn-Teller distortions which make them more insulating. The bulk T_c and α will then be obtained from these four parameters together with the isotope-dependent domain diameter d and the domain-wall width w, with[3] $w/d \sim 0.1$ in $YBa_2Cu_3O_7$ and $w/d \to 0$ as y increases.

It would clearly be naive to model this multiparameter system numerically. Two points can be made: (1) while $\alpha \to 0$ as $T_c(y)$ increases, this is what one would expect on general grounds,[7] thus this is no reason for discarding[9] electron-phonon interactions as unthinkable, and (2) the smooth linear behavior shown in Fig. 1 is quite reasonable considering the large number of internal parameters and the smooth numerical curves[8] for $\alpha(T_c, \mu^*)$. Note especially that near $\alpha = 0$, $dT_c/d\mu^* \sim 7 dT_c/d\lambda$, so that thin domain walls with small Coulomb screening and large μ^* can have large effects on T_c.

If the structure of $YBa_2Cu_3O_7$ is described by two building blocks, then other rare-earth compounds R-Ba-Cu-O with $T_c \sim 90$ K should have similar micromorphologies. Inhomogeneous micromorphologies[3] explain not only the composition dependence of the isotope shift α but

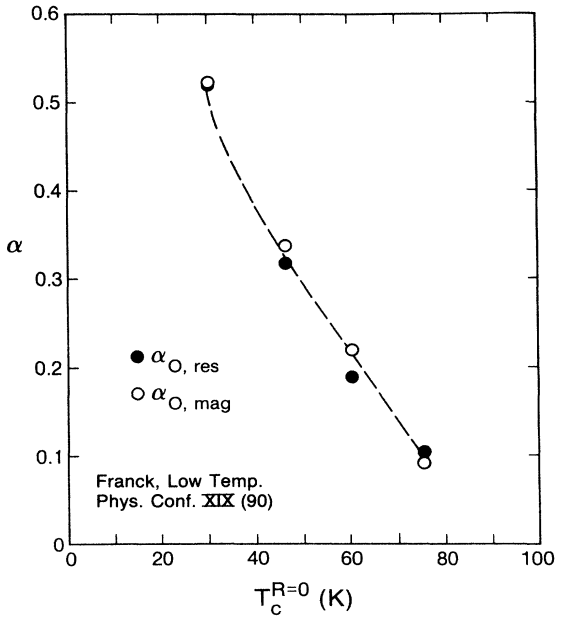

FIG. 1. The isotope exponent α_O, for oxygen replacement $^{16}O \to {}^{18}O$, as a function of T_c in $Y_{1-y}Pr_yBa_2Cu_3O_7$ alloys, from Ref. 6, reproduced here by permission of the authors and publisher for the reader's convenience.

also the anomalous temperature-dependent broadening $\Delta\gamma$ of phonon modes measured by Raman scattering.[10] The strength of this broadening varies with rare-earth (R) radius and with oxygen isotopic mass (partial exchange) m_O, but it is questionable whether this variation can be used to determine $E_g = 2\Delta$ with an accuracy of 2%, as has recently been claimed.[11] To obtain $2\Delta = 316(6)$ cm^{-1} it was necessary to estimate $\Delta\gamma \lesssim 2$ cm^{-1} from data where γ itself is uncertain to ~ 2 cm^{-1}. To map both $\gamma(B_{1g})$ and $\gamma(A_g)$ onto a single curve derived from strong-coupling theory with a single gap parameter, 2Δ requires using[11] electron-phonon coupling parameters λ_t calculated theoretically from an ideal-crystal model which neglects the 6% apical oxygen vacancies found in high-precision x-ray studies of an untwinned $YBa_2Cu_3O_7$ sample.[12] Finally, the value of Δ obtained differs by 40% from the values obtained directly by Raman scattering[13] and by optical reflectivity from untwinned samples.[14] It is possible, however, that the smaller gap inferred from $\Delta\gamma(\omega)$ is associated with one of the two building blocks, probably the disordered domain walls, where the apical oxygen vacancies could be concentrated, while the larger gap observed directly is associated with domain interiors. One would expect that the smaller domain-wall gap could agree with one observed in some tunneling experiments,[15] because the disordered domain walls form a connected network.

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