Simple model for the Hall effect in $YBa_2Cu_3O_{7-\delta}$

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The strong temperature dependence of the Hall effect in $YBa_2Cu_3O_{7-\delta}$ can be understood in terms of a two-band model, with holes on the planes virtually identical to those of $La_{1.85}Sr_{0.15}CuO_4$, and (highly anisotropic) electrons on the chains.

The two families of high-T_c superconductors, represented by $La_{2-x}Sr_xCuO_4$ (La-Sr-Cu-O)[1] and $YBa_2Cu_3O_{7-\delta}$ (Y-Ba-Cu-O)[2] share very similar planes of CuO_2. Given the strongly two-dimensional (2D) nature of conduction in these materials, it is very tempting to assume that the electronic properties of the planes are also very similar and to speculate that they may be responsible for the high values of T_c.[3] Band-structure calculations confirm their very similar form, and both share the same highly unusual form of normal-state resistivity.

However, the Hall effect in the two materials is extremely different. While La-Sr-Cu-O shows only a weak temperature dependence, the temperature dependence of the Hall coefficient R_H in Y-Ba-Cu-O is very strong[4,5] with R_H approximately linear in T. There is an extremely simple explanation for this striking difference, and the purpose of this report is to show that the simple idea works—that it can provide a consistent model of the data.

The strong T dependence naturally suggests a two-band model for conduction in Y-Ba-Cu-O. I propose that the holes arise from the CuO_2 planes, and are very similar to the holes in La-Sr-Cu-O, while the carriers in the Cu-O chains are electrons. This assignment is consistent with the band-structure calculations of Whangbo, Evain, Beno, and Williams.[6] The transport properties of the separate bands would then be given by a two-band model

$$\sigma=\sigma_h+\sigma_e\,, \tag{1}$$

$$R_H\sigma^2=R_{Hh}\sigma_h^2+R_{He}\sigma_e^2\,, \tag{2}$$

with σ_i and R_{Hi} being the contributions to the conductivity and Hall coefficient due to the ith carriers, $i=e,h$. In comparing the values for Y-Ba-Cu-O and La-Sr-Cu-O, account must be taken of the fact that the unit cells in these materials have very different volumes, V_0. Since R_H should scale with V_0, the normalized hole density $\hat{n}=V_0/eR_H$ would be expected to be the same in both materials. The proper scaling for $\sigma=ne^2\tau/m$ is less obvious. If the scattering of the holes is dominated by carrier-carrier scattering,[7] then $\tau^{-1}=n\phi$, where ϕ is a phase-space factor. For a three-dimensional system $\phi\approx(k_BT/E_F)^2$. However, in the CuO_2 planes, the Fermi level is believed to be pinned near the van Hove singularity,[3,6] so ϕ would be a function only of k_BT/t_0, where t_0 is the 2D bandwidth. In this case, σ would be nearly independent of V_0.

To test this idea, I analyze the magnetotransport data using Eqs. (1) and (2). While all of the experimental data[4,5] are qualitatively similar, it is convenient to use the data of Penney, Shafer, Olson, and Plaskett[4] since both ρ and R_H are presented for both compounds studied. In the analysis, I assume that $\hat{n}_e$ is T independent, and $\sigma_h=\alpha\sigma$ (La-Sr-Cu-O) and adjust $\hat{n}_e$ and α until $\hat{n}_h$ most nearly resembles $\hat{n}$(La-Sr-Cu-O). The smallest value of $|\hat{n}_e|$ which gives reasonable agreement is $\hat{n}_e=-0.4$, somewhat larger than might have been expected from Whangbo *et al.*[6] The reason for this large value can be seen from Eq. (2). Since $\sigma_e\sim\sigma_h$, the sign of R_H is determined by the carriers with *lower* concentration. As expected, the value of α is close to one, $\alpha=0.9$. The resulting parameters are shown in Fig. 1.

The real test of this model will come from direct Fermi-surface measurements. Positron annihilation studies are probably simplest, as being relatively insensitive to disorder (a model for the hole Fermi surfaces is given in Ref. 8). Recently, several workers[9–11] have reported Fermi-surface measurements using this technique. Unfortunately, there is very little agreement between them, and it would be premature to place much confidence in any of the results. Nevertheless, it is interesting to note that the Fermi surfaces found by Peter and co-workers[10] agree closely with the predictions of Whangbo *et al.*,[6] including the observation of an elongated electronlike surface. Indirect checks of this two-band model can come from testing its predictions on other transport properties—thermoelectric power, thermal conductivity, etc. Should untwinned single crystals become available, mag-

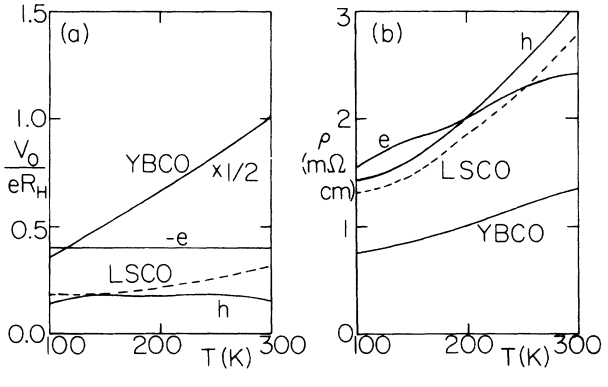

Fig. 1. Hall coefficient (a) and resistivity (b) vs temperature for Y-Ba-Cu-O (solid line) and La-Sr-Cu-O (dashed line); data of Ref. 4. Lines labeled e and h show proposed two-band decomposition of the Y-Ba-Cu-O data.

netotransport measurements on these would provide further tests of the model.

Should the model proposed herein prove correct, it will shed some light on present band-structure calculations of Y-Ba-Cu-O. All calculations[6,12-14] agree that the Fermi-surface sections associated with the CuO_2 planes are holelike, while the CuO chains contribute carriers near the bottom of a nearly empty band, which are thus electronlike. However, most calculations find that the corresponding Fermi surface is *open* along the *a* axis, and, hence, should not contribute to the Hall effect. In contrast, the calculation of Whangbo *et al.* finds that interlayer coupling leads to a closed electronlike Fermi surface for the chains.

Traditional band-structure calculations are known to have difficulty describing transition-metal oxides. In particular, the closely related compound La_2CuO_4 is known to be insulating, but is predicted to be metallic. This is believed to be a failing of the local density approximation, due to the rapid density variation in these materials.[15] It has been suggested[16] that a remedy for this defect might be to perform a layer calculation—representing the material as alternating strips having high and low electronic density, and carrying out local density calculations in the high-density layers. Such an approach has proven highly successful in graphite intercalation compounds, which are considerably more two dimensional.[17] This might explain the success of Whangbo *et al.*[6] at reproducing the closed electron Fermi surface, since their calculation is based on the slab containing just two planes and one chain layer.

Finally, the T dependence of R_H in La-Sr-Cu-O suggests that this material may be a multiband conductor. From the form of Eqs. (1) and (2) it can be seen that this complication does not modify the present analysis. The terms labeled ρ_h and R_{Hh} are characteristic of the CuO_2 layers, but could be due to one or several groups of carriers.

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