PHYSICAL REVIEW B VOLUME 47, NUMBER 18 1 MAY 1993-II

Temperature dependences of the resistivity and Hall coefficient of untwinned single-crystal $YBa_2Cu_3O_{7-\delta}$ at constant volume

D. M. Ginsberg, W. C. Lee, and S. E. Stupp*
Department of Physics and Materials Research Laboratory, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801
(Received 21 January 1993)

The previously published constant-pressure temperature dependences of the resistivity eigenvalues and Hall coefficient of untwinned single-crystal $YBa_2Cu_3O_{7-\delta}$ are used, together with the coefficient of expansion and the compressibility, to calculate the constant-volume temperature dependences of these transport coefficients, since the constant-volume values are the quantities that have been predicted by theories of high-temperature superconductivity. It is found that the in-plane resistivity eigenvalues at constant volume are slightly lower and more nearly linear in the temperature than at constant pressure. The c-axis resistivity at constant volume is also slightly lower than at constant pressure, and approximately as linear. G_H, the reciprocal of the Hall coefficient R_H, at constant volume is slightly higher and just as nearly linear in the temperature as at constant pressure. The cotangent of the Hall angle, as a function of T^2, is essentially the same at constant pressure as at constant volume, and remains linear in T^2.

I. INTRODUCTION

Many of the normal-state properties of high-temperature superconductors are qualitatively different from those of ordinary materials. It is widely believed that an understanding of these unusual normal-state properties will be of great importance in the development of a complete microscopic theory of high-temperature superconductivity. We concentrate here on electrical transport properties, and focus the discussion on the electrical resistivity[1] ρ and the Hall coefficient[2] R_H. In the high-temperature superconductors, ρ varies linearly or nearly linearly over a wide range of temperatures. R_H is also very unusual in these materials, varying approximately as $1/T$ over a wide temperature range. In other words, the reciprocal Hall coefficient, $G_H \equiv 1/R_H$, is linear in T.

The linear temperature dependences of ρ and G_H that we discuss here are followed particularly precisely for untwinned single-crystal $YBa_2Cu_3O_{7-\delta}$ with $\delta \cong 0.1$ and $T_c \cong 90$ K.[3,4] This compound has been carefully investigated by various groups because it can be prepared in the form of very pure, single-phase, untwinned, single crystals with no appreciable antisite disorder and with excellent morphology showing no visible stacking faults.[5,6] We therefore devote our discussion to electrical transport in this compound.

The published temperature dependences of ρ and G_H were measured at a constant pressure p_0, equal to either zero or one atmosphere.[3,4] (These two pressures would give indistinguishable results.) The crystal expands beyond its initial volume V_0 as it is heated from the initial temperature T_0 to obtain the temperature dependence of ρ or G_H. On the other hand, the theoretical expressions for the temperature dependences of these parameters are calculated for a sample at constant volume. It is therefore useful to calculate the predicted constant-volume parameters $\rho(V_0,T)$ and $G_H(V_0,T)$ and their temperature derivatives from the measured constant-pressure parameters $\rho(p_0,T)$ and $G_H(p_0,T)$. We show how to make these transformations and determine whether the temperature dependences are changed appreciably by them.

It should be noted that we correct only for the volume expansion of the sample, not for its change of shape, which would be a result of the anisotropy of the thermal expansion coefficient[7] and compressibility.[8] The shape correction cannot be made at this time, since the resistivity and Hall coefficient have not been measured yet for a sampler under uniaxial pressure in the three directions. Since both the thermal expansion coefficient and the compressibility are roughly twice as high in the c direction as in the a and b directions, the change in shape is roughly, but not exactly , taken into account. Because $YBa_2Cu_3O_{7-\delta}$ is orthorhombic, the resistivity is anisotropic. In our discussion, "resistivity" refers to any of the three eigenvalues of the resistivity tensor, ρ_a, ρ_b (for current in the Cu-O chain direction), and ρ_c (for current perpendicular to the Cu-O planes). The Hall coefficient referred to here is measured with the magnetic field in the c direction.

II. METHOD

The transformations of ρ and G_H are done the same way, so we will discuss the calculation as being carried out on any state function $f(p,V,T)$. Standard thermodynamic analysis[9] shows that

$$\left[\frac{\partial f}{\partial T}\right]_V = \left[\frac{\partial f}{\partial T}\right]_p + \left[\frac{\partial f}{\partial p}\right]_T \left[\frac{\partial p}{\partial T}\right]_V . \tag{1}$$

Furthermore, one has available the usual relation[9]

$$\left[\frac{\partial p}{\partial T}\right]_V = \frac{-(\partial V/\partial T)_p}{(\partial V/\partial p)_T} = \frac{\alpha}{\kappa_T} \, , \tag{2}$$

where α is the volume thermal expansion coefficient (the sum of the three linear expansion coefficients) and κ_T is the compressibility:

$$\alpha \equiv \frac{1}{V}\left[\frac{\partial V}{\partial T}\right]_p \tag{3}$$

and

$$\kappa_T \equiv \frac{-1}{V}\left[\frac{\partial V}{\partial p}\right]_T \, . \tag{4}$$

Thus,

$$\left[\frac{\partial \rho}{\partial T}\right]_V = \left[\frac{\partial \rho}{\partial T}\right]_p + \left[\frac{\partial \rho}{\partial p}\right]_T \left[\frac{\alpha}{\kappa_T}\right] \tag{5}$$

and

$$\left[\frac{\partial G_H}{\partial T}\right]_V = \left[\frac{\partial G_H}{\partial T}\right]_p + \left[\frac{\partial G_H}{\partial p}\right]_T \left[\frac{\alpha}{\kappa_T}\right] \, . \tag{6}$$

Equations (5) and (6) can be used to find the constant-volume temperature derivatives that are predicted by theories. One may, on the other hand, wish to find the constant-volume functions $\rho(V_0,T)$ and $G_H(V_0,T)$ themselves. We use a "thought experiment" to do this as follows. We could heat the crystal at constant volume from (V_0,T_0) to (V_0,T_1), causing f to change by an amount

$$\Delta f = \int_{T_0}^{T_1}\left[\frac{\partial f}{\partial T}\right]_{V=V_0} dT \, . \tag{7}$$

On the other hand, we could accomplish the same process in two steps by heating the crystal at constant pressure from (p_0,T_0) to (p_0,T_1) and then squeezing it down to its original volume V_0 at constant temperature T_1. The first of these steps would change f by an amount

$$(\Delta f)_1 = \int_{T_0}^{T_1}\left[\frac{\partial f}{\partial T}\right]_{p=p_0} dT \, . \tag{8}$$

During this step, the crystal would expand to a new value V_1 given by

$$V_1 = V_0 \exp\left[\int_{T_0}^{T_1}\alpha(p_0,T)dT\right] \, . \tag{9}$$

Bringing the volume back to V_0 would require the application of a pressure p given by

$$\begin{aligned} p &= p_0 + \int_{V_1}^{V_0}\left[\frac{\partial p}{\partial V}\right]_{T=T_1} dV \\ &= p_0 + \int_{V_0}^{V_1}\frac{1}{\kappa_T(T_1)V} dV \, , \end{aligned} \tag{10}$$

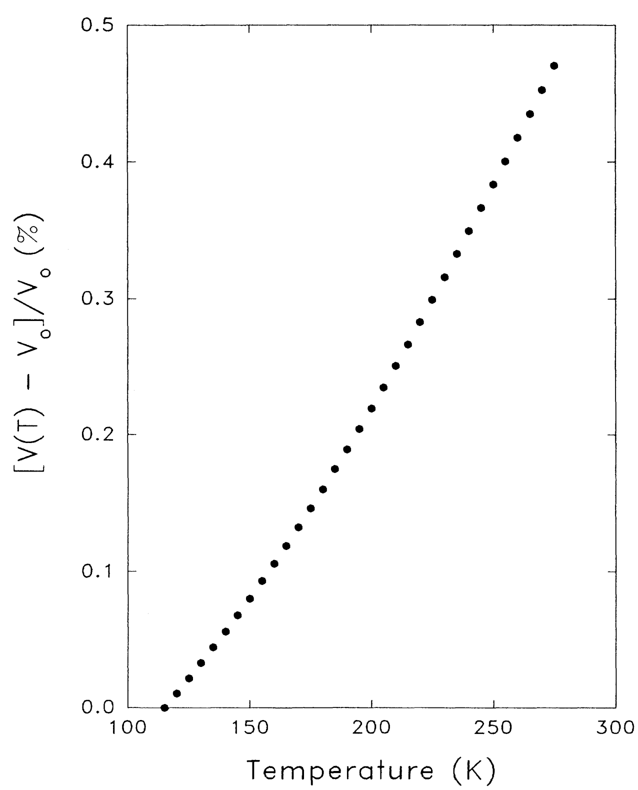

FIG. 1. Percentage volume change on heating a crystal of $YBa_2Cu_3O_{7-\delta}$ up from 115 K to temperature T.

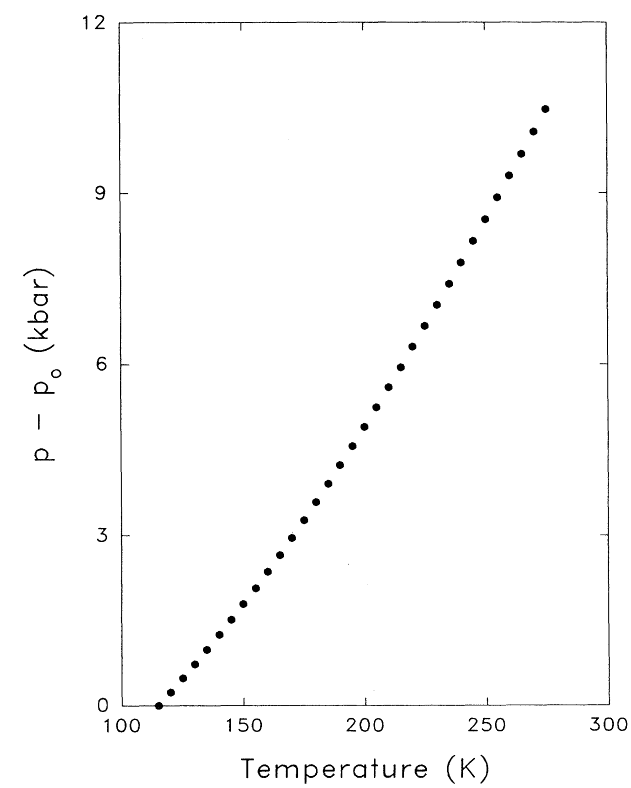

FIG. 2. Pressure that would be required to bring the volume of the crystal back to its value at 115 K, after heating it to temperature T.

changing f by an amount

$$(\Delta f)_2=\int_{p_0}^{p}\left[\frac{\partial f}{\partial p}\right]_{T=T_1}dp \ . \tag{11}$$

Thus, equating Δf given by Eq. (7) to $\Delta f_1+\Delta f_2$, and noting that

$$f(V_0,T_0)=f(p_0,T_0) \ , \tag{12}$$

we obtain the desired relations:

$$\rho(V_0,T_1)=\rho(p_0,T_1)+\int_{p_0}^{p}\left[\frac{\partial \rho}{\partial p}\right]_{T=T_1}dp \tag{13}$$

and

$$G_H(V_0,T_1)=G_H(p_0,T_1)+\int_{p_0}^{p}\left[\frac{\partial G_H}{\partial p}\right]_{T=T_1}dp \ , \tag{14}$$

where p is given by Eq. (10). For $YBa_2Cu_3O_{7-\delta}$ in the pressure and temperature ranges we are considering, κ_T is independent of p,[10] and therefore of V, so

$$p=p_0+\frac{1}{k_T(T_1)}\ln\left[\frac{V_1}{V_0}\right]=p_0+\frac{1}{\kappa_T(T_1)}\int_{T_0}^{T_1}\alpha(p_0,T)dT \ . \tag{15}$$

III. RESULTS

In calculating $\rho(V_0,T)$ and $G_H(V_0,T)$ and their temperature derivatives, we take data for $\rho(p_0,T)$, $(\partial\rho/\partial p)_T$, α, κ_T, $G_H(p_0,T)$, and $(\partial G_H/\partial p)_T$ from the literature (Refs. 3, 11, 12, 10, 4, and 13, respectively). For the reference temperature, we take $T_0=115$ K, the lowest temperature at which data for ρ and the pressure dependence of G_H are available.

At 200 K, for example, the compressibility of $YBa_2Cu_3O_{7-\delta}$ is 4.48×10^{-4}/kbar and the thermal expansion coefficient α is 3.07×10^{-5}/K, so Eqs. (5) and (6) indicate that the constant-volume derivatives of ρ and G_H are different from the constant-pressure derivatives by -4.88×10^{-2} $\mu\Omega$ cm/K $(=-11\%)$ and 9250 T/Ω cm/K $(=15\%)$, respectively, at that temperature. (It should be noted that the compressibility of $YBa_2Cu_3O_{7-\delta}$ has been measured not only by Feitz *et al.*,[10] providing the temperature-dependent values that we have used in our calculation, but at room temperature by Olsen *et al.*[14] and by Jorgensen *et al.*[8] These two groups obtained values of κ_T which were greater than the room-temperature result obtained by Feitz *et al.* by 31 and 45%, respectively.)

Figure 1 shows the percentage change in the volume of a $YBa_2Cu_3O_{7-\delta}$ crystal as it is heated up above 115 K, calculated from Eq. (9). Figure 2 shows the pressure that

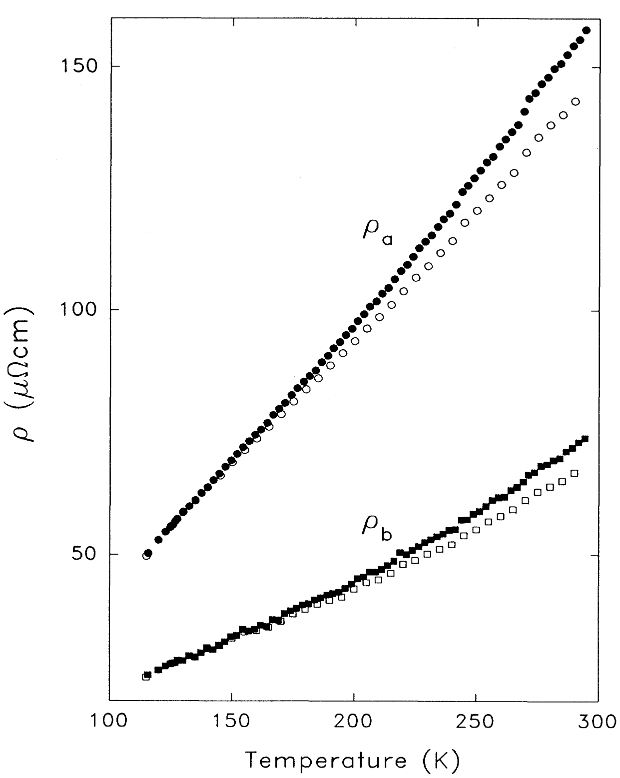

FIG. 3. Constant-pressure (filled circles and squares) and constant-volume (open circles and squares) values of the electrical resistivity in the a direction and the b (Cu-O chain) direction.

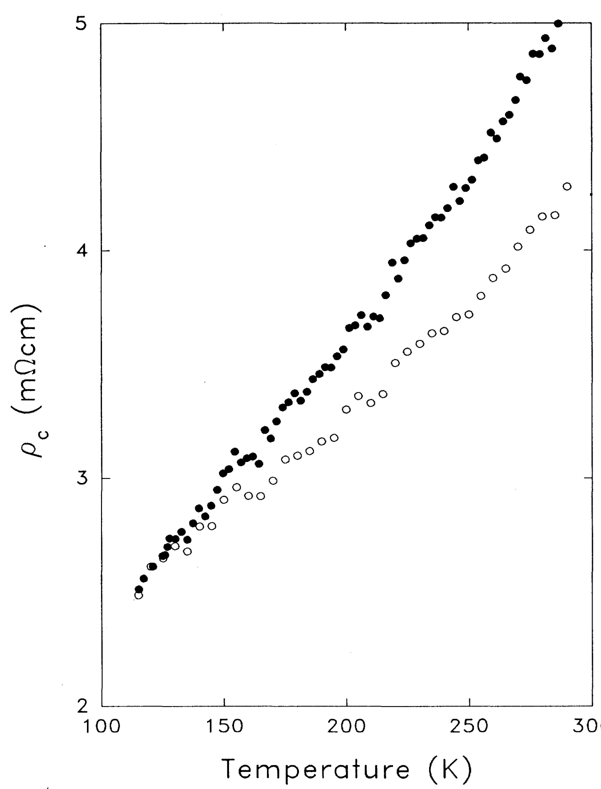

FIG. 4. Constant-pressure (filled circles) and constant-volume (open circles) values of the electrical resistivity in the c direction.

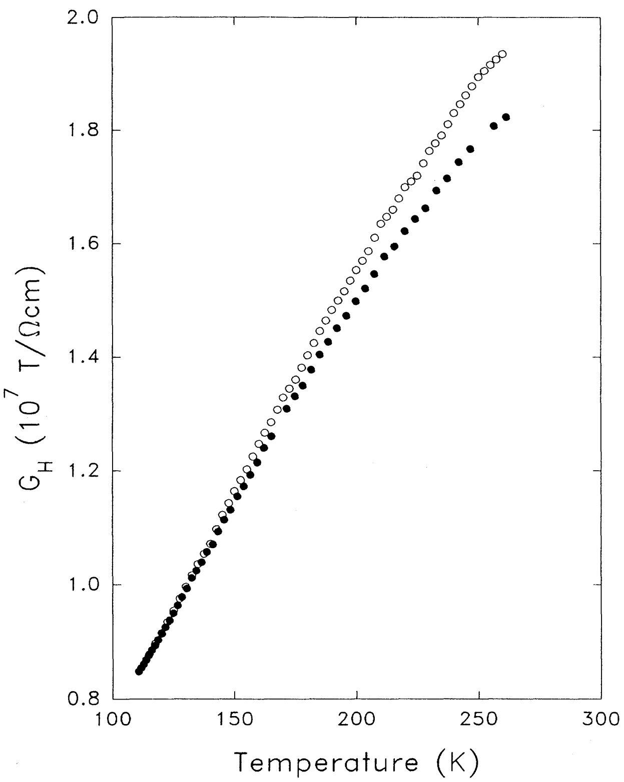

FIG. 5. Constant-pressure (filled circles) and constant-volume (open circles) values of G_H, the reciprocal of the Hall constant R_H with the magnetic field oriented in the c direction.

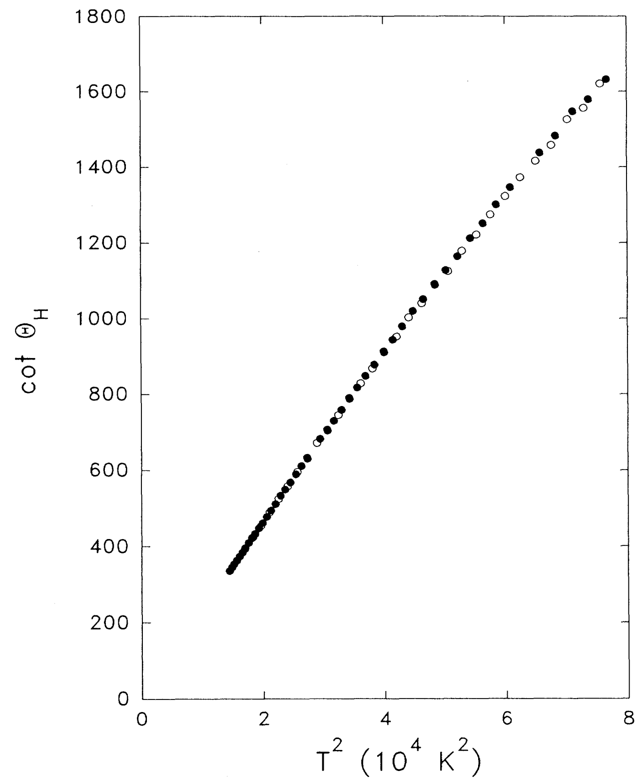

FIG. 6. Constant-pressure (filled circles) and constant-volume (open circles) values of the cotangent of the Hall angle, with the magnetic field oriented in the c direction.

would be necessary to bring the crystal back to its initial volume, from Eq. (10). The figure shows that our analysis involves pressures up to 12 kbar.

Figures 3–5 show the constant-pressure (filled symbols) and constant-volume (open symbols) temperature dependences of ρ_a, ρ_b, ρ_c, and G_H. (For ρ_a, ρ_b, and ρ_c, the data for sample A in Ref. 3 were analyzed; those for sample B would yield nearly identical results.) These figures show that the temperature derivatives of the constant-volume resistivities and G_H at 200 K are different from those of the constant-pressure functions by about -11 and 15%, respectively, confirming the results we obtained above. (Our resistivity results are slightly different from those of Sundqvist and Andersson;[15] they analyzed in-plane resistivity data only, obtained for a twinned sample having a resistivity two to four times higher than the data analyzed here, and they corrected the data only to first order in the thermal expansion.)

In Fig. 6, similar results are shown for the cotangent of the Hall angle Θ_H, which equals ρ_b/ρ_{ab}. The figure shows that the correction for the effect of volume expansion on ρ_b almost exactly cancels that on ρ_{ab}, leaving $\cot(\Theta_H)$ unchanged.

In summary, the constant-volume resistivity eigenvalues are slightly lower than the constant-pressure values. The constant-volume values of ρ_a and ρ_b are more nearly linear functions of T than the constant-pressure values. For ρ_c, the scatter in the data makes the nonlinearity difficult to discern, but it is approximately unchanged. For the reciprocal Hall coefficient G_H, the constant-volume values are slightly higher than the constant-pressure values, and about as linear in T. The cotangent of the Hall angle is nearly the same at constant volume as at constant pressure.

ACKNOWLEDGMENTS

This research was supported in part by National Science Foundation Grants No. DMR 89-20538 (SES) and by DMR 91-20000 through the Science and Technology Center for Superconductivity (DMG and WCL).

*Present address: Philips Research, P.O. Box 80.000, 5600 JA, Eindhoven, The Netherlands.

[1] Y. Iye, in *Physical Properties of High Temperature Superconductors,* edited by D. M. Ginsberg (World Scientific, Singapore, 1992), Vol. 3, Chap. 4, p. 285.

[2] N. P. Ong, in *Physical Properties of High Temperature Superconductors,* edited by D. M. Ginsberg (World Scientific, Singapore, 1990), Vol. 2, Chap. 7, p. 459.

[3]T. A. Friedmann, M. W. Rabin, J. Giapintzakis, J. P. Rice, and D. M. Ginsberg, Phys. Rev. B **42**, 6217 (1990).

[4]J. P. Rice, J. Giapintzakis, D. M. Ginsberg, and J. M. Mochel, Phys. Rev. B **44**, 10 158 (1991).

[5]J. P. Rice and D. M. Ginsberg, J. Cryst. Growth **109**, 432 (1991).

[6]J. P. Rice, D. M. Ginsberg, M. W. Rabin, K. G. Vandervoort, G. W. Crabtree, and H. Claus, Phys. Rev. B **41**, 6532 (1990).

[7]C. Meingast, O. Kraut, T. Wolf, and H. Wühl, Phys. Rev. Lett. **67**, 1634 (1991).

[8]J. D. Jorgensen, S. Pei, P. Lightfoot, D. G. Hinks, B. W. Veal, B. Dabrowski, A. B. Paulikas, and R. Kleb, Physica C **171**, 93 (1990).

[9]F. Reif, *Fundamentals of Statistical and Thermal Physics* (McGraw-Hill, New York, 1965), pp. 167 and 168.

[10]W. H. Feitz, M. R. Dietrich, and J. Ecke, Z. Phys. B **69**, 17 (1987).

[11]V. Ilakovac, L. Forro, C. Ayache, and J. Y. Henry, Phys. Lett. **161**, 314 (1991).

[12]C. Meingast, B. Blank, H. Bürkle, B. Obst, T. Wolf, H. Wühl, V. Selvamanickam, and K. Salama, Phys. Rev. B **41**, 11 299 (1990).

[13]C. Murayama, Y. Iye, T. Enomoto, A. Fukushima, N. Mori, Y. Yamada, and T. Matsumoto, Physica C **185-189**, 1293 (1991).

[14]J. S. Olsen, S. Steenstrup, K. Johannsen, and L. Gerward, Z. Phys. B **72**, 165 (1988).

[15]B. Sundqvist and B. M. Andersson, Solid State Commun. **76**, 1019 (1990).