Competition between oxygen reordering and internal strain for the pressure effect of the Hall coefficient in $Y_{1-x}Ca_xBa_2Cu_3O_y$

T. Honma and M. Tanimoto

Department of Physics, Asahikawa Medical College, Midorigaoka-Higashi 2-1-1-1, Asahikawa 078-8502, Japan

N. Môri

Institute for Solid State Physics, University of Tokyo, Kashiwanoha 5-1-5, Kashiwa 277-8581, Japan

The pressure effect on the Hall coefficient R_H has been studied in Ca and oxygen co-doped $Y_{1-x}Ca_xBa_2Cu_3O_y$ systems. R_H is not altered by pressure in samples without a Cu-O chain, whereas samples with an oxygen-deficient chain are altered in response to pressure, thus demonstrating the contribution of the oxygen reordering effect. However, even in samples with full chain ordering, R_H changes at a rate of -8.3%/GPa. This suggests the contribution of internal strain due to the presence of a Cu-O chain structure. We independently estimated the effect of two factors, oxygen reordering and internal strain, on the pressure effect on R_H. The oxygen-content dependence of the pressure effect on R_H can be explained by competition between oxygen reordering and internal strain.

Superconducting transition temperature T_c vs hole concentration, induced by cation and/or anion doping, exhibits a well-known bell-shaped dependence. The pressure coefficient of T_c, dT_c/dP, is positive in underdoped samples and negative in overdoped samples.[1] The driving force associated with high pressure is expected to be a pressure-induced change in hole concentration. In most high-T_c systems, the Hall coefficient R_H changes at a rate of $\sim -10\%$/GPa.[2] At ambient pressure, the Hall number $N_H \equiv 1/eR_H$ dependence of T_c, $T_c(N_H)$, has the same bell-shaped dependence as the T_c vs hole concentration plot. Under high pressure, dT_c/dP vs dN_H/dP has been shown to be qualitatively consistent with the expected increase in T_c due to the pressure-induced change in carrier concentration in $YBa_2Cu_3O_y$ (Y123) and $YBa_2Cu_4O_8$ (Y124).[2] This indicates that for these systems, the pressure effect on T_c can be qualitatively understood by a simple charge-transfer model.[2–4] An exception is $La_{2-x}Sr_xCuO_4$ (LS214), where dT_c/dP is positive even in overdoped samples and $d(\ln R_H)/dP$ is $\sim 0\%$/GPa in both under- and overdoped samples.[5]

However, in $Y_{0.9}Ca_{0.1}Ba_2Cu_3O_y$, we found that the change in T_c in response to pressure is greater than that expected from the simple charge-transfer model in the sample with $y \geq 6.72$, while for the sample with $y < 6.72$ it is consistent with the charge-transfer model.[6,7] Further, in $Y_{1-x}Ca_xBa_2Cu_4O_8$ (YC124) the maximum T_c observed under high pressure is greater than that observed by Ca doping.[1,8] Recently, the T_c of a Y123 sample ($y=6.66$) with an initial $T_c=64.1$ K was observed to be over 100 K at 17 GPa with no sign of saturation in response to a further increase in pressure.[9] In this system, the maximum T_c never goes beyond 95 K by the oxygen and/or Ca doping.[10,11] These results cannot be explained by the simple charge-transfer model.[6]

$Y_{1-x}Ca_xBa_2Cu_3O_y$ (YC123) and YC124 have the same basic structure except that the charge reservoir for YC123 is a single Cu-O chain, whereas that for YC124 is a Cu-O

double chain. In oxygen-deficient YC123, incomplete chain ordering allows for a dramatic pressure-induced oxygen reordering effect manifested as a huge pressure increase in T_c around $y=6.72$ in Y123 (Ref. 12) and pressure-induced superconductivity in $NdBa_2Cu_3O_{6.67}$.[13] Recently, in Y123 with perfect chain ordering ($y=7$), the importance of internal strain due to the presence of a Cu-O chain was proposed as a way to explain the uniaxial pressure effect on T_c.[14] The pressure effect on T_c appears to be due to two contributing factors: interplane charge transfer through oxygen reordering and intraplane charge rearrangements induced by internal strain.

We have studied the pressure effect on R_H in Ca and oxygen co-doped $Y_{1-x}Ca_xBa_2Cu_3O_6$ ($0.15 \leq x \leq 0.2$) and $Y_{0.9}Ca_{0.1}Ba_2Cu_3O_y$ ($6.59 \leq y \leq 7$). The pressure effect on R_H can be explained by competition between oxygen reordering in the Cu-O chain site and internal strain due to the presence of a Cu-O chain structure.

YC123 samples were prepared by causing a solid-state reaction in a proportioned mixture of Y_2O_3 (5N), $CaCO_3$ (5N), $BaCO_3$ (5N), and CuO (4N). These powders were ground, pressed, and fired in flowing O_2 at 900 °C for 6 h. This process was repeated several times. For the final firing, pellets of the powder were fired for 10–15 h in flowing O_2 at 930–940 °C, and then were annealed in flowing O_2 at an appropriate temperature or in flowing Ar at 750 °C. Samples with $y=7$ or 6 were prepared by furnace cooling of the samples in flowing O_2 or Ar, respectively. All other samples were prepared by quenching to 77 K after the annealing process. The oxygen content y was determined using an iodometric titration technique. Samples with $x \leq 0.2$ and $6 \leq y \leq 7$ were identified as single phase by examining the x-ray powder-diffraction pattern. The density of these samples was somewhat above 80% of the ideal density. The typical sample size was $4 \times 1.5 \times 0.1$ mm^3. Hall voltage V_H measurements were conducted by rotating the sample 360° (240°) in a magnetic field of 7 T (4 T) under ambient (high)
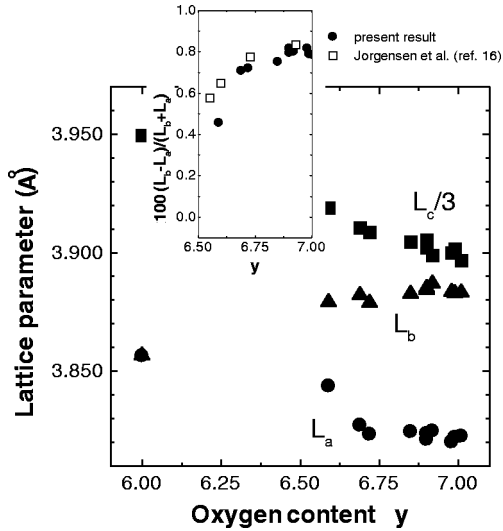
FIG. 1. Lattice parameter for a, b, and c axes L_a, L_b, and $L_c/3$ as a function of oxygen content y in $Y_{0.9}Ca_{0.1}Ba_2Cu_3O_y$. The inset shows orthrombicity $(L_b-L_a)/(L_b+L_a)\times100$ as a function of y. The closed circle and open diamond show the present result and the reported result, respectively, in Y123 of Ref. 16.

pressure. The R_H was determined by fitting the angle dependence of V_H to a sine curve within the scatter of 5% at fixed temperature. At some temperatures, the V_H was confirmed to be linear in the current and magnetic fields. Measurements under high pressure were performed using a Swenson-type piston-cylinder apparatus under a superconducting magnetic field up to 4 T.[1] All other details of the R_H measurement were as described previously.[6,15]

Figure 1 shows the a-, b-, and c-axis lattice parameters L_a, L_b, and $L_c/3$ as a function of y in $Y_{0.9}Ca_{0.1}Ba_2Cu_3O_y$. L_a and L_b at $y=6.92$ were 3.825 and 3.887 Å, respectively. These values were almost equivalent to L_a (3.823 Å) and L_b (3.887 Å) in the Y123 sample ($y=6.93$) with the Cu-O chain structure.[16] The L_a and L_b remained almost unchanged when y was varied above $y=6.72$. Thus, the samples prepared here were shown to have a Cu-O chain structure above $y=6.72$. The degree of chain ordering can be estimated by the orthrombicity. Orthrombicity $(L_b-L_a)/(L_b+L_a)\times100$, which is shown as a function of y in the inset of Fig. 1, decreased in a linear fashion when y was reduced from $y=7$ and decreased rapidly below $y=6.72$, indicating a break in the Cu-O chain structure. The orthrombicity of the sample was almost identical to the reported value in Y123.[16] The formation of chain ordering was not found to be influenced by the Ca doping until $x=0.1$.

Figure 2 shows the Hall coefficient R_H vs T curve in $Y_{0.9}Ca_{0.1}Ba_2Cu_3O_y$ with $y\geq6.72$ under high pressure. R_H at $y=6.72$ showed strong temperature dependence proportional to $\sim1/T$ observed in Y123.[17] The T dependence of R_H, $R_H(T)$, weakened in the same manner as $R_H(T)\sim-T$ with oxygen doping. $R_H(T)$ showed a systematic change in magnitude and T dependence with oxygen doping. R_H remained positive under high pressure, although the magnitude of R_H decreased with increasing pressure. The change in $R_H(T)$ by pressure $dR_H(T)/dP$ showed a similar trend to that by oxy-
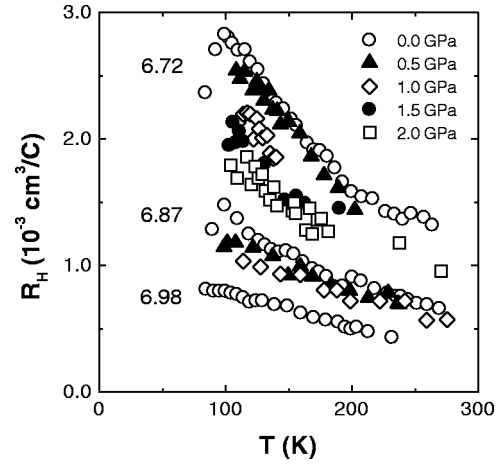

FIG. 2. Hall coefficient R_H vs temperature T curve in $Y_{0.9}Ca_{0.1}Ba_2Cu_3O_y$ with $y\geq6.72$ under high pressure.

gen doping $dR_H(T)/dy$. This finding implies a common origin for the carrier supplied by oxygen doping and by the application of pressure in the YC123 system.

Figure 3 shows the R_H vs T curve in $Y_{1-x}Ca_xBa_2Cu_3O_6$ under high pressure. R_H decreases with Ca doping in addition to oxygen doping, thus suggesting carrier doping by Ca. The $R_H(T)$ here was weaker than that of YC123 with $y\geq6.72$. The inset of Fig. 3 shows R_H as a function of pressure around room temperature in YC123 with $x=0.18$ and $y=6$. R_H remained almost completely unchanged with increasing pressure until 1.6 GPa. We observed a similar result in the sample with $x=0.15$, 0.17, and 0.20. No change in either the sign or magnitude of R_H was found under high pressure in YC123 without the chain.

Figure 4 shows the typical normalized value of R_H at 110 K, $R_H(P)/R_H(0)$, as a function of pressure in $Y_{0.9}Ca_{0.1}Ba_2Cu_3O_y$ with $6.59\leq y\leq6.99$. $R_H(P)/R_H(0)$ decreased in a linear fashion with increasing pressure in all
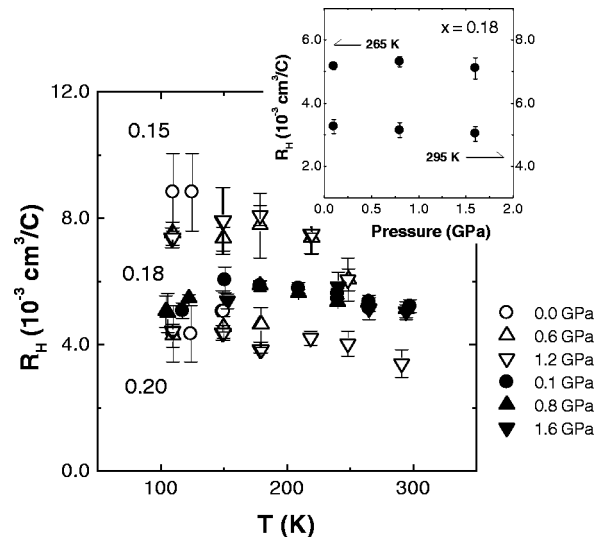

FIG. 3. R_H vs T curve in $Y_{1-x}Ca_xBa_2Cu_3O_6$ under high pressure. The inset shows the R_H as a function of pressure around room temperature. Vertical bars show the measurement error.
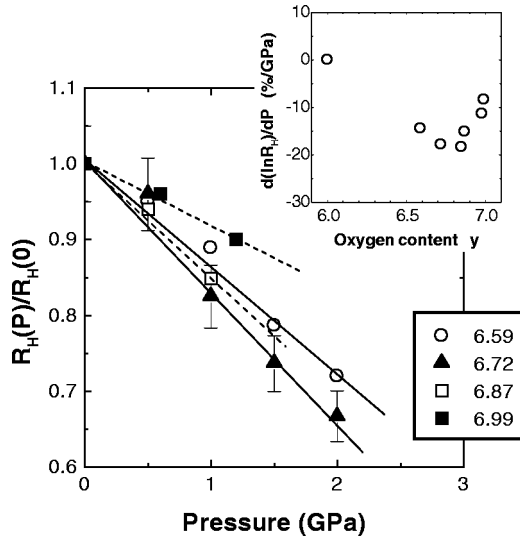
FIG. 4. Normalized value of R_H, $R_H(P)/R_H(0)$, as a function of the pressure curve in $Y_{0.9}Ca_{0.1}Ba_2Cu_3O_y$ samples with various y. The inset shows the derivative $d(\ln R_H)/dP$ vs y curve.

measured samples. The derivative $R_H(P)/R_H(0)$, $d(\ln R_H)/dP$, was found to be within the range $-8.3 \sim -18$ %/GPa. The y dependence of $d(\ln R_H)/dP$ is shown in the inset of Fig. 4. Around $y \sim 6.8$, $d(\ln R_H)/dP$ showed a broad minimum of about -18%/GPa. This was almost two times larger in terms of magnitude than the reported result.[2] Beyond $y \sim 6.8$, $d(\ln R_H)/dP$ increased with increasing y, indicating a suppression of the pressure effect. At $y = 7$, $d(\ln R_H)/dP$ was determined to be -8.3%/GPa. This was almost identical to the reported result in Y123 with $T_c = 91.4$ K and Y124.[2] On the other hand, the $d(\ln R_H)/dP$ value at $y = 6$ was ~ 0%/GPa. The same result was observed in the LS214 system.[5]

We attempted to explain the pressure effect on R_H using a simple model. The dT_c/dP vs dN_H/dP in YC123 with $y < 6.72$ indicated the contribution of charge transfer through pressure-enhanced chain ordering,[6] whereas that in YC123 with $y \geq 6.72$ indicated that some other factor needed to be considered.[7] Here, we considered internal strain due to the Cu-O chain structure. This factor has been proposed as explaining the uniaxial pressure effect on T_c in Y123 with $y = 7$.[14] At $y = 7$, the pressure effect on R_H is due only to internal strain, since no oxygen reordering occurs under high pressure. The internal strain effect could become smaller through breaking of the Cu-O chain structure with decreasing y. Accordingly, the internal strain can be expected to depend on orthorhombicity. Thus, we assumed that the contribution of internal strain for $d(\ln R_H)/dP$, $[d(\ln R_H)/dP]_{IS}$, is roughly proportional to its orthorhombicity. Then, $[d(\ln R_H)/dP]_{IS}$ at $y = 7$ is -8.3%/GPa. The y dependence of $[d(\ln R_H)/dP]_{IS}$ is indicated by the closed downward-pointing triangles in Fig. 5. On the other hand, the contribution of oxygen reordering $[d(\ln R_H)/dP]_{OR}$ can be analytically obtained using the following formula: $[d(\ln R_H)/dP]_{OR} = R_H^{-1}(0) \cdot [dT_c/dP]_{OR} \cdot [dT_c/dR_H]_{OR}^{-1}$. The value of $[dT_c/dR_H]_{OR}$ can be determined from the R_H dependence of T_c, $T_c(R_H)$ observed by oxygen doping. The contribution of
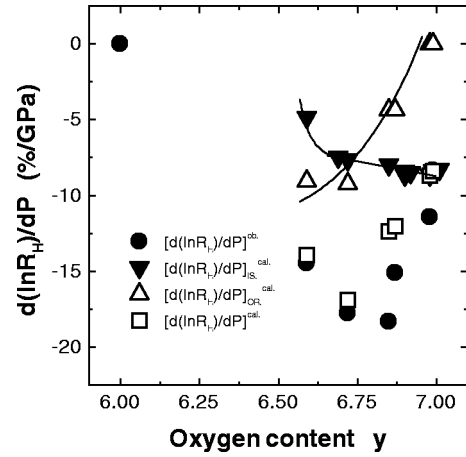

FIG. 5. $d(\ln R_H)/dP$ as a function of oxygen content y in $Y_{1-x}Ca_xBa_2Cu_3O_y$. For $y = 6$, $0.15 \leq x \leq 0.20$. For $y > 6$, $x = 0.10$.

oxygen reordering for dT_c/dP, $[dT_c/dP]_{OR}$, was experimentally determined in Y123 by Fietz *et al.*[12] The $[dT_c/dR_H]_{OR}$ can be calculated from the $T_c(R_H)$ in Y123.[10,18] The calculated $[d(\ln R_H)/dP]_{OR}$ for when the oxygen reordering effect for YC123 and Y123 was identical is shown in Fig. 5 as an open triangle. The $d(\ln R_H)/dP$ can be calculated from the formula $[d(\ln R_H)/dP]_{cal} = [d(\ln R_H)/dP]_{IS} + [d(\ln R_H)/dP]_{OR}$. The calculated and observed $d(\ln R_H)/dP$ are presented as open squares and closed circles, respectively, in Fig. 5. The trend in y dependence of $d(\ln R_H)/dP$ can be reproduced well using the above simple model. The slight difference between the observed and calculated $d(\ln R_H)/dP$ was due to the relatively few data points of T_c vs R_H. From the above analysis, the minimum $d(\ln R_H)/dP$ observed around $y \sim 6.8$ was found to occur in response to internal strain due to the chain. Both $[d(\ln R_H)/dP]_{IS}$ and $[d(\ln R_H)/dP]_{OR}$ were 0 at $y = 6$, since there is no oxygen reordering and no internal strain due to the Cu-O chain. In fact, no pressure-induced change in R_H was observed. Therefore, we concluded that the pressure effect on R_H was due to competition between oxygen reordering in the Cu-O chain site and internal strain due to the presence of the Cu-O chain structure.

In the Y123 with $y < 6.6$, the change in carrier number in the Cu-O$_2$ plane Δn via oxygen ordering due to room-temperature annealing was estimated from the time dependence of the T_c and lattice parameters.[18,19] Δn increased with a reduction in y within the range $6.4 < y < 6.6$. This shows that the effect of oxygen ordering at 1 bar becomes larger with a reduction in y from $y \sim 6.6$. An increase in $d(\ln R_H)/dP$ is expected with a reduction of y from $y = 6.6$. This finding is not inconsistent with the present result.

Y124 is a system that does not show oxygen reordering under high pressure. Since it has a perfect Cu-O double chain, internal strain could be induced. The internal strain for Y124 is expected to differ from those for YC123 or Y123 with $y = 7$. However, the reported value of $d(\ln R_H)/dP$ was -7.7%/GPa for Y124 and -9.0%/GPa for Y123 with $T_c = 91.4$ K.[2] These values are almost identical to the

-8.3%/GPa observed in YC123 with $y=7$. In YC123 ($0 \leqslant x \leqslant 0.06$) with a full chain ($y \sim 7$), the value of $d(\ln T_c)/dP$ was from $0 \sim -0.9\%$ GPa.[2] The $d(\ln T_c)/dP$ for pure Y123 with a full chain is reportedly from $+0.72\%$/GPa $\sim -0.7\%$/GPa.[2,4,9,12,20,21] The $d(\ln T_c)/dP$ for Y124 is $+4.6 \sim +7.4\%$/GPa.[2,22,23] The $d(\ln T_c)/dP$ for Y124 is the largest among the above three systems, while the $d(\ln R_H)/dP$ is almost constant $-8 \sim -9\%$ GPa. $d(\ln T_c)/dP$ may be more sensitive to internal strain than $d(\ln R_H)/dP$. The details remain to be determined.

In summary, the pressure effect on R_H has been systematically investigated in the $Y_{1-x}Ca_xBa_2Cu_3O_y$ system. No change in R_H under pressure was observed in samples without the Cu-O chain structure, whereas samples with an oxygen-deficient chain change in response to pressure at a rate of -18%/GPa. Even in samples with a perfect chain ($y=7$), R_H changes at a rate of -8.3%/GPa. The oxygen-content dependence of $d(\ln R_H)/dP$ can be explained well by competition between oxygen reordering in the Cu-O chain site and internal strain due to the Cu-O chain structure.

[1] N. Môri, C. Murayama, H. Takahashi, H. Kaneko, Y. Iye, S. Uchida, H. Takagi, Y. Tokura, Y. Kubo, H. Sasakura, and K. Yamaya, Physica C **185-189**, 40 (1991).

[2] C. Murayama, Y. Iye, T. Enomoto, N. Môri, Y. Yamada, T. Matsumoto, Y. Kubo, Y. Shimakawa, and T. Manako, Physica C **183**, 277 (1991).

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

[4] C.C. Almasan, S.H. Han, B.W. Lee, L.M. Paulius, M.B. Maple, B.W. Veal, J.W. Downey, A.P. Paulikas, Z. Fisk, and J.E. Schirber, Phys. Rev. Lett. **69**, 680 (1992).

[5] N. Tanahashi, Y. Iye, T. Tamegai, C. Murayama, N. Môri, S. Yomo, N. Okazaki, and K. Kitazawa, Jpn. J. Appl. Phys., Part 1 **28**, 762 (1989).

[6] T. Honma, K. Yamaya, N. Môri, and M. Tanimoto, Solid State Commun. **98**, 395 (1996).

[7] T. Honma, K. Yamaya, N. Môri, and M. Tanimoto, Physica C **235-240**, 1457 (1994).

[8] D.E. Morris, P. Narwankar, A.P.B. Sinha, K. Takano, B. Fayn, and V.T. Shum, Phys. Rev. B **41**, 4118 (1990).

[9] S. Sadewasser, J.S. Schilling, A.P. Paulikas, and B.W. Veal, Phys. Rev. B **61**, 741 (2000).

[10] J.R. Cooper, S.D. Obertelli, A. Carrington, and J.W. Loram, Phys. Rev. B **44**, 12 086 (1991).

[11] H. Claus, M. Braun, A. Erb, K. Röhberg, B. Runtsch, H. Wuhl, G. Brauchle, P. Schweib, G. Muller-Vogt, and H.v. Lohneysen, Physica C **198**, 42 (1992).

[12] W.H. Fietz, R. Quenzel, H.A. Ludwig, K. Grube, S.I. Schlachter, F.W. Hornung, T. Wolf, A. Erb, M. Kläser, and G. Müller-Vogt, Physica C **270**, 258 (1996).

[13] V. Dyakonov, I. Fita, N. Doroshenko, M. Baran, S. Piechota, and H. Szymczak, Physica C **276**, 245 (1997).

[14] W.E. Pickett, Phys. Rev. Lett. **78**, 1960 (1997).

[15] T. Honma, K. Yamaya, F. Minami, and S. Takekawa, Physica C **176**, 209 (1991).

[16] J.D. Jorgensen, B.W. Veal, A.P. Paulikas, L.J. Nowicki, G.W. Crabtree, H. Claus, and W.K. Kwok, Phys. Rev. B **41**, 1863 (1990).

[17] T. Tamegai and Y. Iye, Phys. Rev. B **44**, 10 167 (1991).

[18] T. Ito, K. Takenaka, and S. Uchida, Phys. Rev. Lett. **70**, 3995 (1993).

[19] H. Shaked, J.D. Jorgensen, B.A. Hunter, R.L. Hitterman, A.P. Paulikas, and B.W. Veal, Phys. Rev. B **51**, 547 (1995).

[20] J.J. Neumeier and H.A. Zimmermann, Phys. Rev. B **47**, 8385 (1993).

[21] S. Rusiecki, B. Bucher, E. Kaldis, E. Jilek, J. Karpinski, C. Rossel, B. Pumpin, H. Keller, W. Kundig, T. Krekels, and G. Van Tendeloo, J. Less-Common Met. **164**, 31 (1990).

[22] J.-S. Zhou, J.B. Goodenough, B. Dabrowski, and K. Rogacki, Phys. Rev. Lett. **77**, 4253 (1996).

[23] B. Bucher, J. Karpinski, E. Kaldis, and P. Wachter, Physica C **157**, 478 (1989).