

# AMCoR

Asahikawa Medical College Repository <http://amcor.asahikawa-med.ac.jp/>

PHYSICAL REVIEW B (2001) 63(21):2506.

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

Honma T, Tanimoto M, Mori, N

## 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. Mōri

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

(Received 20 October 2000; published 1 May 2001)

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.

DOI: 10.1103/PhysRevB.63.212506

PACS number(s): 74.72.Bk, 74.62.Fj, 74.25.Fy, 74.62.Dh

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.<sup>1</sup> 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  $\sim -10\%/GPa$ .<sup>2</sup> 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).<sup>2</sup> This indicates that for these systems, the pressure effect on  $T_c$  can be qualitatively understood by a simple charge-transfer model.<sup>2-4</sup> 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.<sup>5</sup>

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.<sup>6,7</sup> 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.<sup>1,8</sup> 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.<sup>9</sup> In this system, the maximum  $T_c$  never goes beyond 95 K by the oxygen and/or Ca doping.<sup>10,11</sup> These results cannot be explained by the simple charge-transfer model.<sup>6</sup>

$Y_{1-x}Ca_xBa_2Cu_3O_y$  (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  $NdBa_2Cu_3O_{6.67}$ .<sup>13</sup> 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  $T_c$ .<sup>14</sup> 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  $900^\circ C$  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  $930-940^\circ C$ , and then were annealed in flowing  $O_2$  at an appropriate temperature or in flowing Ar at  $750^\circ C$ . 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<sup>3</sup>. Hall voltage  $V_H$  measurements were conducted by rotating the sample  $360^\circ$  ( $240^\circ$ ) in a magnetic field of 7 T (4 T) under ambient (high)

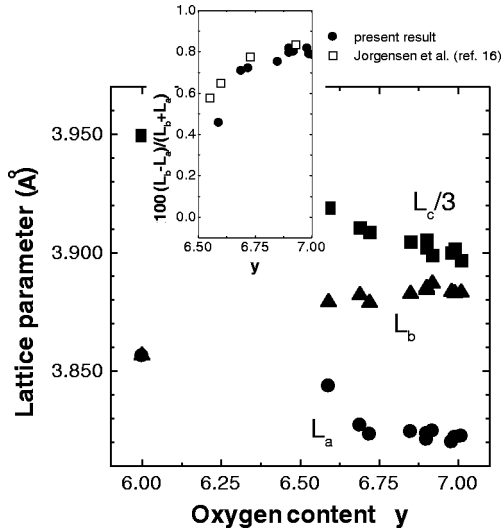


FIG. 1. Lattice parameter for  $a$ ,  $b$ , and  $c$  axes  $L_a$ ,  $L_b$ , and  $L_c/3$  as a function of oxygen content  $y$  in  $Y_{0.9}Ca_{0.1}Ba_2Cu_3O_y$ . The inset shows orthorhombicity  $(L_b - L_a)/(L_b + L_a) \times 100$  as a function of  $y$ . The closed circle and open diamond show the 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.<sup>1</sup> All other details of the  $R_H$  measurement were as described previously.<sup>6,15</sup>

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.<sup>16</sup> 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 orthorhombicity. Orthorhombicity  $(L_b - L_a)/(L_b + L_a) \times 100$ , 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 orthorhombicity of the sample was almost identical to the reported value in Y123.<sup>16</sup> 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  $y \geq 6.72$  under high pressure.  $R_H$  at  $y = 6.72$  showed strong temperature dependence proportional to  $\sim 1/T$  observed in Y123.<sup>17</sup> 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-

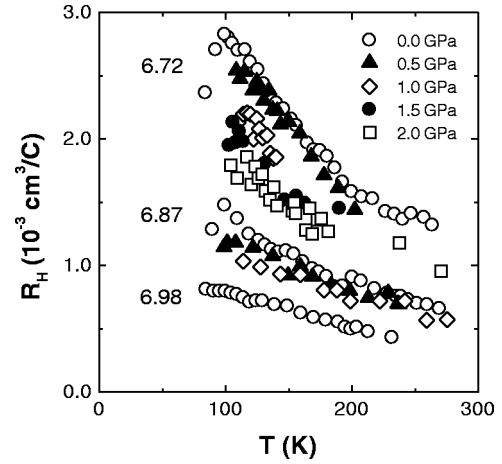


FIG. 2. Hall coefficient  $R_H$  vs temperature  $T$  curve in  $Y_{0.9}Ca_{0.1}Ba_2Cu_3O_y$  with  $y \geq 6.72$  under high pressure.

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  $y \geq 6.72$ . 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  $6.59 \leq y \leq 6.99$ .  $R_H(P)/R_H(0)$  decreased in a linear fashion with increasing pressure in all

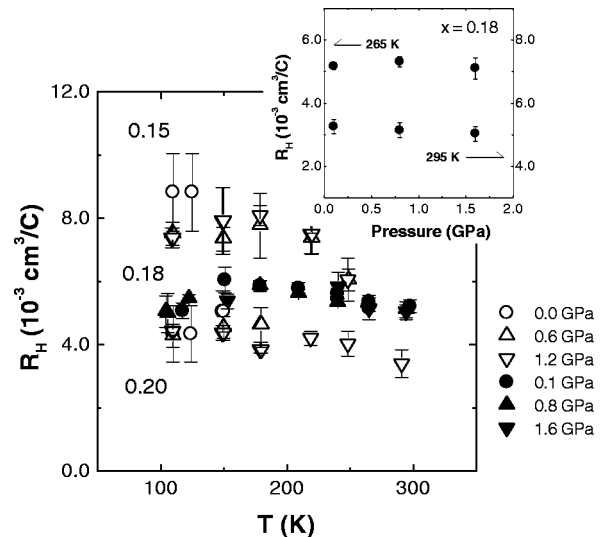


FIG. 3.  $R_H$  vs  $T$  curve in  $Y_{1-x}Ca_xBa_2Cu_3O_6$  under high pressure. The inset shows the  $R_H$  as a function of pressure around room temperature. Vertical bars show the measurement error.

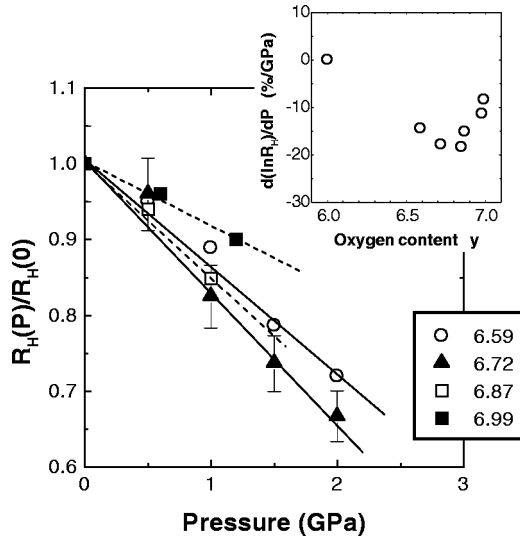


FIG. 4. Normalized value of  $R_H$ ,  $R_H(P)/R_H(0)$ , as a function of the pressure curve in  $Y_{0.9}Ca_{0.1}Ba_2Cu_3O_y$  samples with various  $y$ . The inset shows the derivative  $d(\ln R_H)/dP$  vs  $y$  curve.

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.<sup>2</sup> 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.<sup>2</sup> On the other hand, the  $d(\ln R_H)/dP$  value at  $y=6$  was  $\sim 0$  %/GPa. The same result was observed in the LS214 system.<sup>5</sup>

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,<sup>6</sup> whereas that in YC123 with  $y \geq 6.72$  indicated that some other factor needed to be considered.<sup>7</sup> 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  $y = 7$ .<sup>14</sup> 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

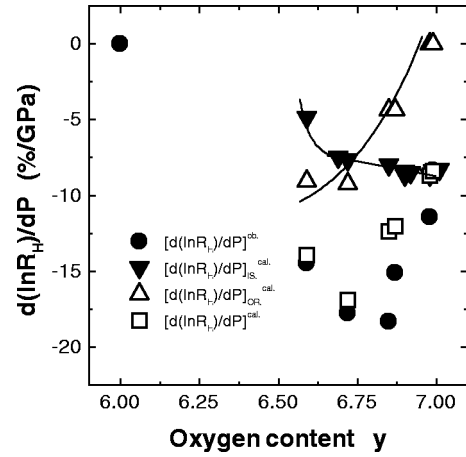


FIG. 5.  $d(\ln R_H)/dP$  as a function of oxygen content  $y$  in  $Y_{1-x}Ca_xBa_2Cu_3O_y$ . For  $y=6$ ,  $0.15 \leq x \leq 0.20$ . For  $y > 6$ ,  $x=0.10$ .

oxygen reordering for  $dT_c/dP$ ,  $[dT_c/dP]_{OR}$ , was experimentally determined in Y123 by Fietz *et al.*<sup>12</sup> The  $[dT_c/dR_H]_{OR}$  can be calculated from the  $T_c(R_H)$  in Y123.<sup>10,18</sup> 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<sub>2</sub> plane  $\Delta n$  via oxygen ordering due to room-temperature annealing was estimated from the time dependence of the  $T_c$  and lattice parameters.<sup>18,19</sup>  $\Delta n$  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.<sup>2</sup> These values are almost identical to the

$-8.3\%/GPa$  observed in YC123 with  $y=7$ . In YC123 ( $0 \leq x \leq 0.06$ ) with a full chain ( $y \sim 7$ ), the value of  $d(\ln T_c)/dP$  was from  $0 \sim -0.9\%/GPa$ .<sup>2</sup> The  $d(\ln T_c)/dP$  for pure Y123 with a full chain is reportedly from  $+0.72\%/GPa \sim -0.7\%/GPa$ .<sup>2,4,9,12,20,21</sup> The  $d(\ln T_c)/dP$  for Y124 is  $+4.6 \sim +7.4\%/GPa$ .<sup>2,22,23</sup> 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.

We would like to thank Professor K. Yamaya of Hokkaido University for supporting the present research at its initial stages and Professor P.H. Hor of the University of Houston for helpful comments at the final stages.

- 
- <sup>1</sup>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).
- <sup>2</sup>C. Murayama, Y. Iye, T. Enomoto, N. Môri, Y. Yamada, T. Matsumoto, Y. Kubo, Y. Shimakawa, and T. Manako, *Physica C* **183**, 277 (1991).
- <sup>3</sup>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).
- <sup>4</sup>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).
- <sup>5</sup>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).
- <sup>6</sup>T. Honma, K. Yamaya, N. Môri, and M. Tanimoto, *Solid State Commun.* **98**, 395 (1996).
- <sup>7</sup>T. Honma, K. Yamaya, N. Môri, and M. Tanimoto, *Physica C* **235-240**, 1457 (1994).
- <sup>8</sup>D.E. Morris, P. Narwankar, A.P.B. Sinha, K. Takano, B. Fayn, and V.T. Shum, *Phys. Rev. B* **41**, 4118 (1990).
- <sup>9</sup>S. Sadewasser, J.S. Schilling, A.P. Paulikas, and B.W. Veal, *Phys. Rev. B* **61**, 741 (2000).
- <sup>10</sup>J.R. Cooper, S.D. Obertelli, A. Carrington, and J.W. Loram, *Phys. Rev. B* **44**, 12 086 (1991).
- <sup>11</sup>H. Claus, M. Braun, A. Erb, K. Röhberg, B. Runtzsch, H. Wuhl, G. Brauchle, P. Schweib, G. Muller-Vogt, and H.v. Lohneysen, *Physica C* **198**, 42 (1992).
- <sup>12</sup>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).
- <sup>13</sup>V. Dyakonov, I. Fita, N. Doroshenko, M. Baran, S. Piechota, and H. Szymczak, *Physica C* **276**, 245 (1997).
- <sup>14</sup>W.E. Pickett, *Phys. Rev. Lett.* **78**, 1960 (1997).
- <sup>15</sup>T. Honma, K. Yamaya, F. Minami, and S. Takekawa, *Physica C* **176**, 209 (1991).
- <sup>16</sup>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).
- <sup>17</sup>T. Tamegai and Y. Iye, *Phys. Rev. B* **44**, 10 167 (1991).
- <sup>18</sup>T. Ito, K. Takenaka, and S. Uchida, *Phys. Rev. Lett.* **70**, 3995 (1993).
- <sup>19</sup>H. Shaked, J.D. Jorgensen, B.A. Hunter, R.L. Hitterman, A.P. Paulikas, and B.W. Veal, *Phys. Rev. B* **51**, 547 (1995).
- <sup>20</sup>J.J. Neumeier and H.A. Zimmermann, *Phys. Rev. B* **47**, 8385 (1993).
- <sup>21</sup>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).
- <sup>22</sup>J.-S. Zhou, J.B. Goodenough, B. Dabrowski, and K. Rogacki, *Phys. Rev. Lett.* **77**, 4253 (1996).
- <sup>23</sup>B. Bucher, J. Karpinski, E. Kaldis, and P. Wachter, *Physica C* **157**, 478 (1989).