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Strain effect on the thermoelectric power of YBa$_{2-x}$Sr$_x$Cu$_3$O$_7$

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Abstract

The temperature dependent thermoelectric power (TEP) for a series of superconducting Y(Ba$_{2-x}$Sr$_x$)Cu$_3$O$_{6.95}$ with $x = 0$ to 0.8 has been investigated. We have kept the oxygen content at the optimal value (6.95 ± 0.02) and have changed the lattice parameters by Sr-doping to study the strain dependent TEP. We have observed that a hump occurs at 240 K for all samples except that with $x = 0$. With increasing the Sr-doping level, S shifts to a higher value and changes its sign from negative to positive. This study demonstrates that the sign as well as the absolute value of TEP has been affected by the lattice strains. © 2000 Published by Elsevier Science B.V.

1. Introduction

The normal state properties of high temperature superconductors have been a key-point to unravel the mystery of high temperature superconductivity (HTS) [1,5]. Especially the transport measurements, including resistivity, Hall coefficient, thermoelectric power (TEP), etc., have provided much information to test various theoretical models. For example, Zhou and Goodenough [6,7] used the data of temperature dependent TEP to test the models of conventional electron–phonon interactions, the marginal-Fermi-liquid theory, and the magnetic models. The authors found that none of the above models could describe

the hump near 240 K in the normal state TEP for (La,Sr)CuO$_4$. Therefore, it prompts a model with a mass-enhancement phenomenon that utilizes vibronic coupling of electrons to optical-mode lattice vibration. Although this model has not been further validated for other HTS systems, it demonstrated that the study of normal state TEP is important for understanding the origin of superconductivity. Based on many previous reports [1,2,6,7], we have summarized the common characteristics of TEP for HTSC:

1. The value of TEP at room temperature, $S(300\ K)$, is positive in underdoped region but negative in overdoped region.
2. The absolute value of S decreases with increasing the number of hole-concentration (n).
3. The functional $S(T)$ curves for the underdoped and overdoped regions are asymmetric with respect to $S = 0$.

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4. For $RBa_2Cu_3O_7$, the contribution from CuO_2-plane gives negative dS/dT while the contribution from CuO-chain yields positive dS/dT.

5. In $S(T)$ curves, a hump was observed above T_c at ~ 240 K for $(La,Sr)CuO_4$ and $(Y,Ca)(Ba,La)Cu_3O_7$. However, there is no hump being observed in Bi-, Tl-, and Hg-based cuprates.

The features of (1) to (3) yielded an empirical rule of S as a function of n [1]. However, it requires a continuous efforts to understand the TEP data of HTS. It had been demonstrated that in the optimal doped $RBa_2Cu_3O_7$ the internal pressure as well as the external pressure affects T_c via another parameter besides the carrier concentration [8], and that the second parameter should be of importance to the development of the microscopic theory for HTS [9]. We, therefore, decided to investigate the stain effect on TEP as well as on the superconducting temperature (T_c) for a series of optimally doped $Y(Ba_{1-x}Sr_x)_2Cu_3O_7$ samples with $0 \leq x \leq 0.8$. We optimized the oxygen content at 6.95 ± 0.02 for each sample and replaced Ba with Sr to reduce the lattice parameters of unit cell. Correspondingly, the internal strain increases with increasing the Sr-concentration.

2. Experiments

The samples of $Y(Ba_{2-x}Sr_x)Cu_3O_{6.95}$ for $x = 0.2$, 0.4, 0.6, 0.8 were prepared by mixing the powders of Y_2O_3, $BaCO_3$, $SrCO_3$, and CuO in appropriate ratios. The mixtures were calcined at 950°C for 20 h in air then grounded and pressed into pellets. The pellets were sintered at 950°C for 20 h in air followed by O_2 annealing at 400°C for 20 h and were then cooled to room temperature at a rate of 2°C/min. Oxygen content of each sample was determined by the iodometric titration method to be 6.95 ± 0.02. Structures of $Y(Ba_{2-x}Sr_x)Cu_3O_{6.95}$ were investigated via Rietveld refinement of the X-ray diffraction (XRD) data. The series of XRD patterns of the fully oxygenated $Y(Ba_{2-x}Sr_x)Cu_3O_{6.95}$ samples show that all the samples are monophasic. In Fig. 1 we display a typical XRD pattern for $x = 0.8$. All the peaks in the XRD pattern can be indexed with a
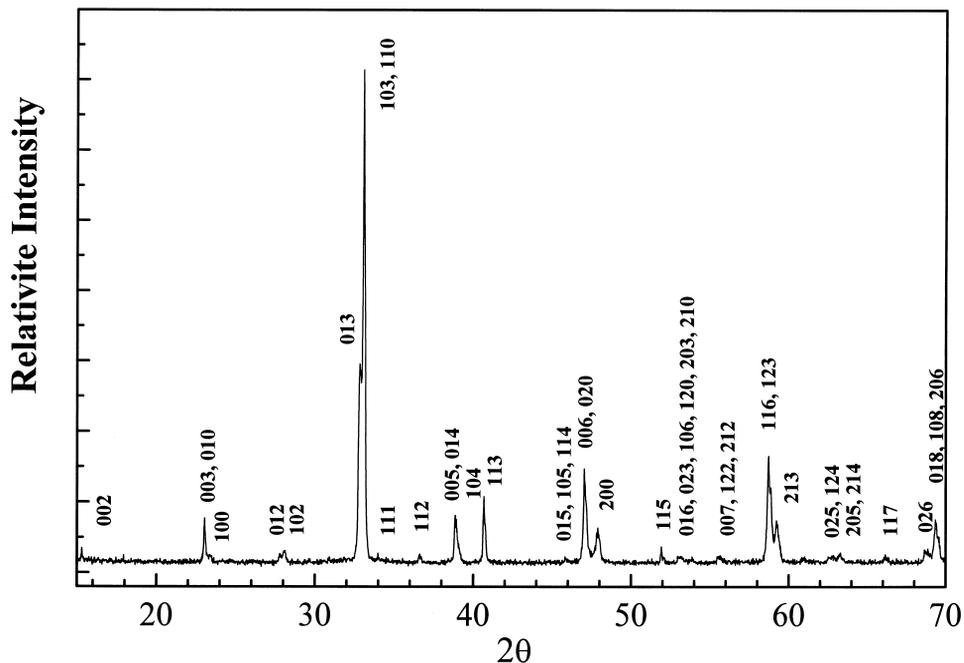

Fig. 1. XRD patterns of the fully oxygenated $Y(Ba_{2-x}Sr_x)Cu_3O_{6.95}$ sample with $x = 0.8$.

orthorhombic crystal structure in the *Pmmm* space group.

The standard four-probe method was used to obtain the pellet resistivity. The absolute thermoelectric power S of the sample was obtained by dc method and calibrated against Pb standard. Cu/Chromel thermocouple was used to detect the temperature gradient which was kept in a range of $0.8 \sim 1.2$ K. Each measurement point was stabilized for more than 25 min in order to avoid non-equilibrium effects. No hysteresis was observed for the cooling and warming measurements.

3. Results and discussion

The structural data obtained from the Rietveld refinement are shown in Fig. 2 with respect to different Sr-contents. It indicates that all lattice parameters, a, b, and c, decrease near linearly with increasing Sr concentration. Since Sr^{2+} (1.13 Å) is smaller than Ba^{2+} (1.35 Å) but larger than Y^{3+} (0.93 Å), this figure clearly demonstrates that Sr indeed replaces the Ba site rather than the Y site.

Fig. 3 shows the resistivity (ρ)data for $x = 0$, 0.2, 0.4, 0.6 and 0.8 w.r.t. the curves from top to bottom. A drop of ρ from $x = 0$ to $x = 0.2$ was observed, but there is no much change of normal ρ for $x = 0.2$, 0.4, 0.6 and 0.8. Defining the T_c value to be the intersect of the extension line of normal state ρ and the tangent line at the transition, T_c decreases from to 92 to 80 K with increasing x from 0 to 0.8.

Fig. 3. The resistivity for $Y(Ba_{2-x}Sr_x)Cu_3O_{6.95}$ with $x = 0$, 0.2, 0.4, 0.6 and 0.8 w. r. t. the curves from the top to the bottom.

Fig. 4 shows S vs. T for $Y(Ba_{2-x}Sr_x)Cu_3O_{6.95}$ with $x = 0$ (the bottom curve) to 0.8 (the top curve). Apparently, the curve of S(T) for $x = 0$ is different from others by a sharp negative slope before the transition. It is a typical $S(T)$ data for an overdoped state. On the other hand, the curves of $x = 0.2$ to $x = 0.8$ are all very similar. There is a trace of hump occurring at ~ 240 K for $x = 0.4$ and 0.6, but it disappears at $x = 0.8$.

The earlier studies of TEP on the high T_c superconductor have revealed a universal relation between hole concentration and the room temperature S [1,2]. In the underdoped region, $S(300$ K$)$ is always positive; while in overdoped region, $S(300$ K$)$ is negative. For $YBa_2Cu_3O_7$ (YBCO), recent experiments
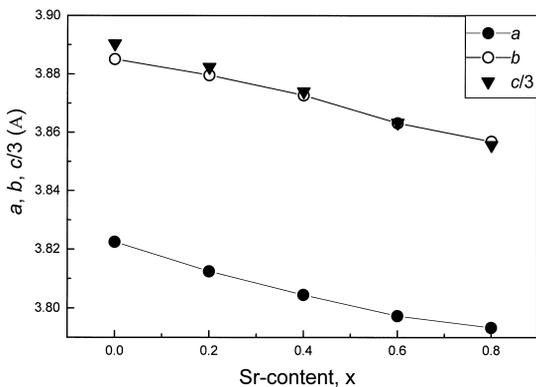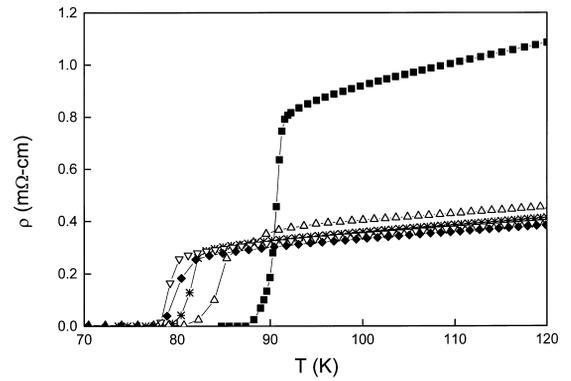

Fig. 2. Lattice parameters for different Sr concentration, x. All of a-, b- and c-parameters show a nearly linear dependence of x.
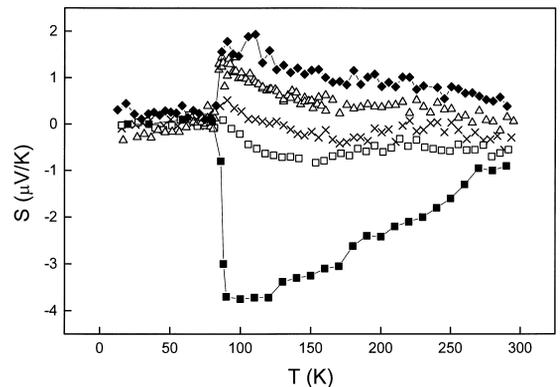

Fig. 4. Temperature dependent TEP for $Y(Ba_{2-x}Sr_x)Cu_3O_{6.95}$ with $x = 0$ (the bottom curve) to 0.8 (the top curve), respectively.

on thermal conductivity [2], NMR [3], dc conductivity [4,5] etc., have revealed that the CuO chain has equally rich phenomena as that of the CuO_2 plane. Studies of TEP on YBCO single crystals [10–12] and thin films [13] suggest that for optimally doped YBCO superconductor, the CuO_2 plane contributes to the positive TEP whereas the CuO chain is responsible to the negative TEP. Based on the two-band model, the total TEP for polycrystalline YBCO was proposed to be the linear combination of both. On the other hand, the single-layer copper oxides $La_{2-x}Sr_xCuO_4$ (La-214) does not follow the same rule as YBCO system [14]. In La-214, S remains positive in both underdoped and overdoped regions, which may be due to the lack of CuO-chain. Thus, the change of sign in the normal state S should be closely related to the two-band structure in YBCO.

There exists another paper showing that S changes from a negative to a positive value by applying the lattice pressure. A study on the overdoped region has been reported by Zhou et al. [6] on $(Y_{1-x}Ca_x)(Ba_{2-x}La_x)Cu_3O_{6.96}$. Zhou at al. showed that S changes dramatically from negative to positive for $x = 0.3$ to $x = 0.4$ with the CuO_2 plane remaining at a constant oxygen content. They observed a corresponding increase of resistivity from $x = 0.3$ to $x = 0.4$ in their study and, thus, attributed the abrupt change of TEP to the onset of disordering of the CuO chain. However, in our samples, there is no increase of ρ with Sr-doping. This excludes the argument that the change of TEP is due to the disordering of the CuO chain. Furthermore, In the work by Zhou et al., the c-parameter of $(Y_{1-x}Ca_x)(Ba_{2-x}La_x)Cu_3O_{6.96}$ was nearly unchanged while the a and the b parameters changed in an opposite direction with increasing x. Such a lattice change definitely involved a more complicated mechanism to describe the lattice effects. In our samples of $Y(Ba_{2-x}Sr_x)Cu_3O_{6.95}$, all of the a, b, c parameters decrease nearly linearly with increasing Sr, suggesting that the lattice pressure was enhanced with increasing x. Furthermore, the resistivity data leads us to assume that our fully oxidized samples of $x = 0$ is at the overdoped state and that the charge redistribution occurs in the samples of $x = 0.2$, 0.4, 0.6 and 0.8.

One of the related works is the hydrostatic pressure effect on TEP for optimal-doped YBCO [7]. The

authors found a negative enhancement at 140 K, decreasing from -1.2 to -2.7 μV/K with increasing the pressure from 1 bar to 13.9 kbar. The authors have attributed the change of TEP under pressure to the transition from a vibronic coupling to an optical-mode deformation since 140 K is considered to be too high a temperature to account for the acoustic mode vibration. They further suggested that the elastic coupling between CuO_2 plane and CuO chain may be responsible for inducing superconductivity in the chains.

In our data, S gets more positive when the lattice contracts. This observation contradicts with the result of hydrostatic pressure on S in YBCO and demonstrates an example that the effect of external pressure does not necessarily the same as that of internal pressure. For $x > 0.6$, S becomes positive and plane-like, implying that a component of S from the CuO chain is suppressed when the lattice strain increases. We, therefore, believe a charge re-distribution between CuO-chain and CuO_2 plane to be responsible for our observation of sign change in S.

4. Conclusion

We have measured the thermoelectric power and the resistivity for a series of $Y(Ba_{2-x}Sr_x)Cu_3O_{6.95}$ samples with $x = 0$ to 0.8. The linear decrease of lattice parameters with x suggested that the internal pressure was enhanced with Sr-doping. We have observed a decrease of T_c and an increase of S with increasing x and have attributed these results to the strain-induced charge redistribution between CuO-chain and CuO_2 plane.

Acknowledgements

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