Relationship between superconducting mechanism and the crystal structure in T'-structured cuprate oxide

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There increases the evidence showing an importance of crystal structure on the physical properties of high-T_c cuprates. The R_2CuO_{4-y} (R: Pr, Nd, Eu$\cdots$) with Nd_2CuO_4-type (abbreviated as T') structure is believed to be an antiferromagnetically ordered Mott insulator. However, the emergence of superconductivity was reported for the moderately annealed thin film of " undoped " T'-R_2CuO_{4-y}. If this is the real case, mother compound of so-called " electron-doped " superconductor is not exactly Mott insulator, and the new way for the superconducting mechanism should be studied. The T'-structure is characterized by the absence of apical oxygen above and below Cu sites. According to the recent theoretical works, the existence of apical oxygen can modify the electronic structure and could change the ground state [1, 2]. In the real T'-structured material, the as-prepared sample is non-superconductor and the annealing procedure is necessary for the emergence of superconductivity. It is recognized that the removal of apical oxygen and/or the repair of defect of CuO_2 plane, which probably exists in the as-prepared sample, is the crucial role of annealing for the emergence of superconductivity [3]. However, the structural study is quite limited so far. Thus, the detailed information about the crystal structure is now indispensable for the determination of true ground state in T'-R_2CuO_{4-y}. We, hence, performed neutron diffraction measurements on (Pr, Nd)$_{2-x}Ce_xCuO_{4-y}$ (x = 0, 0.15) with y 0.03-0.05 at WOMBAT in ANSTO.

Figure 1 shows the diffraction pattern measured at the room temperature for the as-sintered and the annealed Pr_2CuO_4. The results are quite similar. Although the fitting error with χ of 40 and R-factor of 6.33 are still large, the structural parameters regarding oxygen ions were the same within the accuracy. Since the determination of precise differences in the positions and the occupation of oxygen is difficult at present, we simulated the atomic-selective diffraction patterns to evaluate the effect of apical oxygen and/or the vacancy of oxygen in the CuO_2 plane. However, such a simple model causes finite change in the Bragg peaks and the result is inconsistent with the no clear change in the diffraction pattern by annealing. This means that the structural change induced by annealing is much more complex than the picture proposed by the early study [4].

[1] H. Das et al, Phys. Rev. B 79, 134522 (2009). [2] C. Weber et al, Nature Phys. 6, 574 (2010). [3] M. Naito et al., Supercond. Sci. Technol. 15, 1663 (2002). [4] P. G. Radaelli et al., Phys. Rev. B 49, 15322 (1994)

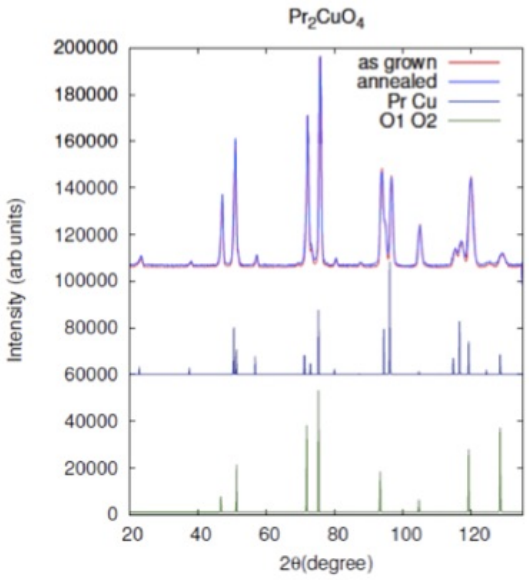

Fig. 1. Neutron diffraction pattern of as-sintered and annealed Pr_2CuO_4. The contribution of the praseodym and oxygen ions was simulated.