Poster Presentation

MS90.P11

Substitution effect in high-Tc mercury-based cuprate superconductor

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HgBa2Ca2Cu3O8+δ superconductor (Hg-1223) still has the highest critical temperature in various superconductors, which is a layered perovskite with the space group of P4/mmm. A structural unit of cation-layers is stacked in a sequence of -HgO-BaO-CuO-Ca- along the c-axis. The substitution of Hg by Pb enhances the stability of the Hg-1223 phase because the high steam pressure of Hg lowers the chemical stability in synthesis. However, the doping into Hg layers is related to an interstitial oxygen defect. On the other hand, the substitution of Ba by Sr improves the hole doping of CuO2 planes. Thus, the element substitution in Hg and Ba sites becomes a key factor in synthesizing high-quality superconductors. Therefore, the cation distribution in the two sites has been examined by the two-wavelengths anomalous dispersion (TWAD) method of synchrotron X-ray resonant scattering. Single crystals of Hg-1223 were grown at T = 1130 K by the liquid-assisted solid-state recrystallization method from the precursor powder prepared by spray drying or evaporation of the nitrate solutions. Oxygen contents in the precursors were determined by iodometric titrations. Four samples of Hg0.45Pb0.30Ba1.63Sr0.50Ca1.94Cu3O8 (Tc = 128 K), Hg0.42Pb0.41Ba1.19Sr1.06Ca1.97Cu3O8 (125 K), Hg0.50Pb0.50Ba0.59Sr1.24Ca1.83Cu3.34O8 (116 K) and Hg0.34Pb0.54Ba0.61Sr1.17Ca1.88Cu3O8 (115 K) were selected for single-crystal intensity measurements. A conventional measurement to determine the Ba-site occupancy was made to use a Rigaku AFC-5 four-circle diffractometer with Mo Kα radiation. After the absorption correction by the arbitrary-shape grid-integration method, crystal-structure refinements were successfully performed with R factors ranging 6.4 to 6.7 %. The site preference of Hg, Pb and Cu in the Hg site was determined with a vertical-type four-circle diffractometer in PF-BL-10A, where wavelengths of λ = 1.3906 and 1.0191 Å were used at Cu K and Hg LIII absorption edges, respectively. In the TWAD method with least-squares calculations, a variation of the residual factors gives a minimum against the contents of Hg or Cu, suggesting, for example, that Cu does not occupy the Hg site for all samples. In the presentation the site preference and structural change will be discussed in the aspects of superconductivity.

Keywords: high-Tc superconductor, substitution effect, resonant scattering