High-Energy X-ray Scattering Study of Optimally Doped YBCO

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Introduction

We present the preliminary results of a high-energy x-ray scattering experiment on an optimally doped YBa₂Cu₃O_{6.92} (YBCO) crystal. The key idea of this study is to investigate the existence and the nature of local-lattice distortions1 and structural coherence of the CuO₂ planes,² which may be relevant to hightemperature superconductivity.³ Due to strong electron-phonon coupling in the cuprates, one can expect such distortions to arise as a manifestation of charge fluctuations or spin-charge separations in the CuO₂ planes. It is well-known that various superstructures are prevalent in the YBCO compound for intermediate oxygen concentrations due to oxygen-vacancy ordering in the CuO-chain planes. Formation of various superstructures makes any unambiguous interpretation of scattering experiments quite difficult. However, since optimally doped YBCO has a stoichiometry close to that for full oxygenation, only the so-called orthorhombic-I phase with full CuO chains is expected to be present. Recent x-ray diffraction work seems to support this structural picture.⁴ Therefore, it seems to be advantageous to study optimally doped YBCO in order to facilitate the isolation of lattice distortions due to charge fluctuations from those of other possible origins.

Experimental Details

The experiment was carried out on the SRI CAT 1-ID beamline. We used a twinned crystal of optimally doped YBCO grown at the University of British Columbia. The sample was a thin rectangular 2 mm X 1 mm plate with a thickness of less than 100 µm. The crystallographic **c** axis is perpendicular to the large facet. The magnetization measurements revealed the onset of diamagnetic behavior at 93.75K in an applied field of 0.2 Gauss. Complete diamagnetic behavior sets in within ~0.5K below this temperature suggesting a high degree of compositional homogeneity in the bulk of the sample. Although the transition is very sharp, we observed the presence of very weak Debye-Scherrer rings using a Weissenberg setup and a CCD camera with an incident energy of 65 keV. This indicates the presence of minute amounts of extraneous phases either on the exterior or in the bulk of the sample. The high-energy study was carried out at 36 keV below the Ba K edge. A Si (3 1 1) reflection was used to monochromatize the beam with the undulator fifth harmonic tuned to provide maximum flux at this energy. Intensity was measured using a Ge solidstate detector. The sample was cooled in a closed-cycle He refrigerator. A diode sensor placed 12 mm from the sample monitored its temperature.

Results

Figure 1 summarizes the main results of our preliminary study. The top panel shows a scan along \mathbf{a}^* through the (-4, 0, 0) charge peak at room temperature (300K), just above T_c (100K), and far below T_c (50K), respectively. Weak superlattice peaks corresponding to (~1/3, 0, 0) are visible on either side of the Bragg peak at all three temperatures. Due to increased thermal diffuse



FIG. 1. Top panel: [H 0 0]-scans between (-4, 0, 0) and (-3, 0, 0) Bragg peaks at three different temperatures (red - 300K, magenta - 100K, green - 50K). Bottom panel: L-scan at 300K and 100K, respectively.

scattering, the data at 100K and 300K are shifted upward, and the tails from the Bragg peak extend further out into reciprocal space relative to those at 50K. These superlattice peaks are rather broad indicating a short-range correlation along the **a** axis. Our observation is consistent with recent neutron diffraction work that has also found (~1/3, 0, 0) superlattice peaks in optimally doped YBCO.⁵ The origin of this peak was suggested to be lattice distortions by charge stripes in the two-dimensional CuO₂ plane.

The bottom panel shows a scan along the c^* axis through the (-3.3, 0, 0) peak at 100K and 300K, respectively. Near sinusoidal oscillations of the intensity are clearly observed. This behavior

suggests that a finite number of scattering planes are correlated along the c axis. These correlations clearly persist at room temperature as well.

Remarks

The observation of weak superlattice peaks corresponding to $(\sim 1/3, 0, 0)$ is intriguing. A more elaborate set of experiments to reveal the nature of the distortions, to study the correlations in the direction of the CuO chain and to measure the temperature dependence is required.

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