Nanoscale Inhomogeneities in a Detwinned, Optimally Doped Yttrium Barium Copper Oxide Superconductor

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Introduction

We present some results of high-energy x-ray scattering experiments in which the nature of microscopic inhomogeneties that are electronic and/or structural in origin was studied in an optimally doped $YBa_2Cu_3O_{6.92}$ (YBCO) crystal. In our preliminary measurements on a twinned crystal, we observed very weak superlattice peaks characterized by a wave vector $\mathbf{q}_0 = (q_x, \delta, 0)$, with ($q_x = 1/4$ and $\delta = 0.04$ reciprocal lattice unit [rlu], respectively), that formed near Bragg points. Such a wave vector is consistent with the formation of 1-D modulations such as charge density waves (CDWs), or "charge stripes," which are tilted with respect to the Cu-O-Cu chain direction in YBCO. This observation is very significant for two reasons. First, evidence that CDWs co-exist with superconductivity in YBCO has been gleaned from a wide array of experiments, including reverse-bias scanning tunnelling microscopy (STM) [1], neutron diffraction [2], nuclear magnetic resonance/nuclear quadrupole resonance (NMR/NQR) [3-5], and far-infrared (FIR) ellipsometry [6]. Second, oxygen vacancies by which the charge-carrier concentration is controlled in YBCO may also order in a quasi-1-D manner in this system. However, because of the twinned nature of the crystal used in our experiment, it was difficult to obtain quantitative information on the anisotropy and temperature dependence of these modulations. In this work, we extended our study of superlattice peaks associated with CDWs and/or lattice modulations and determined $\mathbf{q}_0$ unambiguously in carefully prepared detwinned crystal of YBCO.

Methods and Materials

The detwinned crystal of optimally doped YBCO used in our study had been grown at the ANL Materials Science Division. It was a thin, rectangular, 2×1-mm plate with a thickness of less than 100 μm. The crystallographic **c**-axis was perpendicular to the large facet. The magnetization measurements revealed a sharp transition at ~91.5K, suggesting a high degree of compositional homogeneity in the bulk of the sample. The high-energy study was carried on at X-ray Operations and Research beamline station 4-ID-D by using 36-keV x-rays. A Si(111) reflection was used to monochromatize the beam, with the undulator fifth harmonic tuned to provide maximum flux at this energy. Intensity was measured by using a scintillator detector. The sample was cooled in a closed-cycle He refrigerator.

Results

The two right panels in Fig. 1 show scans along **a*** (along the shortest Cu-O-Cu bonds; H scan) and **b*** (parallel to the CuO chains; K scan) near the (5, 0, 0) charge Bragg peak at several temperatures. A diffuse superlattice peak corresponding to a wave vector of $\mathbf{q}_0 = (1/4, 0, 0)$ is observed above the thermal diffuse scattering (TDS) emanating from the Bragg point. The peak intensity is ~450 counts/second, which is some 10^7 orders of magnitude weaker than that of a Bragg peak. The peak width in the **a*** direction is much larger than the resolution, indicating a shorter range of correlation along the **a** axis. Along the **b** axis, the correlation length is slightly larger. It is clear from H and K scans that as the temperature is lowered, the peak gets stronger. In fact, integrated intensities obtained from the data revealed a linear increase (not shown) with decreasing temperature. Similar behavior was also observed in an underdoped compound $YBa_2Cu_3O_{6.63}$ [7] for which the modulation vector was (~2/5, 0, 0). From the K scans, one can see that the central peak corresponding to the satellite appears exactly at K = 0, thereby establishing the wave vector to be $\mathbf{q}_0 = (1/4, 0, 0)$. The use of detwinned crystal made it clear that $\mathbf{q}_0$ is not (0, 1/4, 0).

In addition to the central satellite peak in the K scans, there is a diffuse component underneath the central satellite peak. The bottom panel on the left (Fig. 1) displays a 2-D scan in the vicinity of the (4, 0, 0) Bragg peak, which reveals the characteristic bow-tie-shaped Huang diffuse scattering (HDS) indicative of lattice strain effects. The middle panel on the left shows a set of line scans at different temperatures. As the

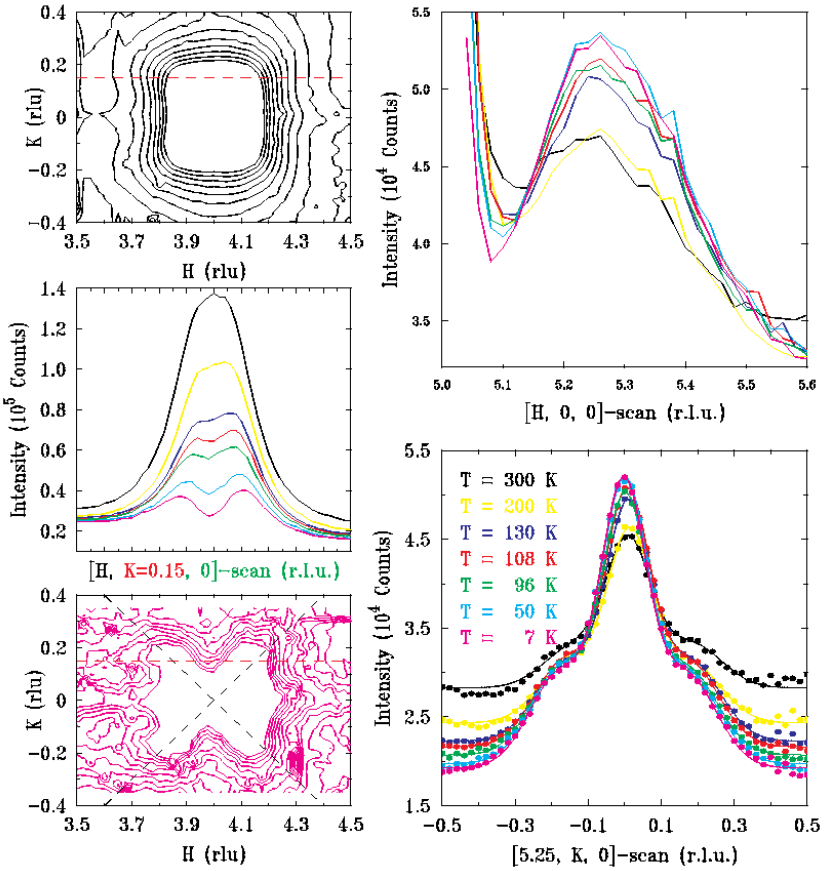

*FIG. 1. Left panels: Bow-tie-shaped HDS around the (4, 0, 0) Bragg peak. The red dashed line in the top and bottom panels indicates the 1-D line scans presented in the middle panel. Right panels: Scans along the **a*** axis (or [1, 0, 0]) and **b*** axis (or [0, 1, 0]), respectively, near the (5, 0, 0) Bragg peak at several temperatures. Low-temperature enhancement of the diffuse peak is clearly visible. The temperatures that correspond to the different colors are shown in the bottom panel on the right.*

temperaure is increased, rapidly growing TDS overwhelms the HDS. At room temperature (top panel on the left, Fig. 1), only TDS characteristic of the orthorhombic YBCO structure is visible.

Discussion

We made the unambiguous observation that a four-unit-cell superstructure, $\mathbf{q}_0$ = (1/4, 0, 0), coexists with superconductivity. Additional data collected to obtain information on the details of the modulation reveal that atomic displacements on CuO chains and on BaO and CuO_2 planes, due respectively to CDWs or oxygen-vacancy ordering, play a critical role in forming these superlattice peaks. However, since oxygen diffusion essentially freezes below ~250K, the growth of oxygen-ordered patches in size or in number seems unlikely to account for the near-linear increase of intensity. Currently, a detailed model of atomic displacements coupled to electronic density modulation is worked out to fit the data.

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