

High-Energy X-ray Scattering Study of Underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6.63}$

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Introduction

Recent inelastic neutron-diffraction measurements observed anomalies in the phonon dispersion curves in YBCO superconductors.¹ These anomalies occur at twice the wavevector, e.g., at $(\sim 0.2, 0, 0)$ for $\text{YBa}_2\text{Cu}_3\text{O}_{6.60}$ (YBCO), of the *incommensurate* spin fluctuations found in the same material.² The phonon anomalies persist even at room temperature and have been attributed to dynamic charge stripes separating the spin stripes. However, dynamic charge fluctuations or charge density waves (CDW) cannot be observed directly by neutrons, which prompted us to undertake an x-ray scattering experiment to search for charge fluctuations. Such measurements have revealed charge stripes in the $\text{La}_{1.48}\text{Nd}_{0.4}\text{Sr}_{0.12}\text{CuO}_4$ compound.³ In this report we present the preliminary results of a hard-x-ray-diffraction study on an underdoped YBCO close in composition to that for which strong phonon anomalies were observed. The study of underdoped YBCO is, however, rather complicated due to the prevalence of oxygen-vacancy ordering in the CuO-chain planes. According to recent x-ray diffraction work,⁴ in the underdoped YBCO studied here, both the so-called orthorhombic-II and orthorhombic-V phases are presumably present.

Experimental Details

Initial characterization was carried out on the SRI CAT 1-ID beamline using a Weissenberg camera with an incident photon energy of 65 keV. We used a small twinned crystal for this study. The sample was a thin rectangular $500 \mu\text{m} \times 500 \mu\text{m}$ plate with a thickness of $\sim 100 \mu\text{m}$. The crystallographic c axis was perpendicular to the flat facet. The magnetization measurements revealed T_c to be 60K with the width of the transition being $\sim 0.5\text{K}$, suggesting a high degree of compositional homogeneity in the bulk of the sample. Although the transition is sharp, we have observed the presence of weak Debye-Scherrer rings, indicating the presence of small amounts of extraneous phases either on the exterior or in the bulk of the sample. Further study was carried out on the SRI CAT 4-ID beamline using 36 keV x-rays. A Si (1 1 1) reflection was used to monochromatize the beam with the undulator fifth harmonic tuned to provide maximum flux at this energy. In order to suppress background and improve resolution, a Ge (1 1 1) crystal was used as an analyzer. For intensity measurements the analyzer was removed. The sample was cooled in a closed-cycle He refrigerator.

Results

The top panel in Fig. 1 shows a scan along \mathbf{a}^* in between the $(4, 0, 0)$ and $(5, 0, 0)$ charge peaks at 14K, taken with the Ge analyzer in place. There appears to be *no* significant scattering above the diffuse tails near the expected incommensurate CDW peaks at $(\sim 4.2, 0, 0)$ and $(\sim 4.8, 0, 0)$, respectively. However, two diffuse peaks corresponding to $(\sim 2/5, 0, 0)$ are clearly visible. The

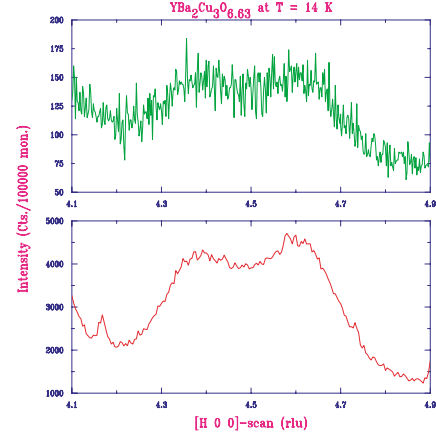


FIG. 1. $[H 0 0]$ scans at 14K between the $(4, 0, 0)$ and $(5, 0, 0)$ Bragg peaks. Top: with Ge analyzer. Bottom: without an analyzer.

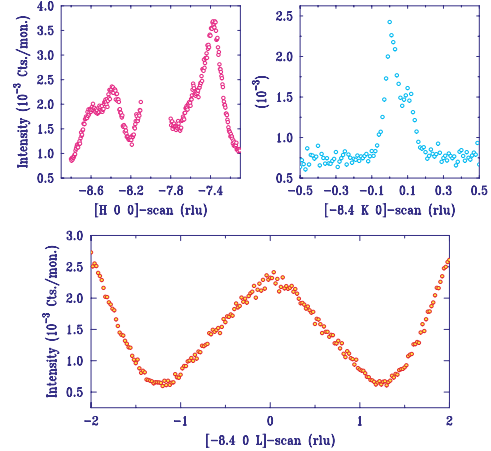


FIG. 2. Top left: $[H 0 0]$ scan near the $(-8, 0, 0)$ peak. Top right: $[K 0 0]$ scan through the $(-8.4, 0, 0)$ diffuse peak. Bottom: L scan through $(-8.4, 0, 0)$. All scans were taken at 14K.

absence of a clear valley at $(4.5, 0, 0)$ suggests the presence of an unresolved relatively weak peak. For comparison the same scan was taken with the analyzer removed and receiving slits left wide open to insure better interception of the diffuse intensities (bottom panel). There is an overall increase in the intensity by an order of magnitude with a larger enhancement of the diffuse peaks. In addition, a weak peak near $(\sim 4.17, 0, 0)$ appears, which is due to some impurity grain. Note that there is no corresponding peak at $(\sim 4.83, 0, 0)$ where the diffuse tail is even weaker. Indeed, careful scans near $(2, 0, 0)$ and all the charge peaks including $(10, 0, 0)$ revealed no sign of weak, broad peaks above the diffuse tails near the Bragg peaks.

Figure 2 shows a set of detailed $[H 0 0]$ (top left), K (top right), and L (bottom) scans near $(-8, 0, 0)$. Diffuse peaks corre-

sponding to $(2/5, 0, 0)$ are present on either side of the Bragg peak. These peaks are broad indicating short-range correlations along the **a** axis. A $[K 0 0]$ scan through $(-8.4, 0, 0)$ shows the peak to be sharper, suggesting a longer correlation length along the CuO chains (**b** axis). The bottom panel shows a scan along the **c*** axis through the $(-8.4, 0, 0)$ peak. Oscillations of the intensity are clearly observed suggesting that a finite number of scattering planes are correlated along the **c** axis. Similar modulations along **c*** were also observed for the $(1/2, 0, 0)$ peak measured through the $(-2, -2.5, 0)$ position.

Remarks

Although we do not have any clear evidence of any CDW peaks due to charge stripes, we have observed diffuse peaks corresponding to $(1/5, 0, 0)$ and $(1/2, 0, 0)$. These peaks are consistent with oxygen-vacancy ordering mentioned above. Oxygen ordering gives rise to lattice distortions, which produce diffuse scattering. The nature of the distortions is currently being studied.

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