

Neutron diffraction investigation of charge-density-wave formation in underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6.67}$

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We report on our neutron diffraction measurement of the charge-density-wave (CDW) modulation in the underdoped cuprate superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{6.67}$. Previous attempts to perform such a study have been hindered by a large background from the sample, sample holder and environments. In this experiment, we make use of the extremely low extrinsic background of D10 in triple-axis mode to measure a single crystal of $\text{YBa}_2\text{Cu}_3\text{O}_{6.67}$. Indeed an indication of a temperature dependent peak is found for one of the Q_{cdw} positions investigated. This constitutes the first evidence for CDW in the cuprates using neutron scattering.

1 Scientific Background

In recent years the competition between different ground states has become a central point in many theories of high-temperature superconductors (HTS). A state with coexisting spin and charge order, known as stripe order, is observed in $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ and $\text{La}_{1.6-x}\text{Nd}_{0.4}\text{Sr}_x\text{CuO}_4$ and has been discussed extensively [1]. Recent observations of quasi-elastic two-dimensional charge-density waves (CDW) for $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ (YBCO) by the use of x-ray diffraction techniques, seem to contradict the universality of the stripe order in the cuprates [2, 3, 4, 5, 6]. It has been shown that the CDW in YBCO competes with HTS, from its temperature and field dependences [5, 6], and with spin correlations in Zn doped samples [6].

The CDW is present in the pseudo-gap phase, where an electronic order is suggested by numerous other probes including high-field NMR [7, 8], and the Hall effect [9]. Quantum oscillations that demonstrated the existence of Fermi pockets are also seen on samples in the doping region where the CDW is observed [10]. In contrast to the other methods x-ray diffraction observes the CDW in YBCO at zero-field. The difference could be due to the different timescales involved, but the energy resolution with x-rays has proven to be too large to accurately determine its lifetime [11, 12]. Therefore an investigation of the charge excitations using neutron diffraction with high energy resolution is needed. Additionally the temperature dependence would give an answer to whether the CDW order is directly related to the pseudo-gap phase.

2 Experimental Setup and Procedure

The sample used is a detwinned single crystal of $\text{YBa}_2\text{Cu}_3\text{O}_{6.67}$ ($T_c = 66$ K) with a mass of 70 mg, mounted on an Al pin to minimize background. After determining the orientation matrix in diffraction mode, the D10 instrument was used with the analyzer mounted. This allowed to reduce the background level to ~ 1 count/min.

In this configuration, we performed measurements close to three positions $Q=(2.3,0,0.5)$, $(0,2.3,0.5)$ and $(0,0.3,6.5)$, where a satellite peak associated with the CDW formation is expected. In figure 1, the results for the first two positions are shown, where no peak above the background level was resolved. The associated Bragg peak intensities divided by 10^6 are shown for comparison, since that is the level ex-

pected from x-ray investigations.

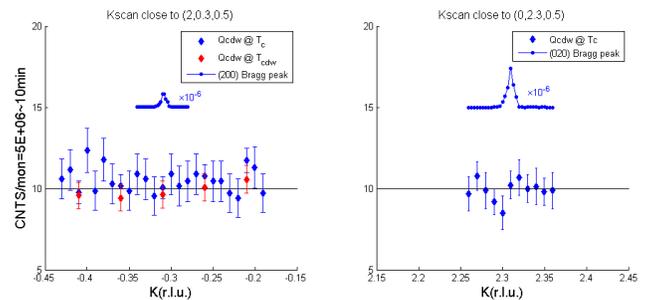


Figure 1: No peak was detected above the background level for $Q=(2.3,0,0.5)$ in the left and $(0,2.3,0.5)$ in the right. The intensity of the closest Bragg peak is shown for reference with scaled down by 10^6 .

Figure 2 shows the rocking curve through the last position $(0,0.3,6.5)$, where a small intensity appears above the background level taken at $T_{cdw} = 160$ K. This is the first evidence for CDW using neutron scattering.

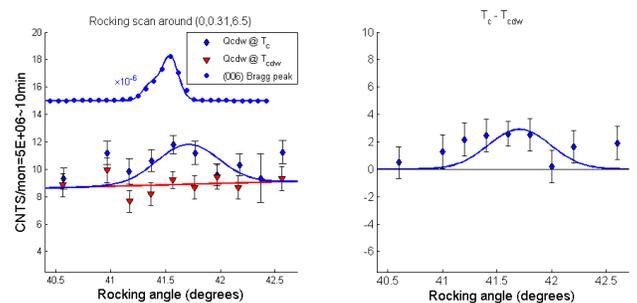


Figure 2: A small peak at the CDW position $Q=(0,0.3,6.5)$ is identifiable in the rocking scan at $T_c = 66$ K that disappears at higher temperature $T_{cdw} = 160$ K. The temperature subtraction is shown on the right giving an amplitude of ~ 0.2 counts/min.

The integrated intensity in the rocking scan corresponds to 3×10^{-6} compared to the $(0,0,6)$ peak, and 0.077 of the ortho-VIII superlattice peak $(2.375,0,0)$, which are roughly consistent with previous x-ray measurements [3].

3 Conclusions and Outlook

Due to the small intensity of the peak found and the previous time spent looking for the best position to get it, a measurement of the energy dependence was not possible to realize in the allotted. Nevertheless, given that the background is currently mostly coming from the instrument (analyzer off tests), a more efficient measurement would be possible by increasing the sample mass by making a compact array of single crystals. Increasing the mass by a factor of 10 and now that the correct position has been found the full measurement at several temperatures could be done in ~ 5 days.

4 References

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