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A Detailed Scanning Tunneling Microscopy Study of the CuO chains in $YBa_2Cu_3O_{7-x}$

D. J. Derro,[a] E. W. Hudson,[b+] K. M. Lang,[b] S. H. Pan,[b*] J. C. Davis,[b] K. Mochizuki,[a#] J. T. Markert,[a] and A. L. de Lozanne[a]

[a]Department of Physics, The University of Texas at Austin, Austin, TX 78712-1081

[b]Department of Physics, The University of California, Berkeley, CA 94720-7300

We have previously reported a 1.36-nm DOS modulation in the CuO chains on the surface of cold-cleaved, atomically-resolved YBCO.[1,2] We have recently completed new experiments in which we obtained detailed spectroscopic data on the same crystal plane, thereby confirming and extending our earlier work. Here we present data showing twin boundaries and steps, and focusing on the effects of these structures on the CuO chain DOS modulations.

1. INTRODUCTION

The study of high T_c superconductors like YBCO is complicated by their layered structure. The superconductivity is thought to solely reside in the CuO planes. Yet the other layers are integral to the structure and electronic properties of YBCO. It has been proposed that the proximity effect may induce superconducting signatures in the CuO chain layer because it resides near the CuO planes. Therefore, it may prove fruitful to probe these other layers by STM after cleaving the YBCO crystal.

Previously, we have probed the CuO chain layer in YBCO using STM. In these earlier studies, we observed a 1.36-nm wavelength in the CuO chain DOS modulations.[1,2] We proposed that these modulations are caused by a Charge Density Wave (CDW).[2] This proposal generates numerous questions as to the origin of the energy gap seen in these CuO chains. For example, could the energy gap be a CDW gap rather than a superconducting energy gap? This prompted a detailed spectroscopic study of the CuO chain layer where a new set of electronics was used for our STM.[3,4] These electronics allowed simultaneous spectroscopic and topographic data acquisition that are then correlated to each other. We found many interesting features related to the spatial dependence of this energy gap upon the surface topography.[3,4] For instance, the energy gap was suppressed near point defects, but enhanced when distant from them.[4] We also were able to explain the large zero bias conductance that other point spectroscopic studies had seen.[4] In addition, other groups confirmed the existence of this charge modulation in YBCO by using scattering techniques to probe the bulk properties. Mook *et al.* found one dimensional fluctuations with a slightly larger wavelength of 1.665 nm by using neutron scattering thereby confirming our discovery in the bulk as well.[5] Also, there is more recent supporting evidence from NMR investigations.[6]

Our most recent investigations, reported here, both confirm and extend our previous detailed spectroscopic studies. We obtained higher resolution spectroscopic data because of the use of lower temperatures (4K) and better electronics. In this case, the spectroscopic data is taken as conductance measurements as a function of position on the surface. Topographic data is taken prior to and during spectroscopic data acquisition. The experimental setup is described elsewhere.[7]

[+]Present Address: National Institute of Standards and Technology, Gaithersburg, MD 20899
[*]Present Address: Department of Physics, Boston University, Boston, MA 02215
[#]Present Address: KLA-Tencor Corporation, San Jose, CA 95134

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2. YBCO CuO CHAIN PLANE SURFACE

We took STM topographic images of the CuO chain layer in YBCO after cold cleaving *in situ*. This surface proved to be rich in structural features, as seen in the figure below containing a terrace between step edges (indicated by the double-headed arrow), CuO chains (indicated by the two arrows that meet at 90 degrees), and a twin boundary (which runs diagonally between the two vertical arrows).

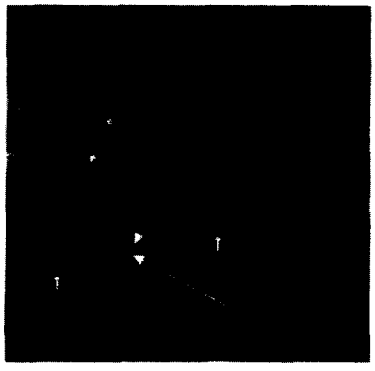

Figure 1. 50 x 50 nm^2 scan with step edges (I = .01 nA, V_{sample} = -100 mV).

Because one can see faint chains in all three levels, the edges step down to different CuO chain planes, separated by 1.2 nm, which is one unit cell length. This is common to step edges seen previously.[8]

2.1 CuO Chains

The CuO chains are the only one dimensional feature in the YBCO structure. A high resolution topographic image of the CuO chains is seen below in Figure 2. The dark regions correspond to missing atoms in either the CuO chain plane or the underlying plane. The charge modulations along the chain direction are clearly visible in the above image. One can also see the constituent atoms that make up the modulations in the left half of the image. For comparison, a larger image is presented below in Figure 3. It is important to point out a difference in the above two CuO chain images: in Figure 3, what appears to be individual CuO chains are actually 3 or 4 neighboring chains that have their charge

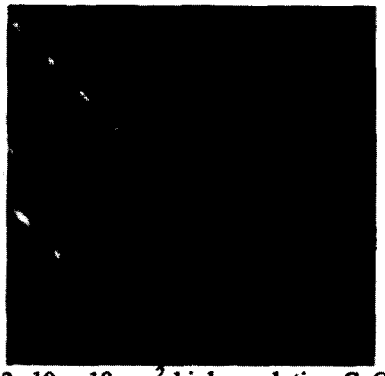

Figure 2. 10 x 10 nm^2 high resolution CuO chain layer image (I = .03 nA, V_{sample} = 60 mV).

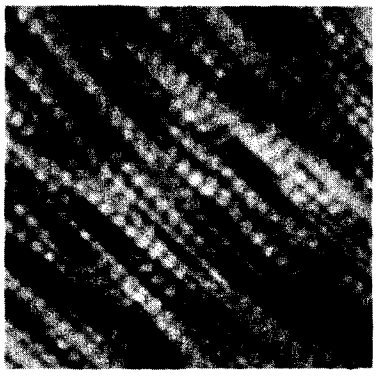

Figure 3. 25 x 25 nm^2 CuO chain layer image (I = .01 nA, V_{sample} = -100 mV).

modulations in phase. One can see this by counting the number of parallel chain modulations seen and comparing it to the unit cell dimension of approximately .4 nm. One can also verify this assertion by noticing that in Figure 2, the charge modulations appear to be correlated to a length of about 3 or 4 neighboring chains. Therefore, it makes sense that larger scans effectively blur together individual chain modulations.

2.2 Twin Boundary

Because a twin boundary imposes a natural boundary to the one dimensional nature of the CuO chains, we studied them in detail. A high resolution larger scan of a twin boundary is shown below.

Figure 4. 50 x 50 nm^2 high resolution image of twin boundary (I = .1 nA, V_{sample} = -100 mV).

The CuO chains are seen to meet at 90 degrees along a nearly horizontal line in this image.

Another very curious feature of this data set is that the correlations themselves appear to have an average persistence length of around 15 nm. This behavior is easily seen in either Figure 2 or in Figure 3. By focusing on CuO chains that are not terminated by defects, one can see a beginning and end to the correlation. The end of the correlations are marked by a fuzzy area where the electronic correlations are less pronounced. Therefore, instead of the surface being made up of in-phase DOS modulations that are continuous and thread-like, it appears to the eye that the modulations are more like smaller and shorter lengths of thread that yield a 'weave' pattern instead of a uniform homogeneity.

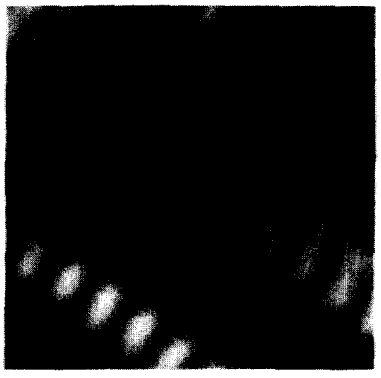

Figure 5. 10 x 10 nm^2 close up of twin boundary (I = .01 nA, V_{sample} = -100 mV).

An interesting feature which is also seen is that the modulations go right up to the boundary. Therefore, the twin boundary apparently does not affect the appearance, behavior, and properties of the DOS modulations. This can be easily seen in the close up image in Figure 5 of the twin boundary from Figure 1. An estimation of the width of the twin boundary from this close-up image yields approximately 1 nm.

2.3 Step Edge

Step edges also provide a boundary condition to the one dimensional nature of the CuO chains and their associated DOS modulations. We were interested in how the modulations interact with this interruption. A close up topographic image was taken of another step edge. One can identify with difficulty the CuO chains moving diagonally from upper left to lower right. It is striking that although the step edge is very jagged, there is a uniformity as the steps appear to be parallel to each other, which is also seen in Figure 1. This may say something about the ease of cleaving this particular plane, which would support our findings as we have imaged this plane many times in the past.[1,2,3,4]

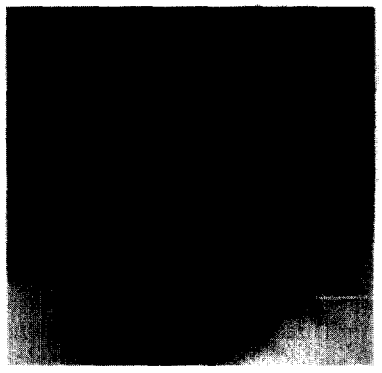

Figure 6. 31.2 x 31.2 nm^2 scan of double step edge (I = .2 nA, V_{sample} = -200 mV).

3. SPECTROSCOPY

The spectroscopic data was acquired using a lock-in amplifier. A topographic image is taken prior to and simultaneously with the spectroscopy, therefore, one can verify that there is negligible

thermal drift for this instrument which has been described elsewhere.[7] The conductance (dI/dV) as a function of position for three different energies is displayed below in Figure 7 for the step edge seen in Figure 6. The step edge in Figure 6 provides a boundary condition to both sides of the one dimensional CuO chains in the middle step. Therefore, this unique scenario can be studied in detail and compared to a similar case where chain modulations are terminated by point defects as seen above. The entire data set consists of 101 conductance planes, taken in 1 mV steps. To get a feel for the whole picture, the data set is more spectacularly viewed as a continuous movie showing all 101 energy planes. The sheer complexity of the independent behavior of different chains then becomes apparent. We are presently investigating this complicated behavior.[9] We display below three representative planes, two inside the energy gap and one outside.

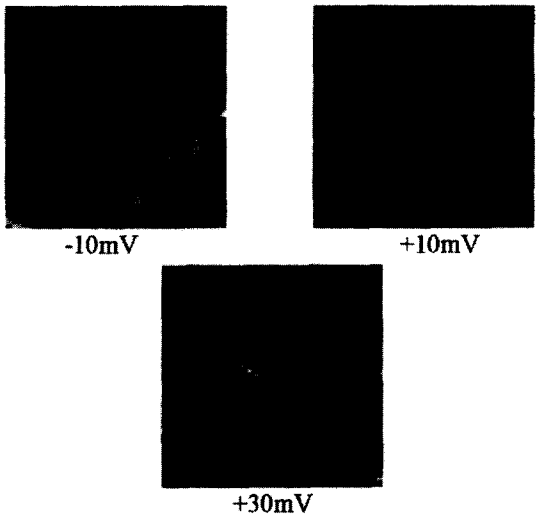

Figure 7: Three 31.2 x 31.2 nm^2 conductance (dI/dV) images for the step edge in Figure 6.

A truly remarkable feature of these images is the fact that different CuO chains have different conductances (light up) at different energies. Therefore, when taking a normal topographic STM image on the CuO chain surface, different chains contribute variable amounts to the integrated density of states (DOS). The explanation of this effect is still under investigation but the simplest explanation would be that each DOS modulation scatters off of point defects and step edges and, therefore, acts like a particle in a 1-dimensional box.

4. CONCLUSION

The YBCO CuO chain plane has a unique 1-d electronic structure, significant in its effects on high T_c superconductivity and also fascinating for its own physics. STM measurements have revealed several extraordinary properties of this system. The new high resolution spectroscopic data (in conjunction with topographic features such as twin boundaries, and step edges) that we present here confirms our previous work and provides new information as to the electronic structure of the CuO plane at the atomic scale. This research area should prove a fertile ground for further investigation.

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