MAGNETIC AND CHARGE FLUCTUATIONS IN HIGH-\(T_c\) SUPERCONDUCTORS

H. A. Mook,\textsuperscript{a} F. Dogan,\textsuperscript{b} and B. C. Chakoumakos\textsuperscript{a}

\textsuperscript{a}Solid State Division, Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831-6393

\textsuperscript{b}Department of Materials Sciences and Engineering
University of Washington
Seattle, Washington 98195, USA

"The submitted manuscript has been authored by a contractor of the U.S. Government under contract No. DE-AC05-96OR22464. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes."

prepared by
SOLID STATE DIVISION
OAK RIDGE NATIONAL LABORATORY
Managed by
LOCKHEED MARTIN ENERGY RESEARCH CORP.
under
Contract No. DE-AC05-96OR22464
with the
U.S. DEPARTMENT OF ENERGY
Oak Ridge, Tennessee

September 1998
DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, make any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.
DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.
MAGNETIC AND CHARGE FLUCTUATIONS IN HIGH-$T_c$ SUPERCONDUCTORS

H. A. Mook, F. Dogan, and B. C. Chakoumakos

Neutron scattering has been used to study the spin fluctuations in the YBa$_2$Cu$_3$O$_{7.5}$ and Bi$_2$Sr$_2$CaCu$_2$O$_8$ materials. Evidence is found for both incommensurate fluctuations and a commensurate resonance excitation. Measurements on the lattice dynamics for YBa$_2$Cu$_3$O$_{6.6}$ show incommensurate structure that appears to stem from charge fluctuations that are associated with the spin fluctuations.

INTRODUCTION

Neutron scattering measurements continue to provide information of direct relevance to some of the most important issues in the high-$T_c$ cuprate superconductors. The magnetic excitations of these materials are the spin fluctuations, and recent measurements have shown that the low-energy spin fluctuations in YBa$_2$Cu$_3$O$_{6.6}$ (YBCO6.6) are incommensurate in nature while a commensurate excitation that is relatively sharp in energy called a resonance is found at about 35 meV. The incommensurability was originally discovered by the filter integration technique that integrates over the outgoing neutron energy in a direction along $c^*$ and thus provides a high data collection rate for the study of lower dimensional excitations. The disadvantage of the technique is that no discrete energy information is available. Thus when a discovery is made by the integration technique further measurements are made by triple-axis or time-of-flight techniques to determine the energy spectrum. Fig. 1a shows the direction of the integrating scan that is made through the point ($\pi, \pi$) to observe the incommensurate fluctuations shown by the dots at the position $\delta/2$ from the commensurate position. Such a scan employs high resolution along the scan direction, but coarse resolution perpendicular to the scan direction and thus cannot determine the exact wave vector position of the incommensurate peaks. The result of the scan for YBCO6.6 is shown in Fig. 1b. The ($\pi, \pi$) position is at (0.5, 0.5) in reciprocal lattice units (r.l.u.).

A recent measurement using a pulsed spallation source with time-of-flight energy determination has used a two-dimensional position-sensitive detector bank to determine the wave vector and energy of the YBCO6.6 incommensurate peaks. The peaks are found to be along the (0, $\pi$)

---

$^a$Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6393, USA

$^b$Department of Materials Sciences and Engineering, University of Washington, Seattle, Washington 98195, USA
and (n, 0) directions as shown in Fig. 1a. The peaks are therefore not exactly on the scan direction shown in Fig. 1a, but are above and below it being observed in the integrated scan through the relaxed vertical resolution. The peaks in the scan in Fig. 1b are found at about 0.055 on either side of the commensurate point. The wave vector of the incommensurate scattering is then $\sqrt{2}$ times 0.055 from the geometry in Fig. 1 and this value must be multiplied by $\sqrt{2}$ again as the scan is in units of (h, h) giving $\delta/2 = 0.11$ or $\delta = 0.22$. The number determined from the time-of-flight measurement is $0.21 \pm 0.02$ r.l.u.. This incommensurability is essentially identical to that observed in similarly doped $^4$La$_{1-x}$Sr$_x$CuO$_4$ (214). It was found that the intensities and the correlation lengths are also very similar in the (214) single-layer and YBCO (123) bilayer materials, thus the low energy spin fluctuations appear to be universal for the high-$T_c$ cuprate materials measured to date.

**MAGNETIC FLUCTUATIONS IN BSSCO**

$^5$Bi$_2$Sr$_2$CaCu$_2$O$_8$ (BSSCO) or (2212) is a high temperature superconductor of considerable importance as one can cleave the material easily to obtain a good surface for photoemission measurements and other surface sensitive techniques. Unfortunately it is difficult to obtain the large single crystals needed for neutron scattering for the BSSCO composition. We were successful in growing rods of the material which have a [110] reciprocal lattice direction along the rod direction (using the same definition of a and b as for YBCO). It was then possible to align a number of these rods together to form a sample of 35g for neutron studies. We then have a crystal with one set of the [110] directions aligned and this permits some information to be obtained.

A difficulty with the sample for the study of magnetic excitations is that the material has bilayers similar to those in YBCO and thus we expect that the magnetic fluctuations are coupled in a similar way. In this case the low energy magnetic fluctuations have no structure factor unless a finite value of $c^*$ is used and $c^*$ is randomly orientated perpendicular to the aligned direction of the crystal. One must then set the spectrometer to sample a point off the [110] direction which means that only some of the $c^*$ values desired fall within the resolution volume of the spectrometer, considerably reducing the magnetic signal.

One might expect that a resonance excitation might exist in BSSCO in a similar way as for YBCO and one can search for it in the same way$^5$ using a triple-axis spectrometer. Our sample of BSSCO has an oxygen composition near optimum doping and we expect that the resonance will not be observable much above $T_c$ in this case. The simplest experiment is thus to scan energy at the momentum value where the resonance is expected and take the difference between data taken well below $T_c$ and data taken above $T_c$. This works in YBCO, but fails in BSSCO for two related reasons. The first is that the signal is small relative to the phonons as we cannot achieve the full magnetic intensity that would be available at a fixed value for $c^*$. The second
problem is the phonons are much more temperature sensitive in BSSCO than they are in YBCO so that the difference in data at high and low temperatures strongly reflects the phonon differences. The only way to circumvent these difficulties is to use a polarized neutron beam to isolate the magnetic scattering. This unfortunately results in even less intensity as polarized beams are much weaker than unpolarized ones. Nevertheless, after considerable counting reasonable results were obtained. Momentum values near (0.5, 0.5) and (1.5, 1.5) were both tried and similar patterns were obtained with the magnetic scattering near (1.5, 1.5) being considerably weaker because of the magnetic form factor. The results are shown in Fig. 2. A peak in energy about 10 meV wide, which is equal to the energy resolution of the experiment, is observed at 10K while the result at 100K appears rather featureless. The peak is only found in the spin flip channel guaranteeing that it is magnetic. The peak is observed at about 37 meV which is near the value expected if the $T_c$ of the BSSCO of 84K is scaled to that of YBCO for the same doping level. The results strongly suggest that BSSCO has a resonance excitation rather similar to that of YBCO. However, the results should be checked with single crystals when they become available.

The same BSSCO sample was employed to search for magnetic incommensurate fluctuations. The integration technique was used in the same way as for YBCO6.6. The experiment works in a similar manner except that the integration now takes place over the directions perpendicular to the [1,1,0] direction and thus is only partly along c*.

For two-dimensional scattering from bilayers this results in an intensity loss in the magnetic signal. However, we see from Fig. 1 the magnetic signal in the integration technique is substantial so that an intensity loss may be tolerated. The results of the measurement are shown in Fig. 3. Fig. 3a shows data presented in the same way as for the YBCO6.6 in Fig 1. The results suggest the possibility of small incommensurate peaks although the counting errors are larger than desired. The data shown are from a number of runs averaged together. Fig. b-d show one of the satellite peaks measured at different temperatures. In this case the background was obtained by a 30 deg. rotation of the sample relative to the position where the scan is performed. The magnetic signal is expected to be small in the 30 deg. rotation case which samples reciprocal space well removed from (0.5, 0.5). The signal decreases with temperature as would be expected for a magnetic excitation. The peak is broad so the center is hard to determine accurately with the errors involved, however, the peak appears to be centered at about 0.42 r.l.u. or 0.08 r.l.u. units from the (0.5, 0.5) position. If the magnetic satellites are arranged as in Fig. 1, $\delta$ would be about 0.32. The value of $\delta$ for fully doped 214 materials is about 0.25 so the $\delta$ value for BSSCO appears to be somewhat larger than for the 214 materials assuming the same type of incommensurability. However, the BSSCO measurement has sizable counting errors and we do not know the actual pattern of the incommensurability. A measurement on a single crystal is needed for a more accurate determination. Until such an experiment is performed the present
result suggests that BSSCO has low energy incommensurate fluctuations which may be similar to those found in 123 and 214 materials.

**CHARGE FLUCTUATIONS IN YBCO**

Neutrons cannot measure charge directly, but can observe a change in the mass density that is either static or dynamic. One can assume that static mass displacements reflect static charge ordering and such effects have been observed in the 214 cuprate materials in special cases. Dynamic charge ordering has not been observed so far and the present results serve as an indication that this occurs in the YBCO materials. We have made measurements on the same YBCO6.6 sample in which the incommensurate magnetic fluctuations are observed. Again we start with the integration technique except we examine the region around the peaks of the reciprocal lattice stemming from the atoms rather than from the magnetism. Fig. 4 shows scans around the (1, 0) reciprocal lattice peak. Data are again shown that use a measurement at 300K as a background. As the sample is cooled distinct peaks form on both sides of the (1, 0) peak that we assume reflects a dynamic incommensurate mass fluctuation that can be considered to stem from an incommensurate charge fluctuation. However, we have not completely ruled out magnetic effects. We note the peaks are small, being an order of magnitude smaller than the magnetic satellite peaks shown in Fig. 1.

The scan is along the (h, 0) reciprocal lattice or the (n, 0) direction and thus is along the direction of the magnetic incommensurate scattering. The charge fluctuation peaks are about 0.22 in r.l.u. units from the commensurate position so that the δ/2 value for them is 0.22 or twice the wave vector of the incommensurate magnetic satellites. However, the absolute direction of the incommensurate wave vector cannot be determined with the integration technique and the peaks could be at a wave vector off of the (n, 0) direction. Fig. 4d shows an identical measurement for YBCO6.35 which has only commensurate magnetic order. No indications of incommensurate charge fluctuations are found for this material.

Work has been underway with triple-axis spectrometry to determine the energy spectra of the charge fluctuations, but that work is still incomplete. It has been noted however, that certain phonon branches show anomalies at the wave vector of the charge fluctuations. The origin of the charge fluctuations is not clear. It would seem extremely likely that the magnetic and charge fluctuations stem from the same source. Obviously the observation of charge fluctuations strongly suggest a dynamic striped phase in YBCO6.6. However, other possibilities exist including Fermi surface effects or dynamic charge density waves. The next step is to determine the energy spectra and absolute wave vector of the incommensurate charge scattering.
CONCLUSION

We have shown new neutron scattering results for the cuprate superconductors. Measurements on a BSCCO sample of crystals with a [110] direction aligned show strong evidence for a resonance excitation and indications of incommensurate magnetic fluctuations. It would be good to have these results confirmed by a high quality single crystal. For YBCO6.6 clear dynamic incommensurate peaks are observed at low temperatures on either side of the (1, 0) reciprocal lattice peak. Since these are found at positions relative to the crystal reciprocal lattice they are assumed to stem from mass fluctuations driven by charge fluctuations. No such peaks are found for a YBCO6.35 sample. The wave vector of the charge fluctuation peaks is twice that of the magnetic fluctuations if we assume the charge peaks are on the (0, \( \pi \)) direction. It would seem likely the magnetic and charge excitations are related. The results give support to a dynamic striped phase model for the cuprate superconductors.
REFERENCES

FIGURE CAPTIONS

1. (a) shows the position of the magnetic incommensurate peaks found for YBCO6.6. The direction of the energy integrating scan used to discover the incommensurability is shown by the arrow. (b) shows the result of the integrating scan. The measurement was made at 10K while 300K data is used as a background since little magnetic scattering is found at 300K.

2. Polarized neutron measurement of the resonance excitation in BSCCO. (a) shows the result at 10K while (b) is the 100K result. The experimental resolution is about 10 meV so that the peak in (a) is resolution limited. A background determined by moving the analyzer off the Bragg position has been subtracted. A number of runs were averaged to obtain the counting errors shown.

3. Integrating scans made to search for incommensurate magnetic fluctuations in BSCCO. (a) shows a scan made in the same way as the scan for YBCO6.6 shown in Fig. 1(b). b-d show scans made over the lower wave vector incommensurate position. The scans are made with more momentum steps and several scans are averaged to obtain lower counting statistics. The background used is obtained by a rotation of the sample so the background samples a region removed from the (0.5, 0.5) magnetic position.

4. Integrating scans made around the crystal reciprocal lattice position (1, 0) for YBCO. (a)–(c) show that incommensurate structure appears at low temperatures at a wave vector twice that of the magnetic incommensurate satellites for YBCO6.6. A measurement made in the same way for YBCO6.35 which has only commensurate magnetic structure is shown in (d).
Fig. 1
Mook et al.
BSCCO

Polarized Beam Spin Flip

Fig. 2
Mook et al.
Fig. 3
Mook et al.
Fig. 4
Mook et al.