Solid State Communications, Vol. 87, No. 11, pp. 1035–1037, 1993.
Printed in Great Britain.

0038–1098/93 $6.00 + .00
Pergamon Press Ltd

MAGNETIC STRUCTURE OF Y_2BaCuO_5

I.V. Golosovsky

St.-Petersburg Institute of Nuclear Physics, Russian Academy of Sciences, Gatchina, 188350, St.-Petersburg, Russia

and

P. Böni and P. Fischer

Laboratorium für Neutronenstreuung, Eidgenössische Technische Hochschule Zürich und Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

(*Received* 5 *March* 1993 *by P. Wachter*)

The antiferromagnetic structure of the Cu spins and the Néel point in Y_2BaCuO_5 were redetermined by neutron powder diffraction. There are two possible collinear models with wave vector $\boldsymbol{k} = [0, 1/2, 1/2]$ and the spins directed along the c-axis. These models cannot be distinguished in powder diffraction. The ordered magnetic moment of the copper atom at saturation amounts to $0.55(3)\mu_B$.

FROM THE DISCOVERY of high temperature superconductivity many experiments suggest that magnetism plays an essential role in CuO_2-based superconductors. Therefore, the magnetic properties of the stable compounds from the triangle BaO–CuO–Y_2O_3 require a better understanding in order to evaluate the magnetic interactions in related high-temperature superconductors.

This is one of the reasons why the cuprates R_2BaCuO_5 known as "green phases" are being extensively investigated now. Magnetic structures have already been reported for Dy, Ho, Er, Tm and Yb compounds [1]. In the Y_2BaCuO_5 compound, where there is only one magnetic sublattice of Cu spins, the ordering with two wave vectors $\boldsymbol{k} = [0, 0, 1/2]$ and $\boldsymbol{k} = [1/2, 0, 1/2]$ has been claimed, following from the observation of two magnetic reflections $1, 0, 1/2$ and $1/2, 1, 1/2$ [2]. This ordering does not correspond to the structures of the Cu sublattice observed in [1]. In [3] the authors believe that the reflection $1/2, 0, 1/2$ attributed to the wave vector $\boldsymbol{k} = [1/2, 0, 1/2]$ is caused by magnetic scattering due to the Cu spins in the $YBa_2Cu_3O_x$ impurity phase. Besides, the structure reported in [2] is not compatible with the results of Mössbauer spectroscopy [4]. Therefore, we have undertaken a new neutron diffraction study of Y_2BaCuO_5. The results of these investigations are described below.

The measurements on a powder sample of Y_2BaCuO_5 were carried out in the high intensity mode on the diffractometer DMC [5] at the reactor Saphir of Paul Scherrer Institute. The neutron wavelength was 1.7036 Å. The 1.7 K pattern clearly showed two resolved magnetic reflections (Fig. 1). In a first step, the accurate cell parameters and the zeroshift were determined from the profile analysis of this pattern. Using them the observed magnetic reflections can be indexed as $0, 1/2, 1/2$ and $2, 1/2, 1/2$ and not as $1, 0, 1/2$ and $1/2, 1, 1/2$ as suggested in [2] (see Table 1). In addition in our experiments only the single wave vector $\boldsymbol{k} = [0, 1/2, 1/2]$ was observed.

The Y_2BaCuO_5 compound crystallizes in the orthorhombic space group *Pnma*. Copper atoms are distributed over the general fourfold positions: (1) $x, 1/4, z$; (2) $1/2 - x, 3/4, z + 1/2$; (3) $x, 3/4, -z$; (4) $x + 1/2, 1/4, 1/2 - z$. Carrying out the group theoretical calculations we found that any combinations of spins are possible. Only the magnetic reflections $0, 1/2, 1/2$ and $2, 1/2, 1/2$ were resolved from the nuclear ones. Therefore, their intensities for different models were calculated and compared with the observed ones. The atomic coordinates for calculating the magnetic structure factors were obtained by profile analysis of data collected in the paramagnetic phase at 20 K (Table 2). The coordinates found were practically the same as reported in a previous study [6] and as those obtained from data collected at 1.7 K.

Fitting the different modes A $(+ - - +)$, C $(+ + - -)$, G $(+ - + -)$ and F $(+ + + +)$, where the brackets designate the signs of four Cu spins, it turned out (Table 3) that the copper spins were

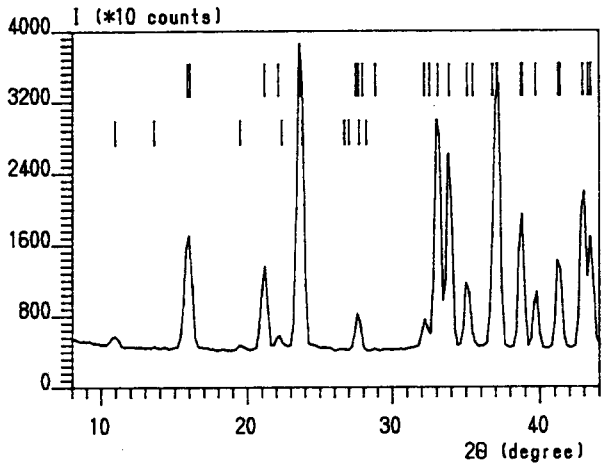

Fig. 1. Neutron diffraction pattern of Y_2BaCuO_5 at 1.7 K. The upper stripes mark the nuclear reflections and the lower ones the magnetic reflections.

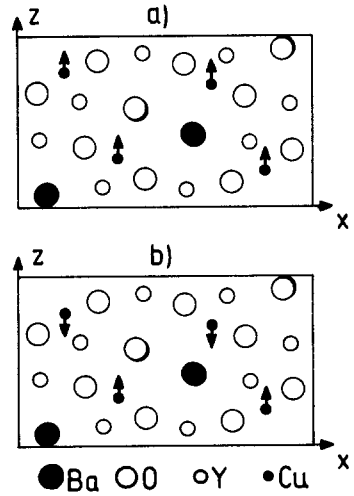

Fig. 2. Magnetic structures of Cu spins (shown by arrows) of Y_2BaCuO_5: (a) F mode, (b) A mode.

Table 1. Scattering angles (in degrees) of the magnetic reflections of Y_2BaCuO_5 *for a neutron wavelength of* 1.7036 Å

h	*k*	*l*	Calculated	Measured
0	1/2	1/2	10.961	10.92(3)
1	0	1/2*	10.487	
2	1/2	1/2	19.508	19.51(5)
1/2	1	1/2*	19.036	

The asterisks indicate the reflections reported in [1].

Table 2. Atomic coordinates of Y_2BaCuO_5 *obtained from neutron diffraction data collected at* 20 K

	x	*y*	*z*
Ba	0.0942(6)	0.25	0.0703(10)
Y1	0.0743(4)	0.75	0.3974(7)
Y2	0.2890(4)	0.75	0.1181(7)
Cu	0.6600(5)	0.75	0.7136(7)
O1	0.5663(4)	0.507(1)	0.8337(5)
O2	0.7726(4)	0.505(1)	0.6458(7)
O3	0.6003(6)	0.75	0.4227(9)

Table 3. Calculated and measured neutron intensities of magnetic reflections of Y_2BaCuO_5

h	*k*	*l*	Calculated	Measured
0	1/2	1/2	328	373(20)
2	1/2	1/2	137	111(17)

directed along the *c*-axis and that the ordering can be described by A or F modes (see Fig. 2). These structures cannot be distinguished in powder diffraction because the intensity of the magnetic reflections are the same. A wave vector $\boldsymbol{k} = [0, 1/2, 1/2]$ means that a translation along the *b* and *c* axes alternates the direction of all spins. Therefore, in spite of a ferromagnetic mode F in a chemical cell, the magnetic structure in a magnetic cell is antiferromagnetic. The ordered magnetic moment of Cu at saturation was found to be $0.55(3)\mu_B$. For its calculation we used the form-factor from [7]. The low value may be the result of a large degree of covalency [8]. The temperature dependence of the intensity of the magnetic reflection $0, 1/2, 1/2$ is shown in Fig. 3. The Néel point is approximately 16.2(5) K in good agreement with the data from optical spectroscopy [9, 10]. The magnetic modes of the Cu sublattice proposed were similar to those

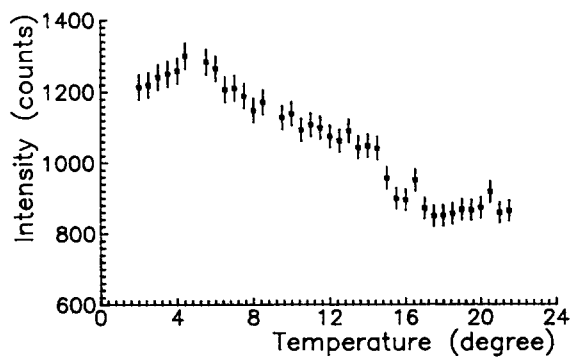

Fig. 3. Temperature dependence of the magnetic reflection $0, 1/2, 1/2$ of Y_2BaCuO_5.

reported for Dy_2BaCuO_5 at low temperature but in the last case the wave vector is $\boldsymbol{k} = [0, 0, 0]$. The observed wave vector $\boldsymbol{k} = [0, 1/2, 1/2]$ was also found in the compound Yb_2BaCuO_5 [1].

It is interesting to compare our results with optic investigations [9, 10]. Those authors have observed two different magnetic fields at the site of the rare earth ion caused by different Cu spin surroundings. They connect these fields with two different magnetic phases, because the ratio of the integral intensities of corresponding lines depends on the sample studied. These phases may be connected with our A or F modes which cannot be distinguished in powder diffraction. In the Y_2BaCuO_5 structure the CuO_5 pyramids are very isolated. Different links Cu–O–O–Cu may result in a coexistence of two magnetic phases described by A and F modes that may have close ground state energies. This question as well as the origin of the anomaly in the temperature dependence of the intensity can only be resolved by appropriate neutron diffraction from a single crystal.

Acknowledgements – The authors are very grateful to J. Zoubkova and B.V. Mill (Moscow State University) for supplying the samples.

REFERENCES

1. I.V. Golosovsky, V.P. Plakhty, V.P. Harchenkov, J. Zoubkova, B.V. Mill, M. Bonnet & E. Roudeau, *Fizika Tverdogo Tela* (*Solid State Physics–Russian*) **34,** N5, 1483 (1992).
2. T. Chattopadhyay, P.J. Brown, U. Kobler & M. Wilheim, *Europhys. Lett.* **8,** 685 (1989).
3. O.D. Kolotii & V.A. Blinkin, "Note to magnetic structure of $YBa_2Cu_3O_x$", Preprint ISC-91-92, Kharkov, Institute for Single Crystal (1991).
4. C. Meyer, F. Hartmann-Boutron, Y. Gros, P. Strobel, J.L. Tholence & M. Pernet, *Solid State Commun.* **74,** 1339 (1990).
5. J. Schefer, P. Fischer, H. Heer, A. Isacson, M. Koch & R. Thut, *Nucl. Instr. and Meth.* **A288,** 477 (1990).
6. S.F. Watkins, F.R. Fronczek, K.S. Wheelock, R.G. Goodrich, W.O. Hamilton & W.W. Johnson, *Acta Cryst.* **C44,** 3 (1988).
7. R.E. Watson & A.J. Freeman, *Acta Cryst.* **14,** 27 (1961).
8. E.W. Ong, B.L. Ramakrishna & Z. Igbal, *Solid State Commun.* **66,** 171 (1988).
9. M.N. Popova & I.V. Paukov, *The 2nd International School on Excited States of Transition Elements*, Wrocław, Sept. 2–6, 1991. World Scientific, Singapore (1991).
10. N.I. Agladze, G.G. Chepurko & M.N. Popova, *Phys. Lett.* **A133,** 260 (1988).