Magnetic structure of $Lu_2Cu_2O_5$

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The magnetic structure of $Lu_2Cu_2O_5$, which is determined from neutron diffraction data, consists of ferromagnetic layers of alternating signs which are parallel to the *ab* plane. The magnetic moment of the copper atom is $0.72(3)\mu_B$.

Interest has recently been manifested in cuprates of the superconducting systems R_2O_3–BaO–CuO_x. In particular, Refs. 1–6 reported on the magnetic properties of the compounds $R_2Cu_2O_5$ with R = Tb–Lu, Y, Sc, and In. Given here is the magnetic structure of $Lu_2Cu_2O_5$, which is determined from neutron diffraction data.

The single-phase polycrystalline sample $Lu_2Cu_2O_5$ was synthesized to accordance with ceramic technology from oxides at 1030–1050 °C in air. The neutron diffraction measurements were carried out on a 48-counter diffractometer[7] at wavelength $\lambda = 1.383$ Å. The neutron diffraction pattern, measured in the paramagnetic phase ($T = 30$ K), was used to refine the crystal structure[8] by Rietweld's method in terms of the $C^9_{2v}(Pna2_1)$ space group. (Let us note that Ref. 8 used the nonstandard setting $P2_1nb$.) In addition to the unit cell parameters $a = 10.701$ (1), $b = 3.4111$ (4), and $c = 12.363$ (1), we refined the coordinates of the oxygen atoms, where difference from the values of Ref. 8 was found to be insignificant (up to five standard deviations).

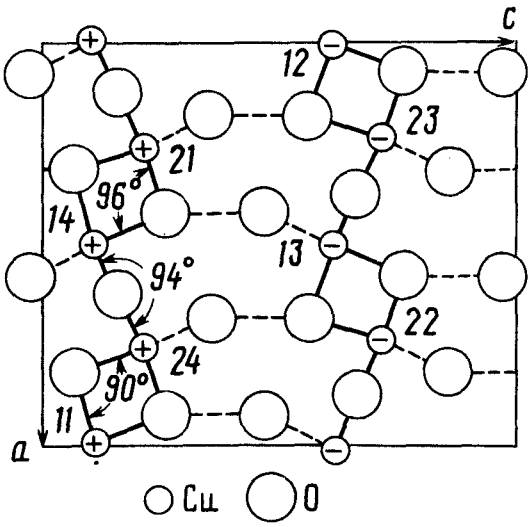

FIG. 1. Magnetic order and exchange bonds in $Lu_2Cu_2O_5$.

TABLE I.

(hkl)	001	201	003
I_{obs}	331 (14)	52 (15)	57 (15)
I_{calc}	336	25	10

In the magnetically ordered phase, the neutron diffraction pattern shows very weak magnetic reflections indexed as 001, 201, and 003; i.e., the wave vector of the magnetic structure is $\mathbf{k} = 0$. The basis functions of the irreducible representations of the group of this wave vector are $\Gamma_1(G_i,A_i,C_i)$; $\Gamma_2(A_i,G_i,F_i)$; $\Gamma_3(F_i,C_i,A_i)$; $\Gamma_4(C_i,F_i,G_i)$, where

$$\mathbf{F}_i = \frac{1}{2}(\mathbf{S}_{i1} + \mathbf{S}_{i2} + \mathbf{S}_{i3} + \mathbf{S}_{i4}),$$

$$\mathbf{C}_i = \frac{1}{2}(\mathbf{S}_{i1} + \mathbf{S}_{i2} - \mathbf{S}_{i3} - \mathbf{S}_{i4}),$$

$$\mathbf{G}_i = \frac{1}{2}(\mathbf{S}_{i1} - \mathbf{S}_{i2} + \mathbf{S}_{i3} - \mathbf{S}_{i4}),$$

$$\mathbf{A}_i = \frac{1}{2}(\mathbf{S}_{i1} - \mathbf{S}_{i2} - \mathbf{S}_{i3} + \mathbf{S}_{i4}),$$

and $i = 1,2$ for the two nonequivalent subsystems of copper atoms, shown in Fig. 1. The presence of the 001 reflection and absence of the 100 reflection indicate unequivocally that the ordering of the spins in both subsystems is described by mode **A**. The intensity ratio of the 001 and 003 reflections gives the relative orientation $\mathbf{S}_{11} = \mathbf{S}_{21}$. (We assume that $|\mathbf{S}_{11}| = |\mathbf{S}_{21}|$.) The intensity ratio of 001 and 201 indicates that the spins are directed along the *b* axis. Thus the ordering of the spins is described by the mode $A_1^y + A_2^y = \frac{1}{2}(S_{11}^y - S_{12}^y - S_{13}^y + S_{14}^y + S_{21}^y - S_{22}^y - S_{23}^y + S_{24}^y)$. The value of the magnetic moment per copper atom, obtained by comparing the experimental and calculated values of the magnetic reflection intensities (Table I), is $0.72(3)\mu_B$.

The magnetic structure of $Lu_2Cu_2O_5$ can be represented by ferromagnetic layers of alternating signs, parallel to the ab plane. Anisotropic interactions should result in weak components G_i^x and C_i^z, which belong to the same irreducible representation Γ^1 as A_i^y.

The Cu^{2+} ions are located in highly distorted trigonal bipyramids of oxygen atoms. The wave function of the ground state is $d_{\xi^2-\nu^2}$, where ξ and η are local axes directed toward the nearest oxygen atoms. In Cu–O–Cu chains with bond angles (solid lines in the figure), close to $\pi/2$, kinetic exchange is; suppressed, and the interactions should be positive. The bonds between the chains are established by pairs of successive oxygen atoms (dashed lines), and they may be expected to be much weaker than the bonds within the chain. It follows from the magnetic structure that the interaction within neighboring chains is positive in the *b* direction and negative in the *a* direction. Suppression by the magnetic field of the weak negative interaction in the

presence of fairly strong anisotropy[9] results in the metamagnetic transition observed in Ref. 6.

[1] R. Troč *et al.*, Phys. Lett. A **125**, 222 (1987).
[2] R. Famery and F. Queyroux, Mat. Res. Bull. **24**, 275 (1989).
[3] R. Troc *et al.*, Physica B **154**, 189 (1989).
[4] R. L. Ramakrishna *et al.*, Solid State Commun. **68**, 775 (1988).
[5] S. W. Cheon *et al.*, Phys. Rev. B **38**, 7013 (1988).
[6] Ya. Zoubkova *et al.*, Pis'ma Zh. Eksp. Teor. Fiz. **49**, 524 (1989) [JETP Lett. **49**, 606 (1989)].
[7] I. V. Golosovskii *et al.*, Preprint LINP, No. 1374, 1988.
[8] H. R. Freund and H. Müller-Buschbaum, X. Naturforsch B **32**, 1123 (1977).
[9] H. A. Groenendijak *et al.*, Physica B **108**, 47 (1981).

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