Polarized neutron scattering study of the CuO_2 chains in $Ca_2Y_2Cu_5O_{10}$

Masaaki Matsuda [a,1], Mitsutaka Nakamura [a], Masayasu Takeda [a], Kazuhisa Kakurai [a], Hirotaka Yamaguchi [b], Toshimitsu Ito [b], Kunihiko Oka [b]

[a] *Advanced Science Research Center, Japan Atomic Energy Research Institute, Tokai, Ibaraki 319-1195, Japan*

[b] *National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki 305-8568, Japan*

Abstract

Polarized neutron scattering experiments were performed in a quasi-one-dimensional magnet $Ca_2Y_2Cu_5O_{10}$, which consists of the edge-sharing CuO_2 chains and shows an antiferromagnetic long-range ordering below T_N=29.5 K with ferromagnetic coupling along the chain. It is confirmed that the magnetic moments point along the b axis perpendicular to the CuO_2 plane. This result combined with that of the previous unpolarized neutron scattering experiments clearly indicates that some fraction of the magnetic moments in the CuO_2 unit exists at the oxygen sites.

Key words: quasi-one-dimensional magnet; magnetic structure; $Ca_2Y_2Cu_5O_{10}$; polarized neutron

1. Introduction

In the edge-sharing CuO_2 chain in which the Cu ions are coupled by the nearly 90^o Cu-O-Cu bond, large magnetic moments can be induced at oxygen sites because of the strong hybridization between Cu d and O p orbitals. An existence of the magnetic moments in the CuO_2 chains is predicted theoretically in Li_2CuO_2. [1] and observed experimentally in $La_9Ca_5Cu_{24}O_{41}$ [2] and in Li_2CuO_2 [3].

$Ca_2Y_2Cu_5O_{10}$ is a quasi-one-dimensional magnet, which consists of the edge-sharing CuO_2 chains. This compound shows an antiferromagnetic long-range ordering below T_N=29.5 K with ferromagnetic coupling along the chain [4,5]. It is worth while studying the magnetic moment at the oxygen sites in this compound in order to check whether the phenomenon is universal. Previous magnetic structural analysis using unpolarized neutrons suggests that the magnetic moments are not localized at the Cu sites but some of the moments also exist at the oxygen sites [4,6]. However, without considering the oxygen moments, there is a slight possibility that the Cu moments are just tilted from the b axis perpendicular to the CuO_2 plane. This study using polarized neutrons confirms that the magnetic moments point along the b axis, strongly supporting the existence of the moments at the oxygen sites.

[1] Corresponding author. E-mail: matsuda@neutrons.tokai.jaeri.go.jp

2. Experimental Details

The neutron scattering experiments were carried out on the 3-axis spectrometer TAS-1 installed at the JRR-3M at Japan Atomic Energy Research Institute (JAERI). Heusler alloy (111) was used as monochromator and analyzer. A flipping ratio of ∼20 was measured on some nuclear Bragg peaks. The horizontal collimator sequence was open-80'-S-80'-open. The incident neutron energy was fixed at E_i=32.4 meV. The single crystal of $Ca_2Y_2Cu_5O_{10}$ was grown using a traveling solvent floating zone method in air [7]. The crystal structure is orthorhombic and the lattice con-

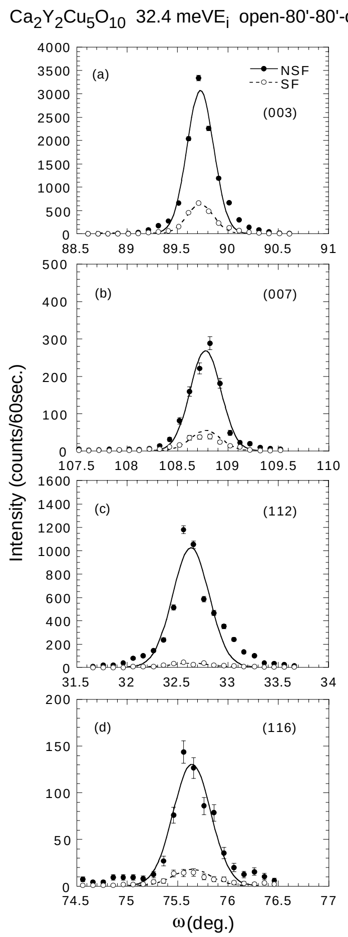

Fig. 1. Elastic neutron scans of $Ca_2Y_2Cu_5O_{10}$ at (0,0,3), (0,0,7), (1,1,2), and (1,1,6) measured at T=15 K with polarized neutrons in the vertical field spin-flip (SF) and non-spin-flip (NSF) mode. A correction originating from imperfect polarization of the neutron beam was made. The solid lines represent the results of fits to a Gaussian. The broken lines show the intensities estimated for the SF mode.

stants are a=2.810 Å (chain direction), b=6.190 Å, and c=10.613 Å at room temperature. The crystal, which is oriented in the (hhl) scattering plane, was mounted in a closed cycle refrigerator. The (00L) and (11L) (L: integer) magnetic Bragg reflections were measured.

3. Results

Figure 1 shows the typical data obtained from the polarized neutron measurements in the vertical field. The non-spin-flip (NSF) and spin-flip (SF) mode experiments give magnetic scattering caused by spin component parallel to the field direction [1,-1,0] and perpendicular to it, respectively. A correction originating from imperfect polarization of the neutron beam was made. The tail of the Bragg peaks probably comes from the poor mosaicity of the crystal and/or the the Heusler monochromator and analyzer. The (00L) intensities originate from the spin component perpendicular to the c axis. From the ratio of the NSF and SF reflection in the (00L) reflections ∼5, as shown in Figs. 1(a) and 1(b), the angle between the field and the spin directions projected in the ab plane is estimated to be ∼25°. This direction almost corresponds to the b axis. From the (11L) intensities the spin component along the c axis can be estimated. Since the SF (11L) intensities are weak, as shown in Figs. 1(c) and 1(d), the c component should be very small even if it exists. The broken lines in Fig. 1 represent the estimated values with the spin structure model in which the moments point along the b axis. [6] The estimated intensities reproduce the observed ones reasonably well. From these results, it can be concluded that the moments point along the b axis.

The previous neutron scattering measurements using unpolarized neutrons shows that a simple model that assumes magnetic moments only at the Cu sites does not describe the magnetic Bragg intensities, especially those of the (11L) reflections [6]. Then, assuming that the moments point along the b axis, it is suggested that the magnetic moments are not localized at the Cu sites but extend to the oxygen sites. Since the present study confirms that the moments point along the b axis, it is clearly concluded that some fraction of the magnetic moments in the CuO_2 unit (∼22%) exists at the oxygen sites.

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