CONF-970814--10

July 31, 1997 Version 6.0

Magnetic Excitation of $CuGeO_3$ under Applied Pressure

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Abstract

Magnetic excitations of the spin-Peierls compound $CuGeO_3$ under applied pressure of 2 GPa have been studied. The dispersion along the chain direction up to zone boundary has been obtained. The spin-Peierls gap energy increases to 4.2 meV and the zone boundary energy decreases to 14.1 meV. The pressure dependence of dispersion relation can be interpreted by the increase of the next-nearest-neighbor intra-chain interaction under applied pressure causing the increase of both the spin-Peierls gap energy and transition temperature.

keywords; spin-Peierls, $CuGeO_3$, high pressure, magnetic excitation

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ORNL is managed by Lockheed Martin Energy Research Corp. under Contract No. DE-AC05-96OR22464 for the U.S. Department of Energy.

DISCLAIMER

During the past four years many experimental studies have been performed on the spin-Peierls (SP) compound, $CuGeO_3$. Previous neutron scattering experiment under high pressure, 1.8 GPa in Ref. 1 revealed that the *c*-axis slightly elongates, while the *b*-axis remarkably shortens by a factor of 4 more than the lattice contraction due to the temperature change from RT to 5 K. It is natural to expect that the interchain exchange interaction J_b increases and the intra-chain interaction J_c remains unchanged upon applying 1.8 GPa. Inagaki and Fukuyama [2] have calculated the phase diagram of antiferromagnetic (AF) and SP states by treating J_b and the spin-lattice coupling η in the mean field approximation. According to this approach, SP phase becomes unstable with increasing J_b at constant η. However, experimental results by Refs.1 and 3 show the increase of SP transition temperature, T_{sp} and SP gap, Δ_{sp} from 14 K to 23 K and from 2 meV to 4 meV, respectively with increasing pressure. The mean field results therefore seem to be in conflict with these pressure experiments.

The temperature dependence of the magnetic susceptibility in $CuGeO_3$ above T_{sp} reported by Hase *et al.* [4] cannot be well described by the spin $S=1/2$ one-dimensional, nearest neighbor Heisenberg AF model by Bonner and Fisher [5]. Riera and Dobry [6] reasonably described the experimental curve of the magnetic susceptibility with nearest-neighbor (nn) and next-nearest-neighbor interaction (nnn), J_c and J_{2c}, respectively with $\alpha=J_{2c}/J_c=0.36$ and $J_c=160$ K. Castilla *et al.* [7] deduced $\alpha=0.24$, $J_c=150$ K and dimerization parameter $\delta=0.03$. The object of this paper is to determine J_{2c} from the pressure dependence in order to estimate the importance of the competing interactions in $CuGeO_3$ system.

A $CuGeO_3$ single crystal with the size 5 mmϕ x 9 mm was grown by the traveling-solvent floating-zone method. The inelastic neutron-scattering experiment was performed on the HB-3 triple-axis spectrometer installed at HFIR of Oak Ridge National Laboratory. The final neutron energy was fixed to be 13.6 meV from the (002) reflection of a pyrolytic graphite (PG) analyzer. The single crystal was mounted with the $(0, k, l)$ scattering plane in an aluminum micro cell using Fluorinert 75 as the pressure-transmitting fluid and clamped type high pressure cell [8] set in CT14 cryostat. The value of applied pressure was estimated consistently by the lattice constants, b and c, of $CuGeO_3$ as compared with the data of Ref. 1.

The magnetic excitation profiles at 5 K are shown in Fig. 1. Both experimental conditions are used with horizontal collimation, 48'-40'-40'-120' and vertical bent PG analyzer as shown in Fig. 1 (a) and with another one, 48'-40'-100'-120' and large flat PG analyzer as shown in Fig. 1 (b). The consistency of both conditions are checked at Q= (0,1,0.68). In Fig. 2, the dispersion curves along c^*-axis both under high pressure, 2 GPa and ambient pressure (AP) are shown together. SP gap energy at 2 GPa becomes about twice of that at AP, but the zone boundary (ZB) energy decreases from 16 meV to 14 meV at 5 K. Just adjusting the parameters of the dimerized chain with only the nn exchange, as calculated numerically by Bonner and Blöte [9] would yield the change in the dimerization parameter δ=0.06 to 0.17 and in the exchange constant from J_c=10.5 meV (121 K) to 9.8 meV (114 K) upon the pressure increase from AP to 2 GPa.. On the other hand the structural study under high pressure [3] unambiguously revealed that the displacement Δz of the Cu atoms, believed to govern the dimerization parameter, does decrease upon applying the pressure. To resolve this inconsistency we tried to estimate nnn interaction in the frame of the spin wave theory [10] to describe the pressure dependent dispersion including the SP gap Δ_{sp} phenomenologically. J_b is estimated from the energy difference at Q=(0, 0, 0.5) and (0, 1, 0.5). The fit results are indicated by the solid lines in Fig. 2 and the ratio $\alpha = J_{2c}/J_c$ increased from 0.1662 ± 0.0059 to 0.1802 ± 0.0075 at 2 GPa. Although the α–values are smaller than the critical value for a finite energy gap reported theoretically [7], the increase of it may indicate the enhancement of the competing interaction between J_c and J_{2c} upon applying the pressure. A more sophisticated analysis of the pressure dependent dispersion including the nnn intra-chain exchange interaction, dimerization and interchain exchange interaction is desirable. The confirmation of double gap and the contribution of J_b will be reported elsewhere [11].

This work was done at the Oak Ridge National Laboratory under US - Japan Cooperation Program in Neutron Scattering and supported by US DOE under contract No. DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.

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Figure Captions

Fig. 1 Neutron inelastic scattering spectra for different Q at 2 GPa and 5 K. Energy scans were done under the conditions of collimations 48'-40'-40'-120' and 48'-40'-100'-120' at (a) and (b), respectively. Solid lines are the results of Gaussian fitting.

Fig. 2 The dispersion curves along c^*-axis at 5 K under 2 GPa and ambient pressure. Solid lines are the fitting curves by spin wave formula added SP gap.

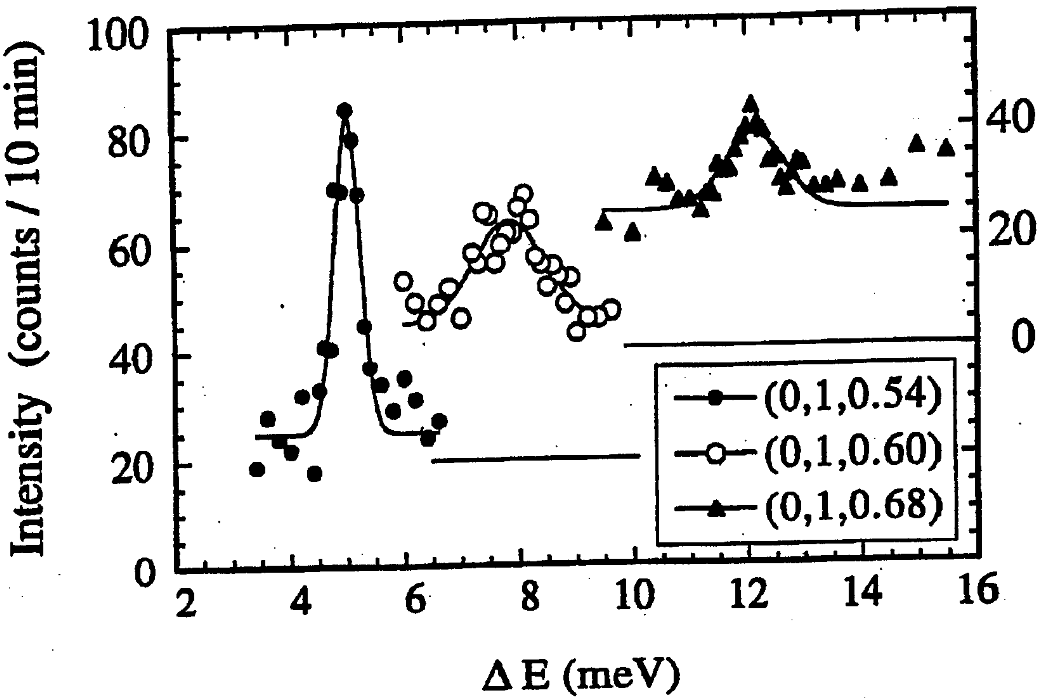

Fig. 1 (a) M. Nishi et al.

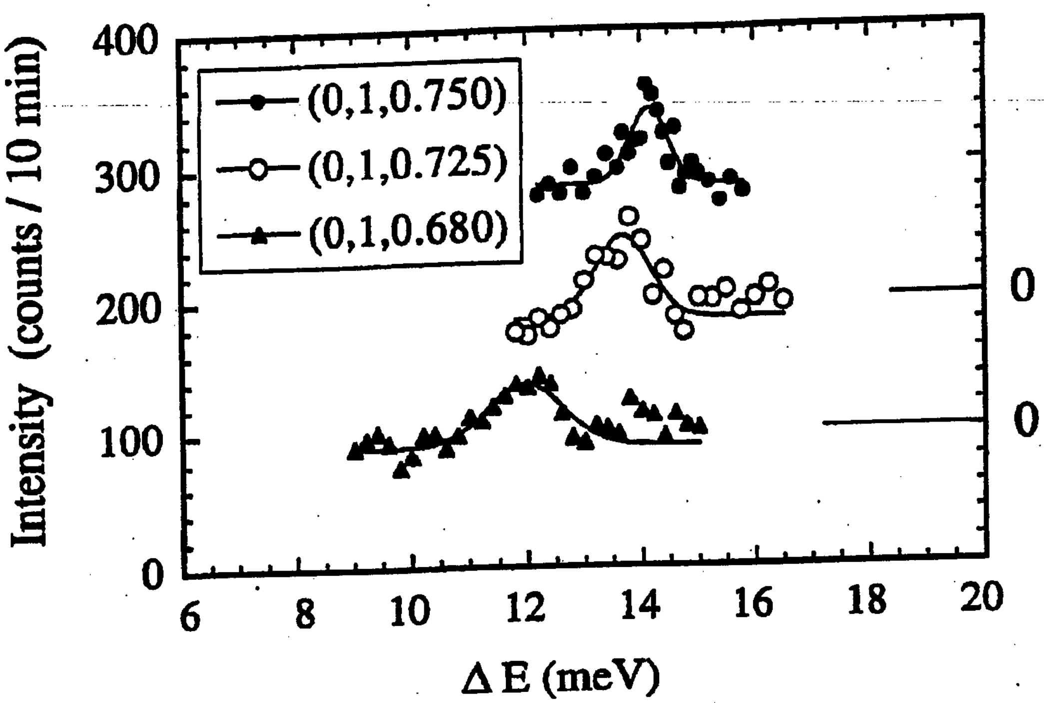

Fig. 1 (b) M. Nishi et al.

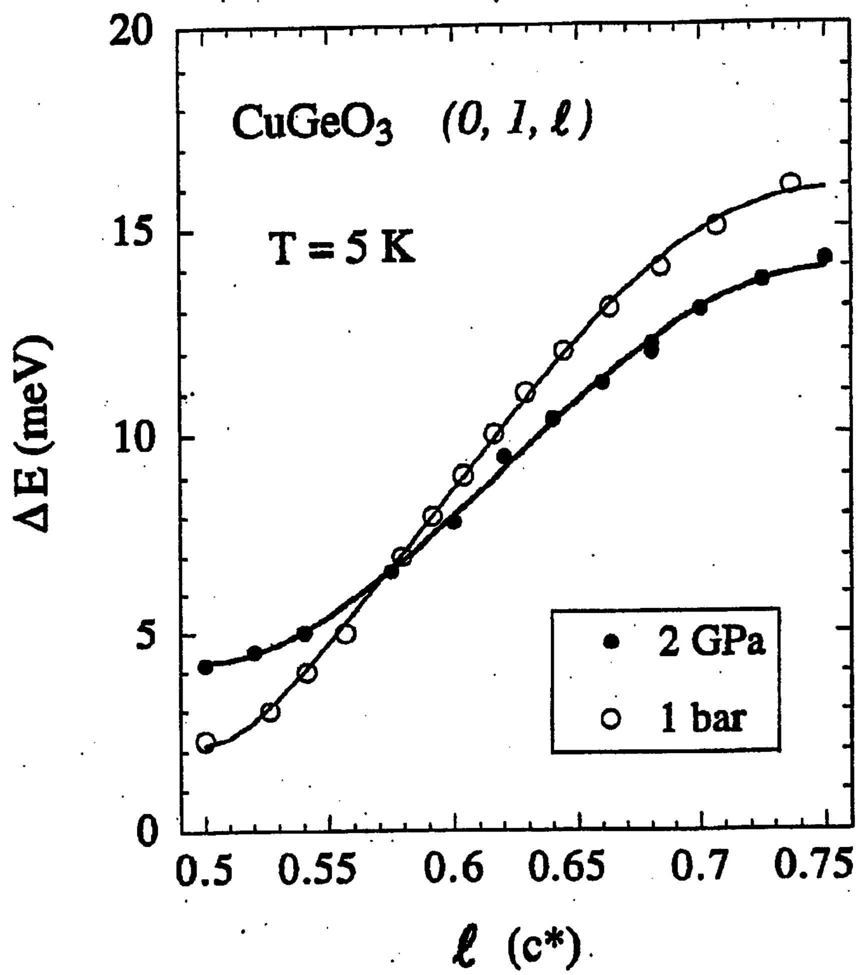

Fig. 2 M. Nishi et al.

M97009380

Report Number (14) CONF-970814--10

Publ. Date (11) 199707

Sponsor Code (18) DOE/ER, XF

UC Category (19) UC-400, DOE/ER

DOE