Magnetic Excitation of S=1/2 Breathing Pyrochlore compound $Ba_3Yb_2Zn_5O_{11}$

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We studied low energy excitation in breathing pyrochlore compound $Ba_3Yb_2Zn_5O_{11}$ to identify the effective spin Hamiltonian using PELICAN spectrometer. The polycrystalline sample with the mass of 17.1 g was prepared by solid state reaction method. We used two setups for the inelastic neutron scattering (INS) experiment; setup I for high energy resolution using incident energy E_i of 2.1 meV, and setup II for coverage of wider Q - $\hbar\omega$ space using E_i of 3.6 meV. Here Q is magnitude of scattering vector and $\hbar\omega$ is energy transfer. Instrumental energy resolutions at the elastic position were 0.059 meV for setup I and 0.135 meV for setup II in full width at half maximum (FWHM). Closed cycle refrigerator was used to control the temperature T in the wide range, 1.5 K < T < 150 K.

Figures 1(a)-1(f) show INS spectra in the setup I measured at various temperatures. Three flat bands are observed at 1.5 K. The absence of dispersion suggests that these bands are approximately cluster excitations. The effect of the intercluster interaction is small and hidden in the instrumental resolution. At 6 K the intensities are suppressed and new flat bands appear at different $\hbar\omega$s. The intensities are small at 80 K, and the excitations are smeared out at 150 K. Several streaks observed in the range of $\hbar\omega < 0.4$ meV in all the panels are acoustic phonons. Figures 1(g) and 1(h) shows the INS spectrum in the setup II.

One-dimensional energy cuts from the INS spectra in Figs. 1(a) and 1(c) are shown by symbols in Figs. 2(a) and 2(b), respectively. The peaks are fitted by Gaussian functions having FWHM of instrumental resolution to estimate the peak energies and the integrated intensities. The peak energies at 1.5 K are estimated as 0.39, 0.52, 0.73, 0.78 meV. At T = 12 K new peaks are observed at 0.21, 0.98, 1.03, 1.24, and 1.37 meV in Fig. 2(b). Temperature dependences of the intensities of the four peaks at 1.5 K are shown in Fig. 2(c), and those of the additionally observed peaks at 12 K are shown in Fig. 2(d). The formers monotonically decrease with the temperature and, in contrast, the latter increase with the temperature. This means that the probabilities of the initial states of the excitations observed at 1.5 K decrease with the increasing temperature and, therefore, the excitations are from the ground state and/or the excited state with small energy compared with 1.5 K. The additional excitations observed at 12 K are from the excited states.

Figure 2(e) shows one-dimensional energy cuts from the INS spectra at 1.5 K in Fig. 1(g) in setup II. A peak is observed at 1.75 meV in addition to the peaks observed in setup I. Q dependence of the intensity integrated in the range of 0.25 meV < $\hbar\omega$ < 0.95 meV in Fig. 2(f) exhibits broad maximum at $Q_{max} \sim 1.25$Å^{-1}. This means that antiferromagnetic correlation between the spins, the characteristic length scale of which is π/Q_{max}, is enhanced. The dispersionless excitations with the Q dependent intensity means that the neutron spectrum is dominated by an antiferromagnetic cluster within the instrumental resolution.

We analyzed the data on the basis of spin S=1/2 tetrahedron Hamiltonian including anisotropic and asymmetric interactions. The calculations are indicated by solid curves in Figs. 2(a)-2(f) and the data is reasonable reproduced. Detailed descriptions of the analysis and discussion will be appeared in a publication in future.

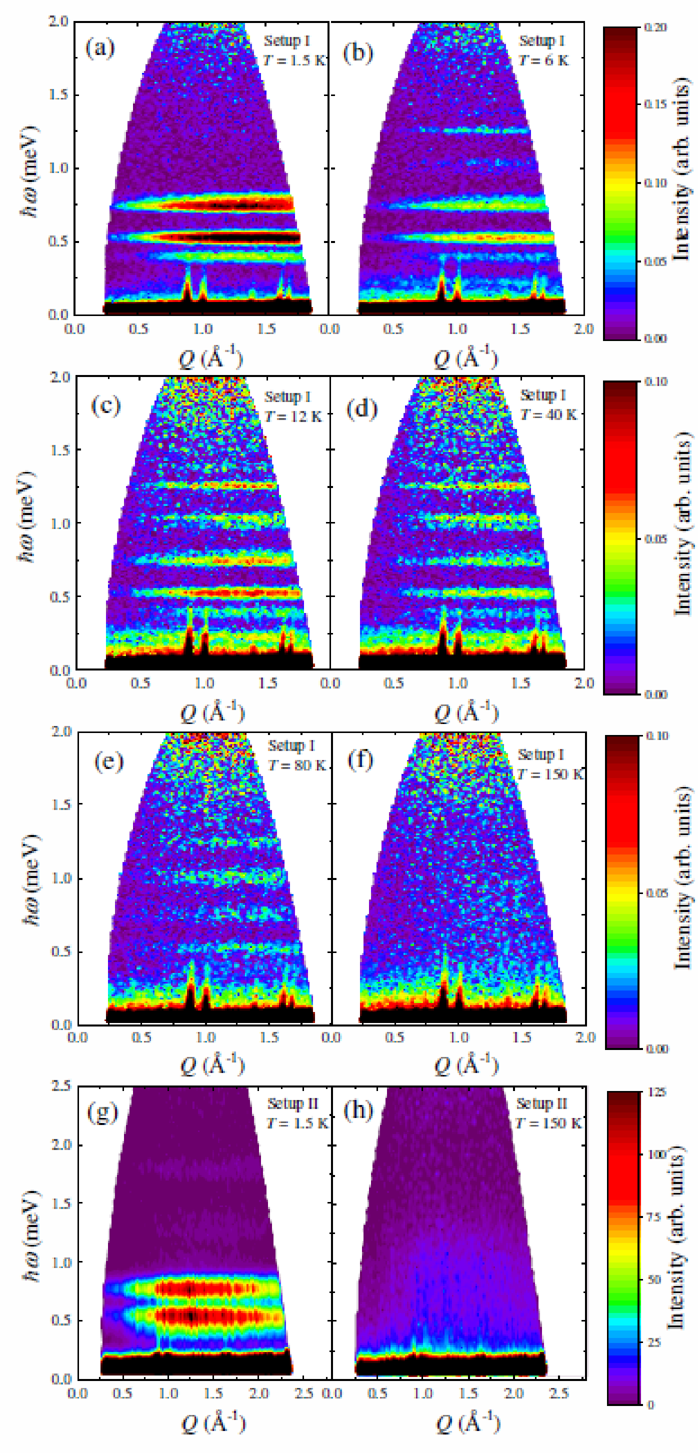
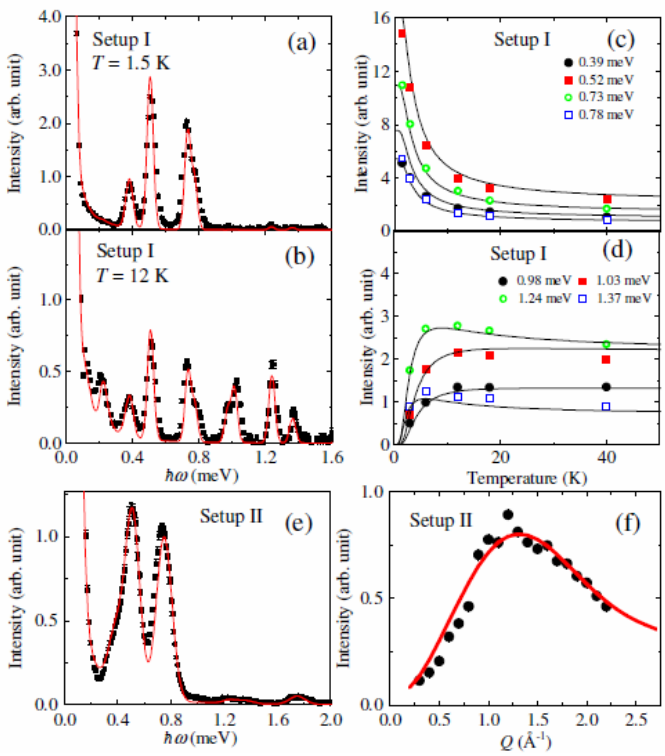


Fig. 1 INS spectra measured at T = 1.5 K (a), 6 K (b), 12 K (c), 40 K (d), 80 K (e), and 150 K (f) using experimental setup I. INS spectra measured at T = 1.5 K (g) and 150 K (h) using the setup II.



(a), (b) Symbols show the $\hbar\omega$ dependences of the neutron intensities integrated in the range of 0.75 $Å^{-1}$ < Q < 1.25 $Å^{-1}$ at T = 1.5 K for (a) and 12 K for (b). (c) Temperature dependences of the neutron intensities of the excitations observed in (a). (d) Those of the excitations additionally observed in high temperatures observed in (b). (e) $\hbar\omega$ dependence of neutron intensity at 1.5 K obtained using setup II. The integrated range is 0.75 $Å^{-1}$ < Q < 1.75 $Å^{-1}$. (f) Q dependence of the intensity integrated in the range of 0.25 meV < $\hbar\omega$ < 0.95 meV. Throughout the panels red and black solid curves are the calculation using the same parameters in an effective spin Hamiltonian.