ESRF	**Experiment title:** Interplay of low-energy phonons and electronic/spin gap in the Kondo-insulator YbB_{12}	**Experiment number**: HS-4649
Beamline:	**Date of experiment**: from: 16/05/2012 to: 22/05/2012	**Date of report**: 25.03.2013
Shifts:	**Local contact(s)**: Michael Krisch	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Pavel Alekseev*, NRC "Kurchatov Institute", Russia

Kirill Nemkovski*, JCNS FRM II, Forschungszentrum Jülich, Germany

Jean-Michel Mignot, Laboratoire Léon Brillouin, France

YbB_{12} is a strongly correlated electron system exhibiting Kondo insulator behavior [1]. This peculiar regime, achieved on cooling below $T^* \sim 50$ K, is characterized by the opening of a narrow gap in the electronic density of states and the quenching of local moment. In spite of intensive investigations, the nature of this transition remains a subject of debate. Though theoretical approaches to this problem are mostly related to the electron subsystem, one cannot disregard a possible interplay with lattice vibrations. A detailed inelastic neutron scattering (INS) study has shown [2] that the phonon spectrum in YbB_{12} is dominated by the boron sublattice. The Yb vibrations contribute only to the low-energy branches in the region 10-25 meV, with the main spectral weight concentrated in the narrow intensive peak at 15 meV. Previously, in the INS experiment we have found an anomalous temperature dependence for this peak. After correction for the Bose factor its intensity demonsrates essential enhancement below the T*. Taking into account the coincidence in symmetry between magnetic and phonon modes which fall into the energy range 15 meV...20 meV, this effect has been ascribed to magneto-vibrational coupling.

For further investigation of this problem we have used the inelastic X-ray scattering (IXS) as it allows to study of the purely vibrational properties without any admixture of magnetic excitations, and the signal measured by IXS is entirely dominated by the Yb vibrations due to the approximately Z^2 dependence of the IXS cross section. The measurements have been performed at ID28 beam-line for powder samples of YbB_{12}, electronically-doped $Yb_{0.75}Lu_{0.25}B_{12}$ and $Yb_{0.8}Zr_{0.2}B_{12}$, and LuB_{12} as referenced compound. Experimental conditions of the experiment at ID28 were as follows: Si (12,12,12) monochromator, incoming wavelength λ_0=0.5226Å energy resolution ΔE_0=1.5meV. The data were recorded for two different analyzer/detector bank positions with average scattering angles ~36.5^0 and 42^0. The resulted momentum transfer was ~80-90 nm^{-1} which is about 10 times more than characteristic size of the Brillouin zone and provides a favorable conditions for "incoherent limit" approximation. Temperature range of the measurements was from 10 to 290K, each temperature point is measured about 5h to get reasonable statistics.

In the experimental spectra (see Fig.1) only one peak have been observed at about 15 meV. The weak one around 30 meV was ascribed to the double phonon scattering based on too strong temperature dependence with respect to the Bose statistics.

An additional problem resulted from the Lorentzian shape of the resolution function. The essential efforts have been made to select the spectra without contamination by the coherent elastic scattering that takes place in both energy and momentum spaces. At each temperature only few spectra have been selected as reliable.

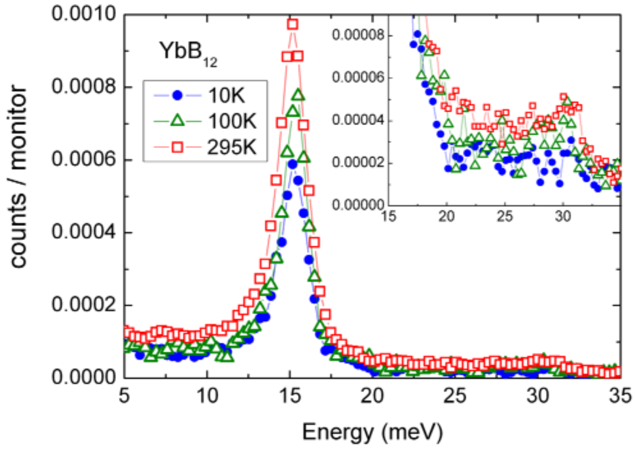

Fig.1. Experimental spctra for YbB_{12} at differnet temperatures. Inset: the peak at 30 meV shown with enhanced scale.

The integrated intensities of the 15 meV peak for all samples under study are shown in Fig.2. In contrast to the clearly observed effect in INS (inset in Fig.2a) no extra contribution is seen in IXS data. In fact the temperature dependencies for YbB_{12}, $Yb_{0.75}Lu_{0.25}B_{12}$ and reference system LuB_{12} are identical and described well by the combination of the Bose-factor and Debye-Waller factor. Certain deviation from this dependence was found only for $Yb_{0.8}Zr_{0.2}B_{12}$ at room temperature (apparently this effect can be ascribed to the trivial difference in Debye-Waller factor due to the substituion of Yb by Zr with almost two-times smaller atomic mass).

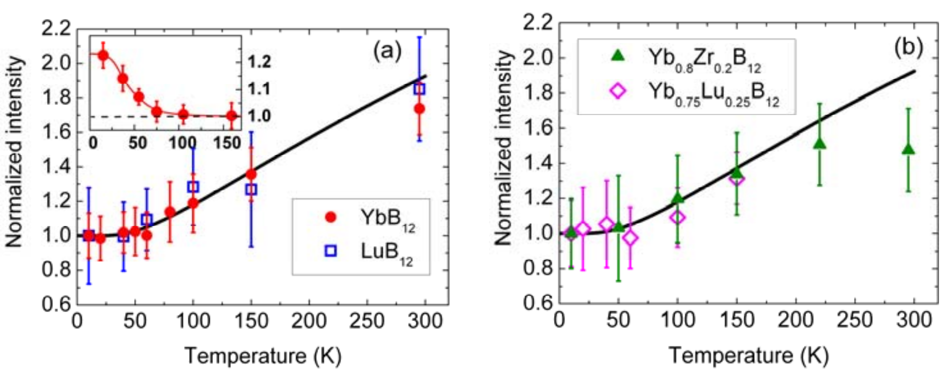

Fig.2. Temperature dependence of the normalized intensity of 15meV phonon peak in YbB_{12}, LuB_{12}, $Yb_{0.75}Lu_{0.25}B_{12}$ and $Yb_{0.2}Zr_{0.8}B_{12}$. Line – production of the Bose-factor and Debye-Waller factor. Inset: temperature dependence of the intensity in neutron experiment corrected for the Bose factor [2]

The momentum transfer in INS experiment was about 100 nm^{-1} which is large enough to exclude any direct magnetic contribution from f-electron excitations. Therefore for subsequent data analysis two possibilities should be taken into account as possible source of the observed qualitative difference between results of neutron and X-ray scattering experiments: 1) the involvement of the B movements into the formation of the phonon density of state intensity which is not detected in the X-ray experiment due to Z^2 dependence of signal intensity, and 2) interference or mixing of magnetic and phonon excitation modes which may be the source of combined Q-dependence of the mutual signal in case of neutron experiment, negligible for X-rays.

References

1. P.S.Riseborough, Adv. Phys. **49** (2000) 257.

2. P.A.Alekseev, J.-M.Mignot, K.S.Nemkovski et al., J. Phys.: Condens. Matter **24** (2012) 205601 and references therein.