The upgraded cold neutron three-axis spectrometer FLEXX at BER II at HZB

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The cold neutron three-axis spectrometer FLEXX is a work-horse instrument for inelastic neutron scattering matching the sample environment capabilities for high magnetic fields up to 17.5 T and low temperatures down to 30 mK at the BER II research reactor at HZB. During the upgrade of the BER II neutron source and its instruments the primary spectrometer of FLEX [1] was completely rebuilt leading to a substantial increase in the flux reaching the sample [2].

The major benefit from the exchange of the entire neutron guide system serving instruments in Neutron Guide Hall I is that it has allowed optimisations of individual instrument positions. As a consequence FLEXX was relocated to a guide-end position in an area of the guide hall with intrinsically low background (Fig. 1). The neutron guide system of FLEXX now hosts m=3 guides including a converging elliptical section to focus neutrons onto a virtual source [3, 4]. The neutrons are subsequently imaged onto a new double focussing monochromator, ensuring a high neutron flux at the sample position with increased monochromaticity [5]. In addition, a new velocity selector is used to remove higher order scattering which eliminates the need for filters. A polarising S-bender may be translated into the beam before the elliptical guide section where the beam is collimated allowing the gains from focussing neutrons onto the sample to be realised for polarised measurements also (Fig. 2). A Heusler analyser is now optionally available replacing the PG analyser when FLEXX is used for longitudinal polarisation analysis or operated with its neutron resonance spin echo option further enhancing polarised neutron capabilities at FLEXX.

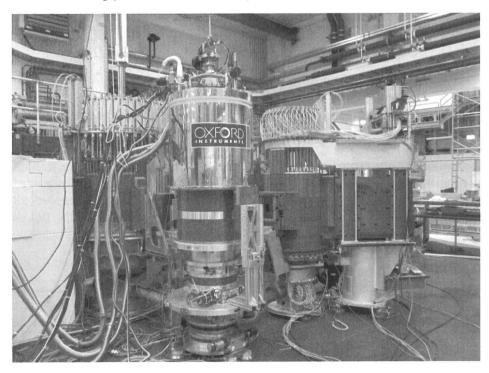


Fig.1: The upgraded cold neutron triple-axis spectrometer FLEXX at its new position in neutron guide hall I at the BER II LK II facility.

Experiments confirmed an order of magnitude gain in intensity (at the cost of coarser momentum resolution), and demonstrated that the incoherent elastic energy widths are measurably narrower than before the upgrade. The much improved count rate allows the use of smaller single crystals samples and thus enables the upgraded FLEXX spectrometer to continue making leading edge measurements. The commissioning phase of FLEXX was completed in 2012 and the instrument is back in full user operation since mid-2012. The new multi-energy analyzer flat cone option MultiFLEXX is in commissioning.

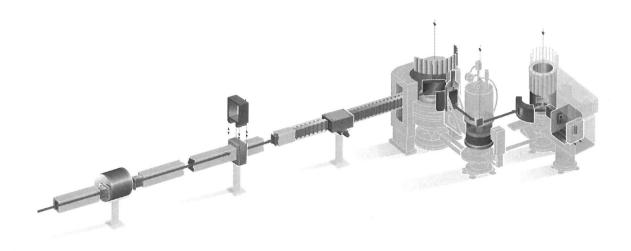


Fig. 2: Schematic drawing of the key components of FLEXX.

FLEXX continues to be highly demanded by the user community and several inelastic experiments have been performed with the new FLEXX. In-house research themes after the commissioning phase have led to new insights in magnetic materials.

Measuring the spin waves in magneto-electric LiCoPO₄

The upgraded FLEXX has recently been used to study the spin waves in magneto-electric LiCoPO₄, which is a pseudo 2D-system with the strongest exchange couplings in the crystallographic *bc*-plane. The Co²⁺-ion is Ising-like in this compound [6], but a crystal field of low symmetry as is the case in LiCoPO₄ could introduce some anisotropy in the hard plane. Previous measurements [6] show a substantial inelastic peak broadening and a low energy dispersion accounted for, which left the determined exchange parameters with a high degree of uncertainty, making a microscopic model for the very strong magneto-electric effect difficult to establish. In addition, the magnetic structure is not completely understood as well [7]; minor deviances from the previously accepted structure reveal a more complicated magnetic Hamiltonian than previously assumed. Such deviances could be important in order to establish a microscopic model for the magneto-electric effect [8].

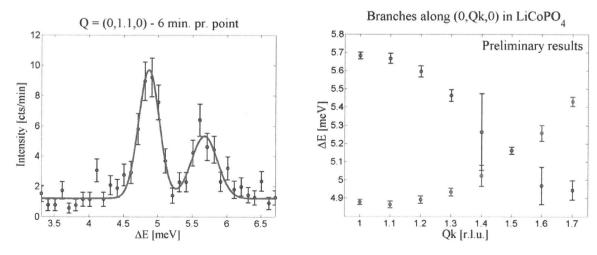


Fig. 3: (Left) Energy scan at Q = (0, 1.1, 0) showing two distinct peaks. (Right) Measured dispersion along K.

We investigated the spin excitations on a merely 70 mg S = 3/2 pebble-like single crystal of LiCoPO₄ during a 3 day beam time using a standard orange cryostat. We used a fixed final energy of 5 meV and completely open geometry to maximize the neutron flux. The excitations in LiCoPO₄ are in the range of 4-6 meV, the flux-maximum of the large dynamical range of FLEXX. We quickly found two distinct branches along K (see figure 1 left), and no sign of a low energy dispersion. In 2.5 days, we were able to measure most of the dispersion along K (see Fig. 3 right). Preliminary results indicate that the hard plane is slightly anisotropic as indicated by the branch splitting, but a more dedicated study of the spin waves in LiCoPO₄ is necessary to understand the details of the magnetic Hamiltonian in order to establish a microscopic explanation for the unusually large magneto-electric effect in this compound.

Crystal field excitations in in SrHo₂O₄

SrHo₂O₄ is a geometrically frustrated rare-earth material with a non-trivial ground state. This material has two non - equivalent magnetic Ho ions with very different single ion anisotropy which competes with geometrically frustrated Ising-type exchange couplings [9]. As a result of this competition, a one-dimensionally correlated magnetic state is formed at low temperatures and it coexists with short range 3-dimensional correlations.

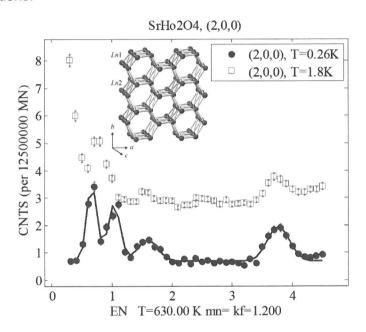


Fig. 4: Constant-wave vector scans measured on FLEXX at Q=(0,0,2) at two temperatures, above and below the magnetic transition. The inset shows the magnetic sublattice of $SrHo_2O_4$, with the two crystallographic positions of the Ho ions.

The crystal field excitations in SrHo₂O₄ have been measured in a single crystal of about 1g on FLEXX, the specific aim of the experiment was to study the low lying crystal field levels and their evolution at low temperatures (T<0.6K) where a partial magnetic order develops. The splitting between the ground state and the excited states is 0.65meV and at low temperatures the excitation splits by about 0.4meV. The ideal instrument to measure such a small splitting is a cold triple axis spectrometer like FLEXX, using low energy incoming neutrons (3meV to 7.5meV) and providing an energy resolution of about 0.07meV. Relatively fast measurements were possible with counting times of less than 10 minutes per point; a ³He dilution stick was used to cool the crystal down below the magnetic transition. These results provide important information to understand the competition between different magnetic mechanisms in the compound. A review article about the magnetic properties of the family of rare-earth strontium oxides can be found in Ref [10].

Neutron Resonance Spin Echo Spectroscopy

Larmor labeling is seen as one of the key ingredients in the development of novel neutron instrumentation. FLEXX puts special emphasis on exploiting the neutron resonance spin echo (NRSE) technique for high-resolution spectroscopy on dispersive quasi-particle excitations. This enables unique measurements in single crystal spectroscopy over large portions of the Brillouin zone. To keep the experimental opportunities at BER II at the forefront the NRSE option available at FLEXX was upgraded along with the change of the primary spectrometer [12].

In user service upgraded V2/FLEXX provides new capabilities for quantum magnetism, heavy-fermion systems and unconventional superconductivity. For example inelastic experiments in magnetic fields up to 17 T are now proven to be feasible. Energy research with inelastic neutron instruments will be strengthened through in-house research, thereby fostering collaborations with external partners. The research themes at the new FLEXX spectrometer in future will be centred on transport properties in thermoelectric materials.

References:

- [1] P. Vorderwisch, S. Hautecler, F. Mezei, and U. Stuhr, Physica B 213-214,866 (1995).
- [2] M. D. Le, D. L. Quintero-Castro, R. Toft-Petersen, F. Groitl, M. Skoulatos, K. C. Rule, and K. Habicht, Nucl. Instrum. Methods Phys. Res. A **729** (0) 220-226 (2013).
- [3] K. Habicht, M. Skoulatos, Optimization of virtual source parameters in neutron scattering instrumentation, Journal of Physics: Conference Series **340** (1) 012029 (2012).
- [4] M. Skoulatos, K. Habicht, K. Lieutenant, Improving energy resolution on neutron monochromator arrays, Journal of Physics: Conference Series **340** (1) 012019 (2012).
- [5] M. Skoulatos, K. Habicht, Upgrade of the primary spectrometer of the cold triple-axis spectrometer FLEX at the BER II reactor, Nucl. Instrum. Methods Phys. Res. A **647** (1) 100–106 (2011).
- [6] Wei Tian, et, al., Phys. Rev. B, 78 184429, (2008).
- [7] T. B. S. Jensen, et. al, Phys. Rev. B 79 092412 (2009).
- [8] D. Vaknin, et. al. Phys. Rev. B 65 224414 (2002).
- [9] A. Poole, et al., arXiv:1401.3265 (2014).
- [10] O.A. Petrenko, Low Temperature Physics/Fizika Nizkikh Temperatur, v. 40, No. 2, pp. 139–147 (2014).
- [11] Felix Groitl, PhD Thesis, TU Berlin (2013).