

[s7.m1.o3] Neutron diffraction studies in the 50 GPa pressure range: recent results on magnetic structures and phase transitions. I.N. Goncharenko^{1,2}, I. Mirebeau¹, J.-M. Mignot¹, A. Ochiai³ and S. Carlson⁴, 1- *Laboratoire Léon Brillouin, CEA-CNRS, CEA Saclay, 91191 Gif-sur-Yvette, France*, 2- *Russian Research Center "Kurchatov Institute" 123182 Moscow, Russia*, 3- *Niigata University, Ikarashi-Nincho 8050, Niigata-shi, Niigata-ken 950-2181, Japan*, 4- *European Synchrotron Radiation Facility, B.P. 220, 38043, Grenoble, France*.
 Keywords: instrumentation, neutron diffraction.

We present an overview of the high pressure magnetic studies on the ORPHEE neutron source of the Laboratoire Léon Brillouin. Progress in pressure techniques and neutron instrumentation¹⁻² allowed us to explore a wide range of pressures (up to 50 GPa in powder studies, up to 10 GPa in single crystal studies) and temperatures (down to 1.5 K).

The huge pressure range was used to study systematically the role of the interatomic distances on the strength of the magnetic exchange in solids and to determine the effect of structural and electronic transitions on magnetic orders^{3,4}. The talk includes several examples of high pressure studies. In particular, we discuss the magnetic and crystal structure of the "model Heisenberg magnets" EuX and GdX (X = chalcogen or pnictogen) studied by X-ray and neutron diffraction in the 50 GPa pressure range.

We discuss future prospects for high pressure studies, including next steps in specialized high pressure neutron instrumentation, application of ultra-low temperatures and high magnetic fields, simultaneous refinements of the magnetic and crystal structures from combined X-ray and neutron data.

[1] I.N. Goncharenko, J.-M. Mignot, G. André, O. A. Lavrova, I. Mirebeau, V. A. Somenkov, "Neutron diffraction studies of magnetic structure and phase transitions at very high pressures", *High Pressure Research* (1995), v. 14, pp. 41-53.

[2] I. N. Goncharenko, I. Mirebeau, P. Molina and P. Böni, *Physica B* (1997), "Focusing neutrons to study small samples", v. 234, pp. 1047-1049.

[3] I. N. Goncharenko and I. Mirebeau, "Ferromagnetic Interactions in EuS and EuSe Studied by Neutron Diffraction at Pressures up to 20.5 GPa", *Phys. Rev. Lett.* (1998), v. 80, pp. 1082-1085.

[4] P. Link, I.N. Goncharenko, J.-M. Mignot, T. Matsumura and T. Suzuki, "Ferromagnetic Mixed-Valence and Kondo-Lattice State in TmTe at High Pressure", *Phys. Rev. Lett.* (1998), v. 80, pp. 173-176.

[s7.m1.o4] Fast Powder Diffraction with a New PSD at the High Intensity Neutron Diffractometer D20. T.C. Hansen, P. Convert, *Institut Max von Laue-Paul Langevin, BP 156, 38042 Grenoble Cedex 9, France*.

Keywords: In-situ diffraction, powder diffraction, instrumentation

D20¹ is a medium-resolution 2-axis diffractometer, providing a high flux of up to $6 \cdot 10^7$ n/s/cm² at the sample position. To achieve the highest detected intensity available in neutron powder diffraction, 1536 detection cells of a stationary, curved linear position sensitive detector (PSD) cover a Θ range of 153.6°. This makes D20 an ideal tool, e.g., for *in-situ* diffraction studies with time constants even below a second. The high stability of that microstrip gas chamber (MSGC) PSD allow for high precision in intensity measurements, as for differential acquisitions in magnetism and physisorption, or studies on disordered systems. Four, vertically focussing monochromators, 15 take-off angles, optional Soller collimators and secondary slits provide a large choice in Q-space, resolution, wavelength and flux. This makes D20 adapted to various levels of crystallographic complexity and rapidity of the observed phenomenon. D20 has been operational in 1997 and 98 and will work again in 2000 after repair of its PSD. First results of the newborn diffractometer shall be presented.

Assisted by the *McStas* package², a *Monte-Carlo* ray-tracing simulation program of the complete instrument has been established. It allows, e.g., a confirmation of the super-GAUSS like deviation from the ideal shape of BRAGG-peaks, observable in conditions of higher flux and less resolution. An analytical approach to these unusual shapes will be suggested. Those simulations additionally permit an optimisation of components, so for the mosaic of the future Germanium monochromator, providing take-off angles up to 120° for high-resolution powder diffraction. When using reflections not normal to the cut face of the crystals, the FANKUCHEN effect may increase the resolution, proportional to the relative rocking angle. Simulations quantify this and the gain or loss in intensity precisely. Further, simulations help preparing experiments, especially those with difficult sample environment. As an example, hydrothermal reaction cells may be checked for background contributions to the pattern, which becomes avoidable, or at least foreseeable and so treatable.

Tools will be provided to determine systematically the optimum out of the variety of configurations at D20. Simulation of a postulated powder pattern for any set-up, and subsequent RIETVELD refinement, reveals the achievable precision of any parameter, and the acquisition time to get a given one. An enhanced instrument control responds to the acquired data reducing waste of beamtime to a minimum, especially in time-resolved experiments requiring fast decisions.

[1] Convert P., Hansen T., Oed A., Torregrossa J. "D20 High Flux Two Axis Neutron Diffractometer", *Physica B*, (1998), **241-243**, 195-197.

[2] Lefmann K., Nielsen K. "McStas", a General Software Package for Neutron Ray-tracing Simulations", *Neutron News*, (1999), **10**, No.3, 20-23.