

OCM08.29.4*Acta Cryst.* (2005). A61, C134

Single crystal neutron experiments under pressures up to 38 GPa
 Igor Goncharenko^a, Arsen Gukasov^a, Paul Loubeyre^b, ^aLaboratoire Léon Brillouin, C.E.A.-C.N.R.S., CEA Saclay, 91191 Gif-sur-Yvette, Franc. ^bDépartement Physique Théorique et Applications, C.E.A., 91680 Bruyères-le-Châtel, France. E-mail: gonch@llb.saclay.cea.fr

Single crystal neutron diffraction is the most powerful technique to characterize magnetic orderings and crystal structures in solids. The “Kurchatov-LLB” pressure cells with sapphire and diamond anvils provide an opportunity to study neutron diffraction in unprecedented range of thermodynamical parameters: pressures above 10 GPa, temperature down to 0.1 K, and applied magnetic fields up to 8 T [1,2]. Recently we used the same pressure technique to study magnetic neutron diffraction under a combination of a hydrostatic pressure and a controlled uniaxial stress [3]. Another “hybrid” pressure cell has been developed to perform both x-ray and neutron diffraction experiments. The cell is compatible with gas loading. This cell was used to study orientational order in solid deuterium under pressures up to 38 GPa and temperatures down to 1.5 K [4]. Neutron experiments on samples as small as 80x80x25 μ^3 have been carried out at the ORPHEE reactor of the Laboratoire Léon Brillouin.

[1] Goncharenko I. N., *High Pressure Research*, 2004, **24**, 193. [2] Mignot J.M., Goncharenko I.N., Link P., Matsumora T., Suzuki T., *Hyperfine Inter.*, 2000, **128**, 207. [3] Mirebeau I., Goncharenko I.N., Dhalenne G., Revcolevschi A., *Phys. Rev. Lett.*, 2004, **93**, 187204. [4] Goncharenko I., Loubeyre P., *in press*.

Keywords: high-pressure, neutron diffraction, single-crystal techniques

OCM08.29.5*Acta Cryst.* (2005). A61, C134

Development of a New State-of-the-art Beamline Optimised for Single Crystal and Powder X-ray Diffraction under Extreme Conditions at the ESRF

Mohammed Mezouar, Wilson A. Crichton, Stany Bauchau G. Blattmann Philippe Marion, Joel Chavanne, Yves Dabin, Olivier Hignette, Christian Morawe, *European Synchrotron Radiation Facility, B.P. 220 38000 Grenoble France*. E-mail: mezouar@esrf.fr

We present a new state-of-the art synchrotron beamline fully optimised for monochromatic X-ray diffraction at high pressure and high (or low) temperature. In comparison with the old high pressure beamline ID30, this new beamline exhibits outstanding performance in terms of photon flux and focusing capabilities. The main components of this new instrument will be described in detail and compared to the performance of beamline ID30. In particular, the choices in terms of X-ray source, X-ray optics, sample environment and detectors will be detailed. The first results of the beamline commissioning are presented.

Keywords: synchrotron beamline, X-ray diffraction, high pressure

OCM08.29.6*Acta Cryst.* (2005). A61, C134

Recent Progress in Large-volume High P-T in situ X-ray Observation at SPring-8

Tomoo Katsura^a, Eiji Ito^a, Ken-ichi Funakoshi^b, Akefumi Nozawa^b, ^aInstitute for Study of the Earth's Interior, Okayama University, Misasa, Japan. ^bJapan Synchrotron Radiation Institute, Kouto, Japan. E-mail: tkatsura@misasa.okayama-u.ac.jp

In 1997, a 15 MN multi-anvil apparatus was installed in the beam line BL04B1 at SPring-8. This apparatus makes it possible to generate pressures up to 26 GPa and temperatures up to 2000 K using WC anvils. Workers have produced a number of experimental results such as determination of precise phase relations, equation of state, and viscosity measurement.

In 2002, another 15 MN multi-anvil apparatus was designed and installed also in BL04B1 [1]. Two major improvements were made in this apparatus. One is a precise guide block system, which prevents

from deformation of the cubic compression space. This system makes it possible to generate further higher pressures using sintered diamond anvils. Pressure of 63 GPa was first achieved by a multi-anvils apparatus.

The other improvement is an oscillation system, which a large-volume press is equipped with in the first time. This system makes it possible to obtain high-quality diffraction patterns against grain growth at high temperatures. The phase boundary of the B1-B2 transition in NaCl was determined by utilizing this function.

[1] Katsura T., *et al.*, *Phys. Earth Planet. Int.*, 2004, **497**, 143-144.

Keywords: high-pressure and high-temperature, in situ X-ray diffraction, multi-anvil apparatus

OCM08.29.7*Acta Cryst.* (2005). A61, C134

High-pressure Magnetic Collapse in Transition-metal Oxides

Jean-Pascal Rueff^a, Aleksi Mattila^b, James Badro^c, Gyorgy Vanko^d, Abhay Shukla^c, ^aLCPMR, CNRS-Université Paris 6, France. ^bUniversity of Helsinki, Finland. ^cLMCP, CNRS-Université Paris 6, France. ^dESRF, Grenoble, France. E-mail: rueff@ccr.jussieu.fr

Pressure plays a key role in transition-metal electronic properties, since it can alter the electron density and hybridization, thereby the localization of the d electrons and their magnetic properties. A satisfying description of d electron in correlated material constitutes in fact an ongoing challenge for theory. This henceforth applies to the magnetic collapse issue. We have studied the 3d magnetism in MnO and CoO under very high pressure using x-ray emission spectroscopy (XES). XES is known as a local probe of the metal magnetism [1]. More specifically, by monitoring changes in the K β emission line as a function of pressure, we were able to identify the disappearance of the transition-metal spin-moment at pressures of 80 GPa and 140 GPa in MnO and CoO respectively [2].

The results were analyzed within a full multiplet approach including crystal field, correlation, charge transfer and O-metal hybridization energies. The pressure dependence of the emission line is well accounted for by changes of the crystal field and ligand bandwidth. This work proposes to reconcile in a unified picture both localized and delocalized aspects of the d-electron properties under pressure. We will discuss about the potentials and perspective of this novel technique for high pressure magnetism studies.

[1] Badro J., *et al.*, *Science*, 2004, **305**, 383. [2] Rueff J.-P., *et al.*, *J. Phys.: Condens. Matter*, 2005, **17**, 717.

Keywords: high-pressure physics, X-ray emission spectroscopy, cluster calculations