lower mantle silicates influence the density and the elastic and seismic properties remain an open question.

Here we develop an energy-domain synchrotron radiation (SR) ^{57}Fe-Mössbauer spectrometer using the single-line Mossbauer source at beamline BL10XU of SPring-8 for enabling simultaneous X-ray diffraction (XRD) and Mössbauer spectroscopy (MS) experiments at high pressures and high/low temperatures in a diamond-anvil cell technique. The diffractometer for the energy-domain SR-MS consists of a high-resolution monochromator and a variable-frequency nuclear monochromator. The single-line Mössbauer sources with an energy width of neV can be extracted from SR using pure nuclear Bragg scattering. For MS measurements on iron-bearing materials, the incident X-rays are tuned to 14.4 keV. For XRD the energy of the incident X-ray beam from undulator source plan to be tuned the high-order harmonic of 14.4 keV. Many geological-relevant materials have no large hyperfine interactions, and exhibit the splitting collapses at high pressure. The energy-domain SR-MS method works in any operation mode for the storage ring. Analysis of MS spectra in energy domain is well established and is easier than that in time domain. Therefore, the energy-domain MS using SR would be suitable for high pressure studies of the magnetic and electronic properties of deep Earth materials, compared with nuclear resonance forward scattering of SR that is a time analogue of MS.

The combined system of XRD and MS can potentially offer the essential information for resolving outstanding issues in mineral physics. The MS method can be used with glass and fluid phase as well as crystalline materials. At present, we are at the stage where the device is started up. The device should be fully available in the second stage of 2011. In this talk, we describe this new facility and report on progress.

Keywords: mössbauer spectroscopy, nuclear bragg scattering, high pressure

MS47.P03

Acta Cryst. (2011) A**67,** C527

Setting up a home high pressure laboratory from scratch – when is it worth it?

Alexander J. Blake,[a] David R. Allan,[b] Neil R. Champness,[a] Jonathan McMaster,[a] Martin Schröder,[a]. [a]*School of Chemistry, The University of Nottingham, Nottingham, NG7 2RD (UK).* [b]*Diamond Light Source, Harwell Science and Innovation Campus, Didcot, Oxfordshire, OX11 0DE (UK).* E-mail: a.j.blake@nottingham.ac.uk

Although high pressure crystallography continues to expand in both scope and popularity [1], the specialized equipment and skills required to pursue such studies in an effective manner mean that it is still regarded as largely the preserve of large, well-established and highly-experienced groups. However, our experience of high pressure studies conducted at central facilities [2], where extensive expertise and support may be available, led us (and other researchers) to consider establishing high pressure facilities within our home laboratories. While these will obviously be modest in comparison to powerful central facilities, they offer the advantage of much greater access, as well as more flexibility and convenience to carry out high pressure experiments.

We have recently set up dedicated in-house high pressure facilities in Nottingham, within a crystallographic laboratory where no such facilities had previously been available [3], and we will describe our experience and the factors which had to be considered during the process. These factors include the nature and extent of the scientific program to be undertaken, grant support, other funding, accommodation and expert advice and support: their influence and interaction must be taken into account when deciding whether in-house high-pressure facilities are viable and, if they are, in designing, commissioning and installing them.

This contribution will also explore some of the different options available, taking into account local requirements and circumstances.

[1] E. Boldyreva, P. Dera, *High-Pressure Crystallography - From Fundamental Phenomena to Technological Applications* - NATO Science for Peace and Security Series B: Physics and Biophysics: Springer **2010**. [2] D.R. Allan, A.J. Blake, D. Huang, T. J. Prior, M. Schröder, *Chem. Commun.* **2006**, 4081-4083. [3] A.J. Blake, O. Presly, D.R. Allan, *Agilent Technologies Application Note on High Pressure Crystallography* **2011**.

Keywords: high pressure, instrumentation, techniques

MS47.P04

Acta Cryst. (2011) A**67,** C527

High-resolution single-crystal neutron diffraction to 10 GPa

C.L.Bull,[a] K.Komatsu,[a] M.Guthrie,[a] R.J.Nelmes,[a] J.S.Loveday,[a] H. Hamidov,[a] M-T.Fernandez-Diaz,[b] M.J. Gutman,[c] [a]*School of Physics and Centre for Science at Extreme Conditions, The University of Edinburgh, Edinburgh EH9 3JZ, (UK)* [b] *Institute Laue Langevin, 6 rue Jules Horowitz BP 156, F-38042 Grenoble Cedex 9, (France)* [c]*ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon, OX11 0QX, (UK). E*-mail: craig.bull@stfc.ac.uk

Single-crystal neutron diffraction is the technique of choice when trying to determine the nature of complex multi-site disorder and anisotropic atomic displacement parameters (ADPs). The absence of form factor effects in the neutron scattering process gives inherent advantages for measurement of disorder and ADPs and the access to three dimensional data provided by a single crystal gives greatly enhanced accuracy on directional dependence.

Now, with the development of new cell, anvil and gasket technologies, a significant breakthrough has been made, allowing us for the first time to take full structure refinement to ~10 GPa on the D9 instrument at ILL, Grenoble, and the Laue TOF instrument (SXD) at the ISIS Facility, UK.

We will describe the results from studies of squaric acid and KDP up to pressures of 10 GPa where we have been studying the proton distributions in nearly centred and centred hydrogen bonds. We will also present results from samples grown in situ at high pressure of phases of ice and ammonia water mixtures. We will describe the technical aspects of performing high-resolution single-crystal studies at high pressure both at neutron spallation and at reactor sources.

Details of analysis techniques will also be described. Finally we will also highlight developments in view to increase the range of both science and pressures that can be achieved.

Keywords: high-pressure, neutron diffraction, single-crystal, hydrogen bond

MS47.P05

Acta Cryst. (2011) A**67,** C527-C528

Low-temperature high-pressure analysis utilizing a novel pressure cell design

Christopher Cameron,[a] Simon Parsons,[a] Stephen Moggach,[a] Konstantin Kamenev,[b] David Allan,[c] [a]*School of Chemistry, University of Edinburgh, (Edinburgh).* [b]*Centre for Science at Extreme Conditions (CSEC), University of Edinburgh, (Edinburgh).* [c]*Diamond Light Source Ltd, Didcot.* E-mail: C.A.Cameron@sms.ed.ac.uk

Inorganic compounds can undergo significant changes in their