MPa) of thermal expansion and phase behavior for some of these materials have made use of a new "Background reducing Internal Mask" to obtain Rietveld quality X-ray data from samples contained in substantial heated titanium pressure vessels. Our studies of local structure evolution in the negative thermal expansion material cubic $ZrMo_2O_8$ as it is heated at ambient pressure and amorphized on compression in a diamond anvil cell will also be discussed.

Keywords: high-pressure diffraction, thermal expansion, local structure

MS.05.3

Behavior of SiO2 in helium pressure medium

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Although helium has been widely used as a good hydrostatic pressure transmitting medium, it sometimes affects considerably to the compression behavior of minerals. Here we report an example that SiO2 glass becomes quite "rigid" when compressed in helium. We have compressed SiO2 glass in helium up to 10 GPa with a diamond-anvil cell [1]. Volume measurements of the bulk size show that SiO2 glass is much less compressible than normal when compressed in a helium medium, and the volume in helium at 10 GPa is close to the normal volume at 2 GPa. X-ray diffraction and Raman scattering measurements suggest that interstitial voids in SiO2 glass are prevented from contracting when compressed in helium. This is probably because a large amount of helium penetrates into these voids. The estimated helium solubility in SiO2 glass is very high and is between 1.0 and 2.3 mol per mole of SiO2 glass at 10 GPa, which shows marked contrast with previous models.

These results may affect discussions on the Earth's evolution as well as interpretations of various high-pressure experiments, and also lead to the creation of new materials.

[1] T. Sato, N. Funamori, T. Yagi. **2011**, to be submitted.

Keywords: SiO2 glass, helium, voids

MS.05.4

**High-pressure polymorphism of ammonia hydrates**

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Ammonia hydrates, $NH_3 \cdot nH_2O$ (where $n = \frac{1}{2}$, 1, 2), are likely to be major constituents of icy bodies in the outer solar system; their phase behaviour and physical properties up to pressures of several GPa are therefore relevant to modelling the structure and thermal evolution of such planetary objects [1]. We report the status of our program to investigate these properties using a combination of high-pressure powder diffraction (carried out at the ISIS neutron spallation source and the Institut Laue Langevin) and quantum mechanical calculations.

Calculations have provided us with predicted crystal structures, constrained only by the experimentally obtained unit-cell dimensions and contents, of both ammonia monohydrate phase II [2] and ammonia dihydrate phase II, as well as predicted structures of other high-pressure phases which can be tested against new powder diffraction data. Moreover, the elastic properties calculated by these methods are a direct complement to equations of state determined from high-pressure experiments [3], [4].

Most recently, we carried out an initial survey of the ammonia monohydrate phase diagram using a Paris-Edinburgh press on the high-intensity D20 beamline at the ILL. Neutron powder data collected over the five day study allowed us to fit an isothermal equation of state for ammonia monohydrate II over a range twenty times larger than previously measured, reproduced earlier observations [5] of phases IV and V, and constrained their phase transition pressures and temperatures (see figure below); ammonia monohydrate phase V was observed up to a pressure of 9 GPa. We will discuss the practical aspects of loading a volatile liquid sample into the CCR-mounted P-E press in use at the ILL, the nature and high quality of the data produced, and implications for our future studies of such systems at high pressure.

Figure 1 below shows the phase diagram of ammonia monohydrate, and the P-T path (pale line) followed during our December 2010 study at the ILL. The darker line shows the P-T path we propose to follow in future work.
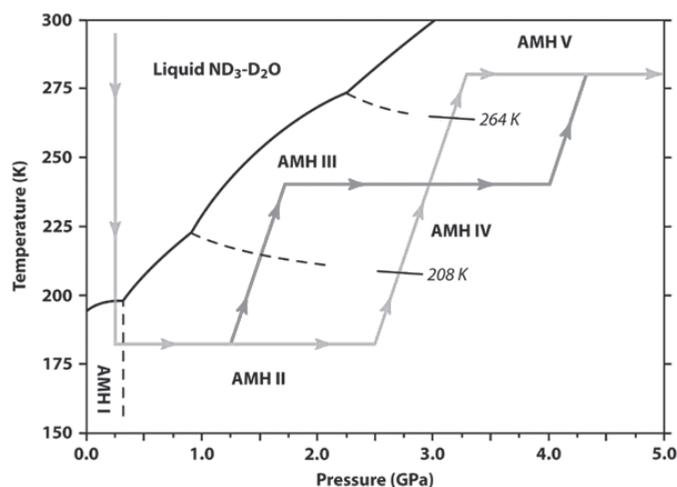
[1] A.D. Fortes, M. Choukroun, *Space Sci. Rev.* **2010**, *153*, 185-218. [2] A.D. Fortes, *et al. J. Am. Chem. Soc.* **2009**, *131*, 13508-13515. [3] A.D. Fortes, *et al. J. Chem. Phys.* **2009**, *131*, article 154503. [4] A.D. Fortes *et al. J. Appl. Cryst.* **2009**, *42*, 846-866. [5] J.S. Loveday, R.J. Nelmes, *High Press. Res.* **2004**, *24*, 45-55.

Keywords: polymorphism, diffraction, pressure

MS.05.5

Structural Evolution of $Ca_{0.4}Sr_{0.4}Nd_{0.2}Mn_{1-x}Cr_xO_3$; $0 \leq x \leq 0.2$ perovskites

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A series of complex oxides of the type $Ca_{0.4}Sr_{0.4}Nd_{0.2}Mn_{1-x}Cr_xO_3$; x