

are similar to the covalently-bonded MOFs, i.e. they can be porous, interpenetrated etc.;

- reconstruction of strongly bound $\text{Mg}(\text{BH}_4)_2$ coordination frameworks is kinetically hindered, giving rise to a coexistence of various metastable polymorphs.

Structural evolution of ammonia borane NH_3BH_3 manifests itself in two phase transitions, below 293 K at ambient pressure and above 1.1 GPa at room temperature, relating a disordered $I4mm$ structure to the ordered polymorphs with $Pmn2_1$ and $Cmc2_1$ structures. The later has been solved from diffraction data, positions of N and B atoms and orientation of NH_3 and BH_3 groups were finally assigned with a help of first principles DFT calculations. Group-theoretical analysis identifies a single two-component order parameter, combining ordering and atomic displacement mechanisms and linking the orientationally disordered parent phase $I4mm$ with three ordered distorted structures. We propose a generic phase diagram for NH_3BH_3 , by mapping three experimentally found and one predicted phases as a function of temperature and pressure, along with the evolution of the corresponding structural distortions. The role of N-H...H-B dihydrogen bonds in the stability of NH_3BH_3 polymorphs is examined.

[1] Filinchuk Y., Cerny R., Hagemann H., *Chem. Mater.*, **2009**, 21, 925. [2] Her J.-H., Stephens P.W., Gao Y., Soloveichik G.L., Rijssenbeek J., Andrus M., Zhao J.-C., *Acta Cryst. B*, **2007**, 63, 561. [3] Ozolins V., Majzoub E.H., Wolverton C. *Phys. Rev. Lett.*, **2008**, 100, 135501. [4] Voss J., Hummelshoj J.S., Lodziana Z., Vegge T. *J. Phys.: Condens. Matter*, **2009**, 21, 012203.

Keywords: high pressure; synchrotron powder diffraction; hydrogen storage

FA5-MS07-O4

High Pressure Anelastic Behaviour of Fe_xO . Leonid Dubrovinsky^a, Anastasia Kantor^a, Innokenty Kantor^a, Michael Krisch^b, Alexei Bossak^a. ^aBGI, Bayreuth University, Germany. ^bESRF, France.

E-mail: Leonid.Dubrovinsky@uni-bayreuth.de

Elastic properties of solids are among the most important for solid Earth geophysics, engineering, and solid-state physics. Elastic moduli can be determined from pressure-volume relations (static or shock-wave compression), from acoustic waves velocity measurements (ultrasonic interferometry), or from dispersion curves of acoustic phonon branches (neutron, x-ray or light inelastic scattering). In the case of an ideal elastic solid the elastic moduli determined using different techniques should coincide within the experimental error (with the conversion factor between isothermal and adiabatic moduli). However, if any anelastic relaxation exists and the equilibrium strain for a given stress is achieved only after certain finite time interval, the effective elastic moduli measured by different methods would systematically vary, depending on sampling frequency. Anelasticity in a solid appears due to defects or other crystal imperfections when the energy minimum is achieved not only by varying the atomic geometry but also by changes in the materials' mesostructure (e.g. structure with a characteristic length larger than the crystal unit cell

size).

We have chosen non-stoichiometric Fe_xO as a candidate for a strongly anelastic material. Although Fe_xO has been intensively studied for several decades, many of its properties including elastic behaviour remain controversial and not well understood. A combined single-crystal inelastic x-ray scattering (IXS) and x-ray diffraction (XRD) study of synthetic wüstite $\text{Fe}_{0.95}\text{O}$ at elevated pressure revealed increasing the difference in the bulk modulus determined from static (XRD) and dynamic (IXS) measurements upon compression. We explain and quantitatively describe this observation by anelastic relaxation in wüstite. The reanalysis of previous results put some more evidence for relative good coincidence for bulk moduli and systematic difference for K' between static and dynamic measurements.

Keywords: high pressure; FeO; anelastic behaviour

FA5-MS07-O5

Pressure Induced Homothetic Volume Collapse in Si and Ge Clathrates Alfonso San Miguel^b, Denis Machon^b, Jean-Christophe Blancon^b, Colin Bousige^b, Sylvie Le Floch^b, Régis Débord^b, Vittoria Pischedda^b, Pierre Toulemonde^a. ^aInstitut Néel, Grenoble, France. ^bLPMCN, Université Lyon 1 and CNRS, Lyon, France.

E-mail: sanmiguel@lpmcn.univ-lyon1.fr

Since the discovery of a pressure induced isostructural homothetic volume collapse (HVC) of silicon type I clathrates [1,2], different models have attempted with limited success to explain this remarkable transition which can be associated with up to ~10% of atomic volume reduction. Recently, different studies [3,4] point out to some form of disorder in the silicon host framework associated to the volume collapse in clathrates, which detail nature has not been well characterized. The pressure induced isostructural HVC in clathrates could be related to pressure induced amorphization preserving the crystal topology recently predicted in zeolites [5] making of the HVC a more general behaviour in nanocage-like materials. We have combined high pressure EXAFS at the Ba L3-edge in $\text{Ba}_8\text{Si}_{46}$ and at the Ge k-edge in the $\text{Ba}_8(\text{Si}_{1-x}\text{Ge}_x)_{46}$ mixed clathrates to obtain a local image of the evolution of the host and guest structures at the HVC transition and understand its physical origin. The full set of obtained data allow us to present a novel picture on the mechanism governing this notable phase transition.

[1] A. San Miguel et al. *Phys. Rev. B* 65 054109 (2002). [2] A. San-Miguel et al. *Europhys. Lett.* 69, 556 (2005). [3] D. Machon, P. Toulemonde, P.F. Mc Millan et al. (*Phys. Rev. B*, accepted). [4] L. Yang et al., *Phys. Rev. B* 74, 245209 (2006). [5] I. Peral and J. Íñiguez, *Phys. Rev. Lett.* 97, 225502 (2006).

Keywords: clathrate; EXAFS; high pressure