INORGANIC CRYSTALLOGRAPHY AND GEOSCIENCES

are similar to those of pure Fe melt [1]. These results imply that the effect of S content in the Earth's outer core may not be so strong.

[1] Alfe D., Kresse G., Gillan M. J., *Phys. Rev.* B, 2000, **61**, 132. Keywords: viscosity, high pressure, Fe-FeS melt

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Accommodation Mechanism of Kr Trapped in Terrestrial and Planetary Materials

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The trapping or adsorption of noble gases in minerals has great interest in solving the "missing Xe" problem. We focus on Kr slightly trapped in terrestrial and planetary materials in a *ppb* level. In this study we have examined the solubility and local structures of Kr trapped in (1) minerals such as quartz, olivine, coesite, stishovite, olivine and wadsleyite and (2) synthetic model-samples of carbon fine powder, silica gel and zeolite.

Samples were synthesized in Kr-atmosphere at high pressure and high temperature, by using the Kawai-type high-pressure apparatus. Kr-doped silica gels, and partly MgO, were used as starting materials and sealed in Pt-capsule to prevent Kr-escape under high pressure. Degassing of Kr for all samples were measured as a function of temperature up to 1850°C by the mass spectrometer. The results showed that the degassing of silica gel causes at temperatures between 500°C and 800°C. On the other hand, Kr-doped natural olivine has the degassing, giving two peaks observed at 800°C and 1800°C. It is notable that small amount of Kr still remains in olivine even at 1800°C. XAFS measurements in the fluorescence mode were made to determine the atomic distances between Kr and the neighboring atoms and the local structures around Kr atoms. There are structural differences in the Kr coordination between terrestrial materials and model samples.

Keywords: gas-solid interaction, high pressure, meteorite

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Pressure-induced Electron Transfer in Cobalt-iron Prussian Blue Complex Studied by RIXS

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Resonant Inelastic X-ray Scattering (RIXS) recently has become one of the most advanced techniques that probe electronic excitations in solids, combining both advantages of a high resolution and bulk sensitivity. In our measurement, we attempted to study the charge transfer in $K_{0.2}Co_{1.4}[Fe(CN)_6] \cdot XH_2O^{[1]}$ as a function of pressure by RIXS. The photoinduced magnetization at low temperature in Co-Fe Prussian blue analogues was explained by the presence of diamagnetic Co(III)-Fe(II) low spin pairs, this step can be pushed by low temperature or high pressure^[2]. Then the photoinduced electron transfer from Fe(II) to Co(III) can be happened. We had performed a preliminary Resonant inelastic x-ray scattering (RIXS) studies on the K_{0.2}Co_{1.4}[Fe(CN)₆]•XH₂O at 0.33GPa under Diamond Anvil Cell(DAC) to study and confirmed the charge transfer behavior successfully during this time. From the comparison of the title compound at 0.33GPa pressure and ambient pressure, we can see the Co(III) ratio increase very clearly, that mean the charge transfer Fe(III)-Co(II) \rightarrow Fe(II)-Co(III)happened. This confirms the outstanding resolving power of RIXS and fruitful quantitative determinate the ligand field strength and also the Co(II)/[Co(II)+Co(III)] ratio can be determinated from this kind of measurement. In here, we will present the measurement results on Iron



K-edge and Cobalt K-edge partial fluorescence yield mode (PFY) by RIXS experiment to get the ligand field strength and charge transfer information related with pressure.

Figure 1. Cobalt Kedge X-ray absorption spectra with 0.33GPa and without pressure by partial fluorescence yield mode (PFY)

[1] Verdaguer M., *Science*, **272**, 698 [2] Ksenofontov V., Levchenko G., Reiman S., Gutlich P., *Phys. Rev. B*, 2003, **68**, 24415.

Keywords: inelastic X-ray scattering, cobalt-iron prussian blue, pressure

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ALS Beamline 12.2.2, A High-pressure X-ray User Facility at the US-West-Coast

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Beamline 12.2.2 is a hard-X-ray beamline making use of the radiation spectrum (~ 5 keV < E < 40 keV) emitted from a superconducting bending magnet. The radiation is conditioned using a plane parabola collimating mirror (M1), a Kohzu monochromator assembly with a Si(111) crystal ($E/\Delta E \sim 7000$) or W/B₄C multilayer ($E/\Delta E \sim 100$), and a toroidal focusing mirror (M2) with variable focusing distance, before it is directed into the experimental hutch

In the hutch, two experimental stations facilitate a variety of highpressure experiments, focusing on *in-situ* high-pressure - hightemperature powder diffraction, EXAFS and X-ray imaging. Endstation 1 is presently optimized for combining externally heated diamond anvil cells (DACs) with powder X-ray diffraction and can be used for high-pressure EXAFS experiments as well. End-station 2 is designed for *in situ* laser heating of DACs using a set of Kirkpatrick-Baez mirrors for secondary focusing (spot size at sample = 0.01 x 0.01 mm²) as well as a double sided YLF laser heating system

Samples are placed on a kinematic mount equipped with 2 rotation stages as well as 4 linear stages in order to center the DAC reproducibly at the same reference position. The overall accuracy of the distance calibration is ~ 0.01 mm corresponding to a theoretical $\Delta d/d$ of 10⁻⁴ at a sample to detector distance of 100 mm. Further benchmarks as well as examples of current research will be presented. **Keywords: synchrotron X-ray instrumentation, high pressure crystallography, mineralogy geophysics high pressure**

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High Pressure Single-Crystal Neutron Diffraction of DKDP

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The initial results of a new initiative of the Paris-Edinburgh (PE) collaboration to develop single-crystal technology for high-pressure neutron diffraction are presented. Single-crystal neutron diffraction data have been collected from D_2KPO_4 at pressures up to 7.5 GPa. At 4.2 GPa it has been suggested by Endo [1] that the hydrogen bond lengths elongate and the proton centres in a single minimum between the two oxygen atoms. However, these results were obtained using x-