The appearance of this inclusions allow as to estimate the temperature of the fusion which did not reach the temperature of hematite melting. Besides, in the glass, we find the inclusions of hematite with the tracks of partial fusion.

Appearance of a great amount skeleton formations with the composition such as FeO is an evidence of a great fusion cooling speed. Such structures forms because of dissociation on the stage of cooling.

Besides we find the numerous inclusions corresponding by structure to baddeleyite glass in the form of thin thready formations, specifying on processes of segregation proceeding in the time of hardening of fusion. These processes of segregation were not observed before in fulgurites. Also, inclusions of baddeleyite glass meets and as separate grains with crystallographic facet and with the raised contents of uranium. Besides there are alumino-silicate inclusions enriched with the titan and phosphorus. In such inclusions are widely used the clusters of ferrian composition.

Keywords: fulgurite, hematite, segregation

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Synthesis and X-ray Study of [Pt(NH₃)₄](ReO₄)₂ Thermolysis Products

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Catalysts based on the Pt and Re play an essential role in reforming processes. About 65% of all the produced rhenium is used for these needs. One of the methods to prepare catalysts is the thermolysis of inorganic complex salts, containing two required metals. In this work we have studied the precursor complex $[Pt(NH_3)_4](ReO_4)_2$ and obtained a solid solution $Pt_{0.33}Re_{0.67}$.

A synthesis of the precursor complex $[Pt(NH_3)_4](ReO_4)_2$, was held in the following way: 0.2 M water solutions of $[Pt(NH_3)_4]Cl_2$ and $NaReO_4$ were mixed at 50°C, then kept for an hour at room temperature. A white residue was separated and washed away with water and acetone. The yield is 75%. The crystal structure of $[Pt(NH_3)_4](ReO_4)_2$ was determined with a X8APEX Bruker diffractometer (MoKα-radiation, θ range 2.85—32.59°, 2007 independent reflections), R = 2.11%. Crystal data: a = 5.1847(6), b = 7.7397(8), c = 7.9540(9) Å, α = 69.531(3), β = 79.656(3), γ = 77.649(3)°, V = 290.19(6) Å³, space group P-1, Z = 1. This complex is isostructural to $[Pt(NH_3)_4](TcO_4)_2$ [ICSD Card 65-766]. The structure consists of the isolated complex $[Pt(NH_3)_4]^{2+}$ and ReO_2^- ions.

The thermolysis of $[Pt(NH_3)_4](ReO_4)_2$ was carried out at 900°C in H_2 atmosphere for 7 hours. According to X-ray analysis, the product is a single phase solid solution $Pt_{0.33}Re_{0.67}$. It is based on the hexagonal close-packed rhenium structure. Crystal data of the solid solution: a = 2.764(2), b = 4.415(3) Å, V = 29.21 Å³, space group P6₃/mmc, Z = 2.
Keywords: platinum group, X-ray analysis, single-crystal structure analysis

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Crystal Structure of KLiSO₄ at High Temperatures

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Above room temperature there are three modifications of $KLiSO_4$; i.e. phase I, II and III. Phase transitions temperatures between them are 435°C and 668°C respectively. The x-ray diffraction intensities of phase I at about 700°C and of phase II at about 600°C were collected on the CAD4 single crystal diffractometer equipped a self-made furnace. During collection of intensities data, a prominent decay of intensities was observed. The crystal structure of phase I is the tridymite derivatives with ordered arrangement of SO₄- and LiO₄-tetrahedra similar to that of phase III. The statistical data of the structure refinement for phase I with polar space group of P6₃mc was R = 0.057, Rw = 0.056 and S (goodness-of-fit) = 1.859. The crystals of phase II usually exhibit misleading hexagonal twinned cell which is composed of three orthorhombic twin domains in the temperature range between 435°C and 668°C. An almost twin-free single crystal of Phase II was observed at the elevated temperature. The crystal structure of phase II was refined with this crystal is orthorhombic with the polar space group Pc2₁n. The final statistical data was R = 0.077, Rw = 0.073 and the S = 1.028 with ordered arrangement of atoms. This data was compared with that of the twinned crystal corrected with twin ratio and further discussed previously reported disordered model with the space group of Pmcn.
Keywords: KLiSO4, structure analysis, high temperature

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***Ab initio* Treatment of Minerals at Extreme Conditions**

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The mantle of the Earth extends from the depth of about 670 km to 2981 km. It consists mainly of $MgSiO_3$-perovskite, (Mg,Fe)O magnesiowüstite and $CaSiO_3$-perovskite. It is possible to calculate thermodynamic properties, structures and energetics of the separate minerals at extreme conditions of the mantle using *ab initio* methods, such as the density functional theory with the generalized gradient approximation (GGA) [1] and the projector augmented wave (PAW) method [2], which are included in the VASP [3] code. To get a better picture of the mantle it is necessary to not only look at chemically pure minerals, but to consider them as a solid solution, as it is the probable case in nature.

Using density functional theory the structure and the stability of the $CaSiO_3$ perovskite in the pressure range of the Earth's mantle (0-150 GPa) have been calculated [4]. Additionally we use the subregular solid solution model together with point defect calculations to model the solvus of the (Ca,Mg)-perovskite phase diagram at 25 GPa. This is a special case, because there is also a symmetry change from a tetragonal to an orthorhombic perovskite structure as you increase the concentration of Mg. This is the first work to treat this subject with ab initio methods.

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Keywords: (Ca,Mg)SiO3 perovskite, Earth's mantle, solid solution

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Viscosity Measurements of Fe-FeS Melts under High Pressures

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The Fe-FeS melt is the important Earth's outer core material and its viscosity has been thought to be very low under high pressure and high temperature. Recent measurements of the Fe-FeS melt have showed the low viscosity values (~ 10^{-2} Pa-s), however, the accuracies are not so good for determining the viscosity values. An x-ray radiography technique with synchrotron radiation is very useful for the falling sphere viscosity measurement, because it enables us in situ observation of the sinking process and determination of the reliable viscosity coefficient.

We measured the viscosities of Fe-FeS ($Fe_{73}S_{27}$, $Fe_{80}S_{20}$, $Fe_{90}S_{10}$) melts, combining the falling sphere method with the large volume press at the SPring-8. Precise viscosities have been obtained up to 9 GPa using Stoke's law. The pressure dependences of the viscosities are very small, however, the viscosities slightly increase with increasing pressures. The activation energies and the activation volumes have been determined from the dependences on pressure and temperature of the viscosities. The viscosities of the Earth's outer core have been calculated using the activation energies and the activation volumes of $Fe_{90}S_{10}$. The calculated viscosities of the Earth's outer core

P10

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.

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Keywords: viscosity, high pressure, Fe-FeS melt

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Acta Cryst. (2005). A**61**, C374
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

P.10.04.9
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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 $K_{0.2}Co_{1.4}[Fe(CN)_6]\cdot XH_2O$ 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)→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
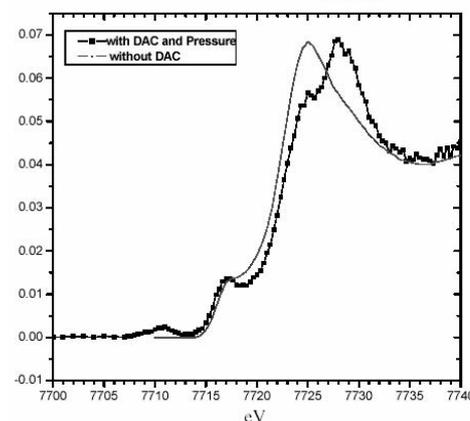
K-edge and Cobalt K-edge partial fluorescence yield mode (PFY) by RIXS experiment to get the ligand field strength and charge transfer information related with pressure.

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

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

P.10.04.10
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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 super-conducting bending magnet. The radiation is conditioned using a plane parabola collimating mirror (M1), a Kohzu monochromator assembly with a Si(111) crystal (E/ΔE ~ 7000) or W/B_4C multilayer (E/ΔE ~ 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 high-pressure experiments, focusing on *in-situ* high-pressure - high-temperature powder diffraction, EXAFS and X-ray imaging. End-station 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 mm^2) 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 Δd/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-