superconductor at high pressure due to the high density of states at the Fermi level. Matsuoka *et al* [2] followed Feng's work and indeed found $CaLi_2$ become a superconductor at 11 GPa. However, the crystal structure of $CaLi_2$ under pressure is still not well established. In this work, the crystallography of $CaLi_2$ at high pressure has been extensively investigated by the evolutionary algorithm USPEX. We explored several new phases of $CaLi_2$ at pressures in range 50 — 250 GPa. The chemical bonding and the electronic structures of the high pressure phases $CaLi_2$ are studied in detail. The high-pressure structures of $CaLi_2$ and the physical mechanisms of phase transitions will be discussed.

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Keywords: *ab-initio* structure determination, high pressure, electronic structure

P10.04.20

Effect of pressure on the crystal structure of α'_L-$Ca_{1.5}Sr_{0.5}SiO_4$

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One of the high-temperature polymorph of Ca_2SiO_4, α'_L phase, which is stable above 973 K [1] is known to become quenchable to room temperature with incorporation of Sr [2]. It is reported that the phase transition between α'_L and α'_H is displacive and α'_L is a hettotype of α'_H which is isostructural with β-K_2SO_4. In order to estimate the structural distortion of the α'_L phase from the α'_H phase, the tolerance factor (t) for the β-K_2SO_4 type structure was defined in this study. For the purpose of studying the effect of pressure on t, the crystal structure of $Ca_{1.5}Sr_{0.5}SiO_4$ was analyzed at 2.9 GPa and 4.6 GPa. A synthesized single crystal of $60 \times 60 \times 30$ µm was placed in a modified Merrill-Bassett type diamond anvil pressure cell [3]. The pressure medium was a 4:1 mixture of methanol and ethanol and a stainless steel (SUS301) plate was the gasket. Pressure was calibrated by the ruby fluorescence method [4]. X-ray intensity measurements were performed using the BL-10A beam line at the Photon Factory (High Energy Accelerator Research Organization, Tsukuba, Japan). Judging from the observed bond compressibilities, t decreases with pressure and the structural distortion of $Ca_{1.5}Sr_{0.5}SiO_4$ increases with pressure.
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Keywords: high pressure, single crystals, X-ray diffraction

P10.04.21

Rietveld refinement of natural fluorapatite from ultrahigh pressure eclogite

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Fluorapatite(FAP), found within eclogite from ultrahigh pressure orogen of China, is attracted for their structural response to pressure. Zhang et al. (2005) estimated the formation conditions of the ultrahigh pressure eclogite as >940ºC and >4.5GPa. Additional stress on FAP was kept away from crashing eclogite with hammer and grinding with agate mortar during the course of sample preparation. Powder X-ray diffraction method was used since the FAP aggregates containing amount of exsolutions on a scale of micrometer. The Rietveld method was performed for structure refinement. Polynomial background and the Pseudo-Voigt function were used for simulating measured profile. K-alpha 2 component was stripped and no smoothing was made. The final structure of the FAP is derived under the agreement index GOF=1.19. The space group of FAP is P63/m, and the refined cell parameters are c=6.8849(7) and a=9.3842(2)Å. That leads to a cell volume V=525.08Å^3. Metaprism twist angle ϕ, defined as the (001) projected angle of O1-Ca1-O2, is measured as 23.91º from the refined structural model. The X$^-$ ionic radius is measured as 1.313Å from tunnel Ca-F minus Ca^{+2} radius. This X$^-$ ionic radius is less than 1.33 Å an expected dimension of closest packing model when c/a=0.734. The formula of the FAP is, on averaged, derived as: $(Ca_{3.98}Sr_{0.01})_{3.99}(Ca_{5.96}Na_{0.01}Sr_{0.02})_{5.99}(P_{5.98}S_{0.02})_6O_{24}F_{1.99}$. As compression on flexible one-dimension tunnel in apatite leads to structurally adjustment through an increase in angle ϕ, it follows that higher pressure correlates with higher angle ϕ. The structure of the FAP from ultrahigh pressure eclogite of China possesses a small cell volume and a large twist angle and demonstrates a good record for the ultrahigh pressure processes underwent.

Keywords: apatite, Rietveld refinement, ultrahigh pressure

P10.04.22

Pressure-induced structural change of Ca and Mg aluminosilicate melts

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Viscosity and density are important physical properties to control the transportation of magma in the Earth's interior, which are strongly correlated to microscopic structure of magma. Magmas have been considered to be densified by changing its structure with increasing pressure. We have studied the static structure of the $Ca_3Al_2Si_6O_{18}$ and $Mg_3Al_2Si_6O_{18}$ melts up to 5 GPa by X-ray diffraction analysis, in order to clarify pressure-induced structural change in topology and aluminium coordination environment. We have found the degenerated T-O peaks splitting into two peaks up to 5 GPa, indicating the coordination change of aluminum with pressure. This observation is consistent with the results of NMR studies on the $Ca_3Al_2Si_6O_{18}$ glasses quenched from high-P melts, showing the increase of population of highly coordinated aluminum

with quenching pressure. Our studies also yields the evidences of the size reduction and the ordering of intermediate range structure with increasing pressure, in which the first sharp diffraction peak (FSDP) in the diffraction pattern shifts toward higher momentum transfer and becomes sharp by compression.

P10.04.23

The *ab initio* high pressure solid solution behaviour of the Al_2O_3-$MgSiO_3$ system

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With the assumption that the lower mantle is pyrolitic, $(Mg,Fe)SiO_3$ perovskite (70 vol%) is thought to be the most abundant phase in the Earths lower mantle, followed by magnesiowüstite $(Mg,Fe)O$ with (20 vol%) and $CaSiO_3$ perovskite, which comprises between 6 and 12 vol%. The Al_2O_3 content of fertile mantle compositions amounts to about 4-6 mol% and is supposed to dissolve mainly into $MgSiO_3$ perovskite. Experimental and theoretical studies have shown that a fair amount of Al_2O_3 can be dissolved in $MgSiO_3$ and that at pressures above 27 GPa $MgSiO_3$ perovskite and Al_2O_3 corundum form coexisting solid solutions. No further aluminous phase has been observed up to the pressure of the Al_2O_3 phase transformation to the Rh_2O_3(II) structure at 80-100 GPa. To what extent the recently discovered high pressure phases of $MgSiO_3$ and Al_2O_3 will change reciprocal solubilities of the phases in the $MgSiO_3$-Al_2O_3 system is still unknown. Using static *ab initio* point defect calculations and simple thermodynamic models, qualitatively correct solid solution behavior of the $MgSiO_3$-Al_2O_3 system was predicted. The solubility of Al in $MgSiO_3$ is large throughout the mantle and increases with pressure and temperature. Even though the high pressure phase transitions reduce the reciprocal solubilities, these are always large enough to completely assimilate the Al of the pyrolitic mantle. Information on the solubility of Al in $MgSiO_3$ might elucidate mineralogically more complex systems in the lower mantle of the Earth. Incorporation of other impurities present in significant quantities in the Earths mantle (Fe^{2+},Fe^{3+}, and to a lesser extent Cr), into the $MgSiO_3$ host might influence the Al-solubility, and thus change the now well established behaviour in the MgO-AlO-SiO system.

P10.04.24

Oxygen partitioning between magnesiowüstite and Fe-liquid: Implication to the earth's core

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Oxygen is potentially an important light element in the Earth's outer core (e.g., Ringwood 1977). In order to constrain the oxygen content of the core, the dependence of the oxygen concentration in liquid iron on pressure, temperature and oxygen fugacity needs to be clarified up to the relevant P-T conditions . We have conducted partitioning experiments of FeO between magnesiowustite and liquid iron at conditions up to 70 GPa and 3500 K with laser heated diamond anvil cell. Focused ion beam (milling) was used to prepare thin foil from run products for transmission electron microscopy. The technique has the advantage of site-specificity at the submicron meter scale and homogeneous thinning of the samples having multi-layers of different phases or the two-phase interface. The compositions of coexisting quenched iron and magnesiowustite were measured using a transmission electron microscope equipped with energy dispersive X-ray spectrometer and electron energy-loss spectrometer. Applying a thermodynamic model to describe the partitioning of oxygen, deltaH0 - T deltaS0 + int.deltaVdP + RTlnKd = 0, we obtained thermodynamic parameters, delta H0 = 170000 (J/mol), delta S0 = 56 (J/K/mol), and the hypothetical equation of state of the Fe-O metallic liquid component (K = 74 GPa, K' = 6.7, V0 = 13.2 cm3/mol). In case of core-mantle equilibrium, the results show that the outer core must be undersaturated in oxygen, which causes a layer at the very base of the mantle to be depleted in FeO. However, such an MgO-rich layer might be very thin because Fe-Mg diffusion, at least in silicate perovskite, is extremely slow at core-mantle boundary conditions (Holzapfel et al. 2005).

P10.04.25

Phase transitions and incommensurate structures in the brownmillerite system $Ca_2(Fe_{1-x}Al_x)_2O_5$

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The solid solution series is reported to exist from x=0 up to x=0.69 (e.g. [1] and references therein) at ordinary pressures. A phase boundary between structures adopting space group *Pnma* and *I2mb* was found close to x=0.28 [2]. Crystals with higher Al-contents can be synthesised using high pressure [3, 4]. HT phase transitions are known for the iron end-member and the structures crystallising in *Pnma* [2]. The HT phases were considered to conform to *I2mb* or *Imma* space group symmetry. Recent single crystal diffraction studies have found that $Ca_2Fe_2O_5$ transforms to a modulated structure in the range of 960-980K. This incommensurate phase can be described in superspace group *Imma(00 γ)s00* [5]. The modulated structure exhibits an aperiodic sequence of tetrahedral (FeO_4) chains. The temperature range of the transition is characterised by phase-coexistence, which can be observed by *in situ* HT single crystal X-ray diffraction experiments. Diffraction data collected in this region