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.

Keywords: silicate melt, aluminium coordination number, melt structure

P10.04.23

Acta Cryst. (2008). A**64**, C497

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.

Keywords: *ab-initio* calculations, solid solutions, high-pressure minerals

P10.04.24

Acta Cryst. (2008). A**64**, C497

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).

Keywords: high pressure, electron energy loss spectroscopy, thermodynamics

P10.04.25

Acta Cryst. (2008). A**64**, C497–498

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