RMC simulation of the experimental structure factor was successfully applied to generate a reliable 3-dimensional atomic configuration. Several partial atomic pair correlation functions, like the $g_{SiO}(r)$, $g_{BO}(r)$, $g_{OO}(r)$, $g_{SiSi}(r)$, $g_{SiB}(r)$, $g_{NaO}(r)$, $g_{BaO}(r)$, $g_{ZrO}(r)$ and most of the corresponding coordination number distributions has been revealed providing information on the short and intermediate range order.

The Si-O network proved to be highly stable consisting of slightly modified SiO_4 units. The B-O surrounding proved to be more complex. We have found that two characteristic well resolved first neighbour B-O distances are present at 1.40 Å and 1.60 Å. The latter agrees with the Si-O first neighbour distance, which is also at 1.60 Å. From the detailed analyses of the B-O and O-B coordination number distributions we have established that both 3- and 4-fold coordinated boron atoms (denoted as $^{[3]}$B and $^{[4]}$B) are present.

We suppose that the boron atoms partly form a mixed continuous network with Si-O network, where several different mixed $^{[4]}$B-O-Si and $^{[3]}$B-O-Si linkages are present in agreement with the findings of NMR [4,5] and Raman spectroscopy [6].

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MS23 O4

Magnetic phase transition of FeS at high pressures

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According to the cosmochemical arguments and the seismological data, the Earth's core must contain some light elements. However, the nature of the light element is still uncertain, and the major proposed candidates have been C, Si, O, H, or S. Therefore, it is important to understand the phase relationships of iron alloys at high pressures and high temperatures. In this study, we conducted high-pressure experiments and ab inito calculations to investigate the phase transitions and the physical properties of iron sulfide. In the case of high-pressure experiments, the laser-heated diamond anvil cell combined with the synchrotron X-ray diffraction technique was used [1]. We also used the first-principle calculations to investigate the magnetic property of high-pressure phase, which was discovered in the high-pressure experiments [2]. According to previous studies at ambient temperatures, FeS exhibits the following sequence of high-pressure phase transitions: troilite (FeS-I), low-P MnP phase (FeS-II), monoclinic phase (FeS-III). In our high-pressure experiments, we confirmed that the monoclinic phase was stable up to 40 GPa. Above 40 GPa, the sample was heated to 1000-2000 K to induce the phase transition. After heating, a new high-pressure phase (high-P MnP phase) was observed. This high-P MnP phase (FeS-VI) remained stable at pressures higher than 120 GPa. We found a significant discrepancy between low-P MnP and high-P MnP phases. The discontinuities for the unit cell volume and the cell parameters between two phases were observed. As the structure of low-P MnP phase is identical to that of high-P MnP phase, these discontinuities indicated that an unknown type of phase transition must occur. Next, we investigated the magnetic properties and the spin configurations of these phases using the ab inito calculations. Previous study [3] confirmed that the low-P MnP phase was antiferromagnetic state. The same results were confirmed in our calculations. We also calculated the non-magnetic state for the MnP structure. The calculated results showed that the non-magnetic MnP structure was more stable than anti-ferromagnetic MnP structure at high pressures. The volume and cell parameters of non-magnetic MnP structure were in good agreement with those of high-P MnP phase observed in our experiments. Therefore, the magnetic transition of the MnP structure occurred at high pressures. The high-pressure stability limit of the high-P MnP phase was also investigated. We found that the phase transition from the high-P MnP phase to the CsCl-type phase occurs at about 300 GPa. Thus, the high-P MnP phase is stable at pressures corresponding to the lower mantle and the outer core. In contrast, the CsCl-type phase is stable in the inner core. Our new findings can contribute to the understanding for the nature of the Earth's core.

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MS23 O5

Sound velocities of $MgSiO_3$ perovskite and post-perovskite: A constraint on the D" discontinuity

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Recent discovery of post-perovskite phase transition has important implications for interpretation of the D" layer at the base of Earth's mantle. Knowledge of the pressure dependence of acoustic wave velocities of post- perovskite phase provides essential and direct constraints for the seismic wave velocity profile at the D" region. In this study, we report the aggregate shear wave velocities in $MgSiO_3$ post-perovskite phase by Brillouin spectroscopy in a diamond anvil cell (DAC) up to 173 GPa, in combination with infrared laser annealing of the samples. High-pressure Brillouin scattering measurements of sound velocities were carried out at room temperature in a symmetric diamond anvil cell with a 60-degree angular aperture. An argon-ion laser at a wavelength of 514.5 nm and 25-150 mW of power was used as a probe beam. The incident laser was focused to a beam size of ~30 μm in diameter on the sample. The scattered light was analyzed by a six-pass tandem Fabry-Perot interferometer. All measurements were performed in a platelet scattering geometry. Polycrystalline samples were synthesized in situ