MS15-P06 | STRUCTURE, CRYSTAL CHEMISTRY, AND COMPRESSIBILITY OF IRON-RICH SILICATE PEROVSKITE AT PRESSURES UP TO 95 GPA

Koemets, Iuliia (Bayerischen Geoinstitut, Universität Bayreuth, Bayreuth, GER); Zhaodong, Liu (Jilin University, Changchun, CHN); Wang, Biao (Bayerischen Geoinstitut, Universität Bayreuth, Bayreuth, GER); Koemets, Egor (Bayerischen Geoinstitut, Universität Bayreuth, Bayreuth, GER); McCammon, Catherine (Bayerischen Geoinstitut, Universität Bayreuth, Bayreuth, Bayreuth, GER); Katsura, Tomoo (Bayerischen Geoinstitut, Universität Bayreuth, Bayreuth, GER); Dubrovinsky, Leonid (Bayerischen Geoinstitut, Universität Bayreuth, Bayreuth, Bayreuth, GER); Hanfland, Michael (European Synchrotron Radiation Facility, Grenoble, FRA); Chumakov, Aleksandr (European Synchrotron Radiation Facility, Grenoble, FRA)

Bridgmanite (Mg, Fe, Al silicate perovskite) is the most abundant mineral in the Earth's lower mantle. We investigated two crystalline iron-rich materials with compositions of FeMg_{0.5}Si_{0.5}O₃ and Fe_{0.5}Mg_{0.5}Al_{0.5}Si_{0.5}O₃, synthesized at 27 GPa and 2000 K using a Kawai-type multi-anvil apparatus and recovered to ambient conditions. We found that as-recovered FeMg_{0.5}Si_{0.5}O₃ has a previously unknown structure that is derived from a corundum (or ilmenite) prototype. On compression above 15 GPa, this phase transformed into a new monoclinic silicate double-perovskite. A characteristic feature of this double-perovskite structure is the presence of two distinct octahedral B-sites; one occupied by Si only, and the other by iron and magnesium. Analysis of compressibility changes of both polyhedra as obtained by single-crystal X-ray diffraction and variation of Mössbauer hyperfine parameter at pressures up to 95 GPa suggest a spin transition of ferric iron at a pressure of ~40 GPa. Thus, our study resolves the long-standing controversy regarding iron behaviour in bridgmanite and its possible impact on the compressibility of the mineral: we found that ferric iron indeed can occupy octahedral site, can undergo spin crossover, and affect compressional behaviour of the material. However, ferric iron does not mix with silicon in octahedra of silicate perovskite. By combining our data on pressure-volume relations of Fe_{0.5}Mg_{0.5}Al_{0.5}Si_{0.5}O₃ and published results for Al-rich bridgmanites we estimate the bulk modulus of FeAlO₃ end-member