**PS18.03.24 COMPARATIVE CRYSTAL CHEMISTRY OF SILICATES BEYOND 20 GPA.** Li. Zhang, H. Ahsbahs, A. Kutoglu, S. S. Hafner, Center of Materials Sciences, University of Marburg, Germany

The crystal chemistry of Mg$^{2+}$, Co$^{2+}$, Fe$^{2+}$, Mn$^{2+}$, Ca$^{2+}$, Fe$^{3+}$ and Al$^{3+}$ at high pressure in relatively incompressible silicates is not well studied. Present knowledge is largely based on limited experimental results at relatively low pressure. As a result, a systematic description of the high pressure crystal chemistry for the above cations is not available. Mg$^{2+}$, Fe$^{2+}$, Ca$^{2+}$, and Al$^{3+}$ cations are major constituents in minerals of the Earth's deep mantle. For understanding especially the chemical processes and the physical properties in that region it is essential to obtain information about the high pressure behavior of the above cations in the mantle minerals.

The high pressure crystal chemistry of those cations was studied by considering their electronic structures, polyhedral coordination as well as the crystal structure. Experiments were performed on synthetic endmember garnets, $Mg_3Al_2(SiO_4)_3$ $Fe_3Al_2(SiO_4)_3$ $Mn_3Al_2(SiO_4)_3$ $Ca_3Fe_2(SiO_4)_3$ $Ca_3Al_2(SiO_4)_3$, olivines, $Mg_2SiO_4$, $Fe_2SiO_4$, $Mn_2SiO_4$, $Co_2SiO_4$ and pyroxenes, $CaMgSi_2O_6$, $CaFeSi_2O_6$. The crystals were loaded in diamond anvil cell with rare gas solids, argon, neon and helium as well as mixtures of ethanol-methanol serving as pressure transmitting media. The unit-cell parameters determined up to 212 GPa show that polyhedral coordination of individual cation controls primarily their crystal chemical behavior. The 6-fold coordinated polyhedra with cations of similar electronic structures like Co$^{2+}$, Fe$^{2+}$, Mn$^{2+}$ do possess compression behavior which obeys prediction of bulk modulus - volume systematics, whereas those with cations of different electronic structure like e.g. Fe$^{2+}$, Mg$^{2+}$ do not follow such predictions. This is evidenced in olivine and pyroxene. The high pressure crystal chemistry of these cations in garnet, olivine and pyroxene as well as its implication to the bulk modulus - volume systematics will be discussed.

**PS18.03.25 PRESSURE-INDUCED PHASE TRANSITION OF $AgGaS_2$.** H. Kitahara, N. Ishizawa, F. Marumo* and Y. Noda** Research Laboratory of Engineering Materials, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226, Japan, *Department of Earth Sciences, Nihon University, 3-25-40 Sakurajosui, Setagaya-ku, Tokyo 156, Japan **Department of Materials Science, Faculty of Engineering, Tohoku University, Aramaki, Aoba-ku, Sendai 980-77, Japan

Single-crystal X-ray diffraction study under high-pressures has been carried out on $AgGaS_2$ to obtain crystallographic information of the high pressure phase in the range 4.2-11.6 GPa employing a diamond-anvil cell. Single-crystals of $AgGaS_2$ with chalcopyrite structure were grown with the Bridgman method. The crystal is tetragonal, I42d, a=5.7626(5) and c=10.3128(9) Å at ambient pressure. Above the transition point 4.2 GPa, the systematic condition of 2h+1=4n for hhl reflections was broken, showing that the diamond glide planes parallel to {110} have been disappeared in the high-pressure phase. In addition, most diffraction spots except 001 split into two or more in the high-pressure phase. They turned into single ones again when the pressure was released. These results indicate that (1) above 4.2 GPa the diamond glide planes are lost, and (2) a twin or a quadruplet seems to be formed in a way which keeps the c direction constant, and (3) the transition is essentially reversible, though the glide twins were left in the pressure-released crystals. The phase transition looks like a displacive type and the high-pressure phase apparently possesses a symmetry of C2, one of the non-isomorphic subgroups for I42d. The compressibility along the c axis is larger than; that along the a axis under pressures up to transition point. Since the intensities of 001 reflections were scarcely affected by the transition, the structural change may involve the atomic displacements on (001).

**PS18.03.26 KINETIC STUDIES ON THE CRYSTALLISATION OF COESITE USING THE HP/HT-DEVICE MAX80 AND SR.** Zinn, P.[1], Hinze, E.[2] & Lauterjung, J.[1]; [1]GeoForschungsZentrum Potsdam, D-14473 Potsdam; [2]University of Giessen, D-35390 Giessen

The kinetic behaviour of the quartz - coesite transition has been studied in the P/T range of 3.2-5.2 GPa and 680-900°C by in-situ X-ray diffraction using synchrotron radiation and a MAX80 cubic anvil high-pressure apparatus at HASYLAB. The quartz - coesite equilibrium phase boundary has been determined and discussed using the experimental results. During the transition, X-ray patterns were collected, and the transformed volume fraction has been estimated from the diffracted intensities of the respective phases as a function of time. By fitting a fundamental rate equation for grain boundary nucleation and interface-controlled growth to the transformation-time data, rates of nucleation and growth have been estimated [1].

During the in situ observed phase transition over a small P-T stability region an intermediate non quenchable stage could be detected [2]. By constructing a Bragg-Bragg Mo-double-crystal-monochromator the resolution of the MAX80-device could be raised up to $\Delta d/d = 0.001\%$. With this configuration the intermediate phase shall be investigated in detail.

Furthermore, by quenching the samples, the reaction products could be investigated by TEM images. A strongly twinning with (100) reflection twins could be observed [3]. Its influence on the thermodynamic behaviour of the a-quartz - coesite phase transition is discussed. Coesite-nuclei in quartz crystals, and in a latter stage penetrating the quartz-crystals could be observed. The growth mechanism and the existing structural relationship between host-quartz and the coesite-nucleus were then analysed.

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## High Pressure IV
## Pressure Cells and Sample Conditions

**MS18.04.01 LARGE VOLUME CELL AT HIGH P/T- NEW LIMITS AND FUTURE PROSPECTS.** W.Utsumi, Department of Synchrotron Radiation Facility Project Japan Atomic Energy Research Institute Tokai-mura, Naka-gun, Ibaraki 319-11, Japan

In contrast to the diamond anvil cell, multi-anvil apparatus are capable of maintaining stable high temperatures under high pressure owing to the larger sample volume. More than 14 years have passed since the first multi-anvil apparatus for synchrotron radiation was installed at the Photon Factory, and similar apparatus have been installed at the HASYLAB and NSLS. These multi-anvil systems combined with synchrotron radiation have brought us a large number of excellent results. The recent biggest advance in the multi-anvil apparatus is the use of sintered diamond as an anvil material. The characteristics of sintered diamond such as high compressive strength and no cleavage plane has enabled us to extend the attainable pressure range greatly. Many attempts have been made to replace tungsten carbide anvils with sintered diamond for the various type of multi-anvil apparatus, and most of them have had successful results.

Among the several multi-anvil type apparatus, the DIA type apparatus, a variation of cubic anvil press, has been most commonly used for the synchrotron radiation experiment in Japan. This system has many advantages; 1) fairly large sample volume which has a simple symmetry, 2) stable high pressure and high tempera-