

Structures and crystal chemistry of mantle minerals from single crystal diffraction at high pressure

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The common minerals in the Earth's crust and upper mantle undergoes phase transitions at high pressures and temperatures. Single crystal diffraction is a powerful technique to have structural information of these phases, with possibility of collecting data in-situ, at high pressures. The current features of synchrotron beamlines (i.e. X-ray beam and detector features) allow fairly good data even after first order transitions and chemical reactions, where an original single crystal domain is transformed into a multi-crystals/domains. Structure refinements, including atomic site occupancy refinement, provide also an in-situ chemical analysis, and this is extremely important after non isochemical transitions. Few examples are provided, on silicates, oxides and carbonates, at lower mantle pressures. Alkali-pyroxenes transform at high pressures and temperatures in alkali-perovskite, indicating that significant amount of these elements may incorporate in perovskite (bridgmanite) mineral. Iron oxide at lowermost mantle conditions transforms into complex structures with stoichiometry unknown at ambient conditions. This is the case of $\text{Fe}_{13}\text{O}_{19}$ oxide, stabilized above Mbar pressure, with a stoichiometry intermediate between magnetite and hematite. Carbonates provide interesting example of coordination change from [3] to [4] at pressures above 80 GPa, and continuous or discrete coordination change is observed as function of pressure. Red-ox reaction in Fe-bearing systems, furthermore, promote different stoichiometries compared to the low pressure ABO_3 carbonate, with extremely rich structural and topological features, such as truncated chain C_4O_{13} groups observed in $\text{Mg}_2\text{Fe}_2(\text{C}_4\text{O}_{13})$ carbonate.