

determined the structural evolution and phase transition behaviour of two natural pigeonites with composition $\text{Wo}_6\text{En}_{76}\text{Fs}_{18}$ and $\text{Wo}_{10}\text{En}_{43}\text{Fs}_{47}$ (ie Ca and Fe) by single-crystal diffraction. Both undergo a first order phase transition, and show that the transition pressure is controlled by the average M2 ionic radius.

Keywords: High-pressure phase transition, pyroxenes, Earth's upper mantle.

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Structural studies of $\gamma\text{-Fe}_2\text{SiO}_4$ ringwoodite and its high-pressure polymorph. E. Greenberg^{a,b}, J.

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One of the most abundant minerals in Earth's mantle is $(\text{Mg,Fe})_2\text{SiO}_4$ olivine. The properties of olivine and its transformation to spinel have been extensively studied due to the effect this transition has on seismic wave velocities. The purpose of this study is to obtain an equation of state for the Fe end-member of ringwoodite (Fe_2SiO_4 spinel) and to determine the high-pressure post-spinel structure. Synchrotron x-ray diffraction and Mössbauer spectroscopy were used to study the structural properties of ringwoodite up to 60 GPa. Starting at ~ 30 GPa, x-ray diffraction shows splitting of several peaks, marking a phase transition to a rhombohedrally distorted spinel structure. According to Mössbauer spectroscopy measurements, this new high-pressure phase has two different Fe sites; each characterized by different quadrupole splitting and isomer shift values. These two sites have an intensity ratio of 3:1, in agreement with the structure determined from x-ray diffraction studies.

Keywords: high-pressure phase transitions, Mossbauer spectroscopy, powder x-ray diffraction

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Solid solution behaviour of lower mantle minerals.

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Under the assumption that the Earth's lower mantle is pyrolytic and isochemical to the upper mantle, $(\text{Mg,Fe})\text{SiO}_3$ perovskite ($\sim 70\%$) is thought to be the most abundant phase in the lower mantle, followed by magnesiowüstite $(\text{Mg,Fe})\text{O}$ with $\sim 20\%$ and CaSiO_3 with between 6 and 12 vol%. One of the open questions concerning Ca in the lower mantle is whether with increasing temperature and depth, the entire amount of Ca could be incorporated into MgSiO_3 perovskite such that the CaSiO_3 perovskite phase would vanish.

Using density-functional simulations within the generalized gradient approximation and projector-augmented wave method (as implemented in the VASP [1] software package) together with thermodynamic modelling, the reciprocal solubilities of MgSiO_3 and CaSiO_3 perovskites were calculated for pressures and temperatures of the Earth's lower mantle from 25 to 100 GPa and 0 to 6000 K, respectively. The solubility of Ca in MgSiO_3 results to be less than 0.02 atoms per formula unit, the solubility of Mg in CaSiO_3 is even lower, and, most important, the extent of solid solution decreases with pressure. To dissolve CaSiO_3 perovskite completely in MgSiO_3 perovskite, a solubility of 7.8 or 2.3 mol% would be necessary for a fertile pyrolytic or a depleted harzburgitic mantle. Thus, for any reasonable geotherm, two separate perovskites will be present in fertile mantle, suggesting that Ca-perovskite will be residual to low degree melting throughout the entire mantle. However, at the solidus, CaSiO_3 perovskite might completely dissolve in MgSiO_3 perovskite in a depleted mantle with <1.3 wt% CaO. These implications may be modified if Ca solubility in MgSiO_3 is increased by other major mantle constituents such as Fe and Al.

[1] Kresse G., Furthmüller J., *Physical Review B*, 1996, 54, 11169.

Keywords: solid solution, high-pressure phases, ab-initio calculations