EGU24-8194, updated on 14 Aug 2024
https://doi.org/10.5194/egusphere-egu24-8194
EGU General Assembly 2024

High pressure phase of Magnesiowustite: Implications to the mineralogy of super-Earths

Anjitha Karangara and Pratik Kumar Das
Indian Institute of Engineering Science and Technology, Shibpur, Department of Earth Sciences, Howrah, India
(anjivaishna3@gmail.com)

Recent years have seen the discovery of a huge number of exoplanets, including several planets with very high densities suggesting that they also have rocky interiors which may be 9 – 10 times more massive than Earth. Mineralogy of these so called 'super-Earth' planets have been an interesting topic, as it gives implications on the planetary processes (Plate tectonics, geodynamo, etc.) and their habitability. Many studies concluded that such planets may contain ultra-high-pressure analogues of Earth's lower mantle minerals. (Mg,Fe)O, a binary solid solution of MgO-FeO system is the second most abundant mineral of Earth's lower mantle. If these super-Earth's interior can have high pressure analogue of perovskite which is another most abundant phase of lower mantle of Earth as shown by some recent studies then there is a possibility of finding high pressure phase of (Mg,Fe)O also in the lower mantle of those super-Earths. MgO is stable in a NaCl structure (B1) in lower mantle condition of earth. It transforms to $CsCl_2$ (B2) at high pressure (*p*) and Temperature (*T*) conditions. However, FeO is stable in B1 structure which transforms to a rhombohedral phase first and then to NiAs-type structure (B8) with increasing *p*. Finally, above 240 GPa and 4000 K, FeO transforms directly from B1 to B2. Along with structural phase transitions, FeO also undergoes a spin transition from high spin (HS) to low spin (LS) state with increasing pressure. In this study, we performed first principles DFT calculations on the structural phase transitions of $Mg_xFe_{1-x}O$ (x % = 0, 25, 50, 75 & 100) from B1 to B2 coupled with spin transition. Their mechanical and thermal properties under pressures ranging from 0 – 500 GPa relevant to super-earth planets have also been estimated. Our investigations have confirmed the presence of B1 phase of (Mg,Fe)O in lower mantle of earth with a spin transition from HS -LS which is thought to be responsible for the seismic anomalies of lower mantle of Earth. Spin transition of magnesiowustite and its effect on mechanical and thermal properties have been the topic for several experimental studies for many years. Most of them tried to explain the shear anisotropy of lower mantle with the help of (Mg,Fe)O with various Fe concentrations. Present study attempts to explore the stable phases of $Mg_xFe_{1-x}O$ relevant to super-Earth conditions. Both mechanical and dynamical behaviour have been investigated in the entire pressure range. Results show a new tetragonal phase of $Mg_{0.25}Fe_{0.75}O$ above 125 GPa, which is found to be both mechanically and dynamically stable. These findings will also attempt to predict the mineralogy and seismicity of those giant planets.