Crystal structure and elasticity of dense hydrous mineral under high pressure

Liu Lei, Liu Hong, Yi Li, Li Ying, Liu Guiping, Lv Chaojia, Yang Longxing, Gu Xiaoyu
Key Laboratory of Earthquake Forecasting, Institute of Earthquake forecasting, CEA, Beijing, China.

1.Introduction

The water in interior of the Earth has various functions, such as dramatically lowering the melting temperature of mantle rocks, causing arc magmatism, decreasing the magma viscosity and density, enhancing magma migration, influencing the elastic and rheological properties of the mantle, and broadening seismic discontinuities.

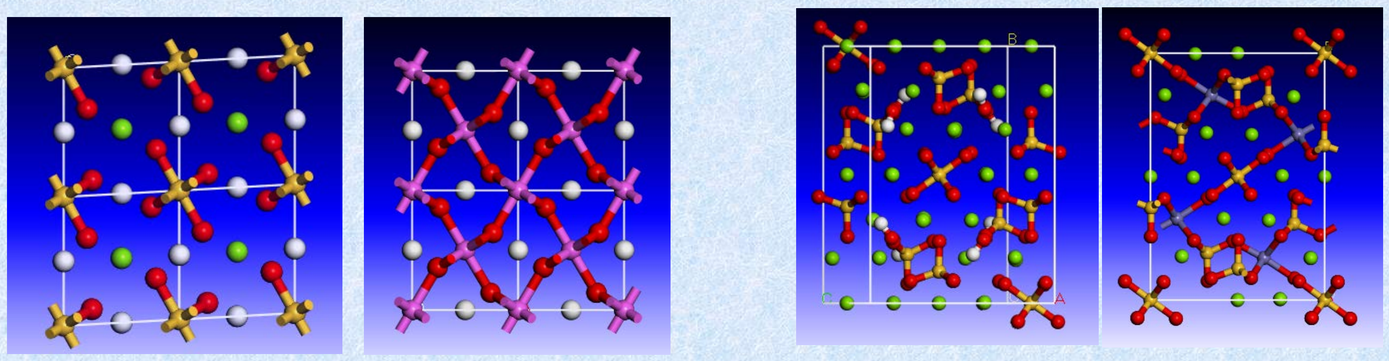
Water can be carried down into the Earth's interior by subducting slabs through hydrous minerals.

Since the first discovery of 10Å phase7, dense hydrous magnesium silicates including 3.65 Å phase, phase A, phase B, Superhydrous phase B, phase D, phase E and so on have received considerable attention because of their presumed role in the water budget of the Earth.

As two of the important hydrous mineral, the properties of the Phase B and Phase D have significant effects on water storage, composition and structure of the deep Earth. So the crystal structure, elasticity of Phase B and Phase H with different Fe, Al and water contents were calculated.

2. Simulation Method

First-principles calculations were performed using density functional theory (DFT) and the planewave pseudopotential technique in the CASTEP codes.

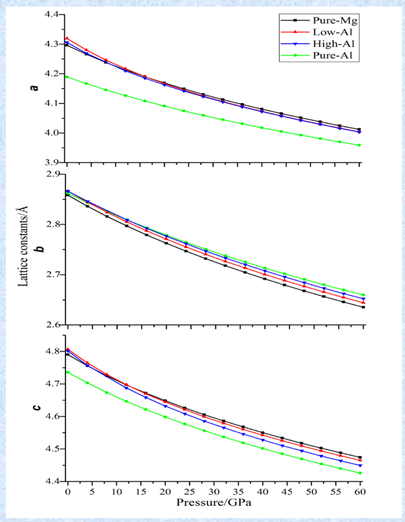


1 2 3 4

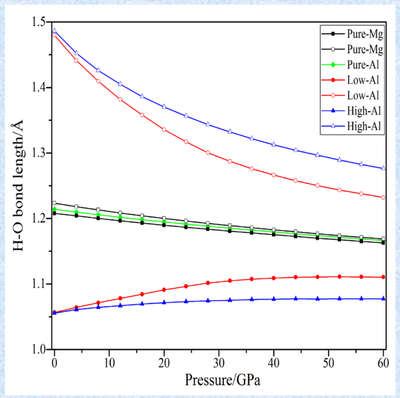
crystal structures of the Phase B and Phase H with different Fe, Al and H contents
1-Phase B, 2-Al-bearing phase, 3-Phase H, 4-Fe-bearing Phase H

3. Result

3.1 The Phase H

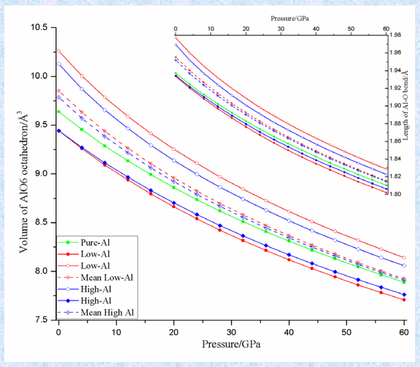


Lattice constants of the Phase H.
Fe, Al and H effect the lattice constants of the Phase H.



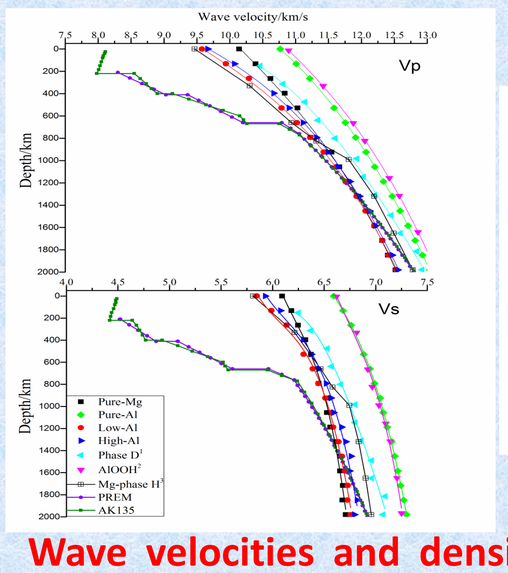
The symmetry of Low-Al and High-Al phase H's structure increases with increasing pressure.

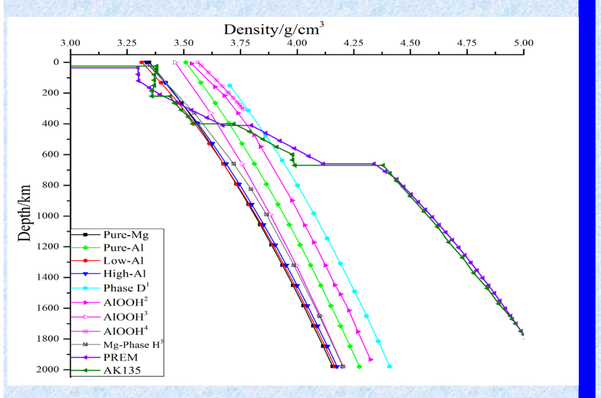
H-O bond length of the Phase H.



Volume of AlO6 octahedron decreases with increasing Al content. The variation of Al-O bonds' length coincides with AlO6 octahedra.

Transformation from phase D to phase H and formation of solid solution of phase H and δ-phase AlOOH would affect the composition and structure of the mantle.

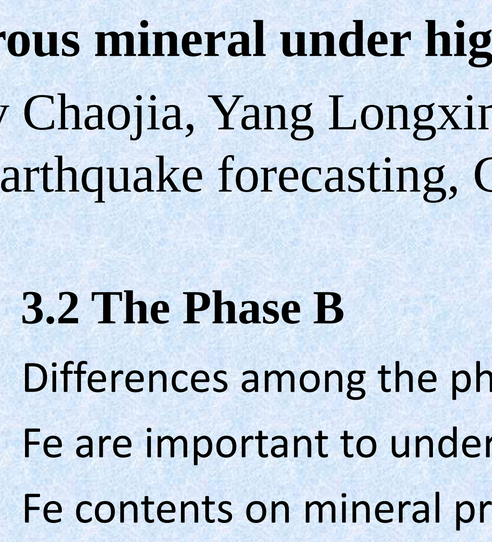




Wave velocities and density of the phase H, phase D and δ-phase AlOOH along with the typical velocity structure of the Earth.

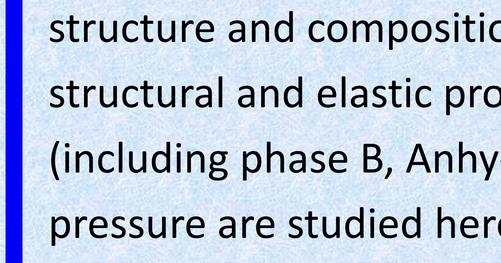
3.2 The Phase B

Differences among the phase B with different water and Fe are important to understand the effects of water and Fe contents on mineral properties along with the structure and composition of the mantle. the crystal structural and elastic properties of the phase B (including phase B, Anhy-PhB and Fe-PhB) under high pressure are studied here.



Lattice constants of Phase B as functions of pressure.

Different results indicate by number as follows: 1-this study; 2-Ottonello et al.; 3-Crichton et al.; 4-Hazen et al.; 5-Finger et al. ; 6-Crichton et al.

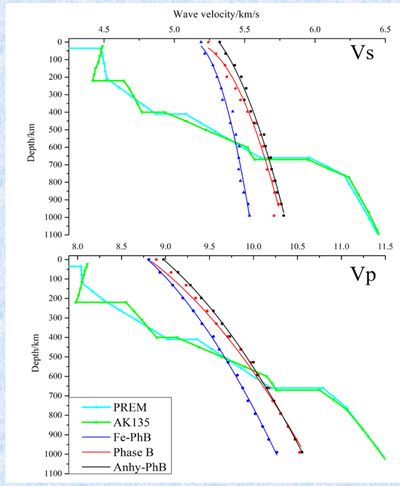


Densities of phase B along the typical Earth's density structure.

1-This study; ***2***-Ottonello et al. 2010; ***3***-Crichton et al. 1999.

Density of Fe-PhB is 9.2% higher than that of Anhy-PhB, whereas those of phase B are 1.4 %.

Results indicated formation of Anhy-PhB by the reaction between forsterite and periclase may be responsible for the X-discontinuity at 260–330km depth of the mantle.



wave velocities of the phase B plotted along with the typical Earth velocity structure

The compressional wave velocity (Vp) and shear wave velocity (Vs) of phase B decreased with increasing water and Fe contents.

Wave velocities results provide an evidence for the stability zone and the formation of X-discontinuity zone of the mantle. The results are consistent with density results.

4.Conclusion

The Fe, Al and water have important effects on crystal structure and wave velocity of minerals and then effect the composition and structure of deep Earth.

Published:

1. Lv Chaojia, Liu Lei*. et al. Structural, elastic, and vibrational properties of phase H: A first-principles simulation.Chin. Phys. B, 26: 067401, 2017.
2. Liu Lei, et al. The structure and elasticity of phase B silicates under high pressure by first principles simulation. Chin. Phys. B, 27: 047402, 2018.
3. Liu Guiping, Liu Lei*. Crystal structure and elasticity of Al-bearing phase H under high pressure. AIP Advances, 8:055219, 2018.