

CONSTRAINTS ON THE INNER CORE COMPOSITION FROM MINERAL PHYSICS

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I determine the necessary amount of several light elements - C, S, P, O, Si, H - as major alloying components of hexagonal close-packed (hcp) iron to match the observed seismic properties of the Earth's inner core. For this I employ first-principles calculations based on density-functional theory in the ABINIT implementation.

First I compute the elastic constants tensors and determine the seismic properties of Fe₃X compounds, with X = C, S, P, O and Si, using first-principles calculations. Assuming independent substitutions, linear relations and similar temperature corrections of velocities, I find that fitting all density, V_p and V_s, obtain Si as the most reasonable light element, in amount of 6-7 wt. %. C and O come next with respectively 3-5 wt. % and 4-9 wt.%. P and S yield unreasonable values. The slope of the compressional wave velocities with respect to pressure also gives Si as the best light element candidate. Second I determine the seismic properties of H-bearing hcp iron and show that hydrogen is a bad alloying element as it increases both compressional and shear wave velocities. In a third step I consider Fe-(Ni,Co,Mn) ideal solid solutions and repeat the above procedure.

Then I use all of the above data to separate reasonable and unreasonable solutions for the recorded seismic data of the inner core in a broad chemical space containing H, C, Si, O, P, S as the light elements and Ni, Co, Mn as the metals alloying hcp iron.

Finally, I model the thermodynamics of the Fe-Si system and show that there is an immiscibility gap, widening with pressure, between Si-bearing hcp-iron and Fe-bearing FeSi. My calculations show that at core conditions one cannot dissolve more than about 5-6 wt. % Si in the hcp iron.