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Constraints on the inner core composition from mineral physics

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We calculate the seismic properties of hexagonal close-packed (hcp) iron alloyed with several light elements - C, S, P, O, Si, H – and metals – Ni, Co, Mn - from first-principles calculations. By trying to match our theoretical results with the observed seismic properties of the Earth's inner core, we can separate reasonable and unreasonable solutions for the recorded seismic data of the inner core in a broad chemical space.

First we work on Fe3X compounds, with X = C, S, P, O and Si. Assuming independent substitutions, linear relations and similar temperature corrections of velocities, we find that fitting all density, Vp and Vs, 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 we 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 we consider Fe-(Ni,Co,Mn) ideal solid solutions and repeat the above procedure.

Finally, we 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.