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Iron Silicides at the Earth's inner core conditions

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The Earth's core plays a fundamental role in the evolution of our planet. It has liquid outer and solid inner regions, and it is accepted that the inner core is formed as a result of cooling and crystallization of the outer core. It is expected to contain around 10 wt % light elements (S, Si, O, possibly C, H, etc.) alloyed with Fe and Ni. Very little is known about these alloys at pressures and temperatures of the core. Silicon has been proposed to be a major alloying light element in the Earth's core based on its cosmochemical abundance, the solubility in liquid Fe at high pressures and temperatures and the thermoelastic properties in Fe-Si alloys. Studying the phase relations and the stabilities of the Fe silicides at the Earth's inner core conditions is thus essential for our understanding of Earth's core. Using the evolutionary crystal structure prediction methodology, we could investigate Fe-Si compounds at pressures of up to 400 GPa, i.e. covering the pressure range of the Earth's core. Evolutionary simulations correctly find that at atmospheric pressure the known non-trivial structure with $P2_13$ symmetry is stable, while at pressures above 20 GPa FeSi undergoes a phase transition to the CsCl-type structure, which is stable up to the Earth inner core pressures. In our Calculations, we searched for the ground states of the following systems at 300 GPa and 400 GPa - Fe_3Si (with 8, 12 and 16 atoms in the unit cell), Fe_2Si (with 9, 12 and 18 atoms/cell), Fe_5Si_3 (8, 16 and 24 atoms/cell), FeSi (8 atoms/cell), $FeSi_2$ (9, 12 and 18 atoms/cell), $FeSi_3$ (8, 12 and 16 atoms/cell). We show that among the above possible Fe silicides only FeSi with CsCl-type structure is thermodynamically stable at core pressures, while the other silicides are unstable to decomposition into Fe + FeSi or FeSi + Si. This is consistent with previous works and suggests that Si impurities contribute to stabilization of the body-centered cubic phase of Fe in the inner core. However, it is somewhat unexpected that the CsCl-type phase of FeSi has such an enormous stability field. This means that it can be an individual mineral phase both in the inner core and at the core-mantle boundary region, where it may be formed by a reaction of the type: $3Fe_{metal}$ + (Mg, Fe)SiO_3 = 2FeO + (Mg, Fe)O + FeSi. We are trying to understand the behavior of silicon in the Earth's inner core and to find the mechanism for Si partitioning between liquid and solid Fe in the core. The findings might make the contributions on the interpretation of the observed seismic anisotropy of the inner core