Iron silicides at pressures of the Earth's inner core

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[1] The Earth's core 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. Here, using the evolutionary crystal structure prediction methodology, we 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 the CsCl-type structure is stable. We show that among the possible Fe silicides (Fe_3Si, Fe_2Si, Fe_5Si_3, $FeSi$, $FeSi_2$ and $FeSi_3$) 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. **Citation:** Zhang, F., and A. R. Oganov (2010), Iron silicides at pressures of the Earth's inner core, *Geophys. Res. Lett.*, *37*, L02305, doi:10.1029/2009GL041224.

1. Introduction

[2] The Earth's core plays a fundamental role in the evolution of our planet. It has a 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. There is an increasing amount of evidence suggesting that the inner core is rather complex and possesses significant seismic anisotropic [*Song*, 1997], is stratified into two or three regions [*Durek and Romanowicz*, 1999; *Ishii and Dziewonski*, 2002], and has low rigidity [*Cao et al.*, 2005] and is possibly laterally heterogeneous. These features are not fully explained, largely because of the lack of reliable information on core-forming materials. There is still much uncertainty [*Brown*, 2001; *Nguyen and Holmes*, 2004] on the phases of iron at high pressures and temperatures. Both the experiments at ambient temperature [*Antonangeli et al.*, 2004] and static theoretical calculations (0 K) [*Stixrude and Cohen*, 1995; *Stixrude et al.*, 1997; *Vočadlo et al.*, 2000], suggested that the hcp phase of iron is the most likely stable phase at pressures of the inner core. However, the stability of hcp-Fe at core conditions has been recently challenged, especially at high temperatures and in the presence of lighter elements, such as S, Ni, Si et al. [*Lin et al.*, 2002; *Beghein and Trampert*, 2003]. Bcc phase can be stabilized by entropic effects at high temperatures [*Belonoshko et al.*, 2003] and small amounts of light element impurities [*Vočadlo et al.*, 2003; *Côté et al.*, 2008b, 2008a]. It is possible that bcc phase might be formed at the Earth's core conditions and it is clear that we need to investigate the effect of alloying elements on the stability of the iron phases [*Dubrovinsky et al.*, 2007; *Belonoshko et al.*, 2008]. Laser-heated diamond anvil cell measurement [*Lin et al.*, 2002, 2009] indicated that Si alloyed with Fe (7.9 weight % Si) can stabilize the bcc phase up to at least 150 GPa (compared to ~10 GPa for pure Fe) and 3000 K. It was found in the diamond anvil cell experiment that the Fe-Si alloys dissociate into almost pure iron and a CsCl-structured (B2) phase of FeSi at pressures of 85–140 GPa and temperatures over 3800 K [*Dubrovinsky et al.*, 2003]. However, recent experimental study [*Lin et al.*, 2009] suggested only hcp $Fe_{0.85}Si_{0.15}$ is the only stable phase between 170 and 240 GPa at high temperatures up to 3000 K, whereas the theoretical study [*Côté et al.*, 2010] suggested the fcc Fe-Si alloy should coexist with hcp in the two-phase region in the inner core. In this paper, we use the evolutionary crystal structure prediction method USPEX [*Glass et al.*, 2006; *Oganov and Glass*, 2006; *Oganov et al.*, 2006] to study possible Fe silicides (Fe_3Si, Fe_2Si, Fe_5Si_3, $FeSi$, $FeSi_2$ and $FeSi_3$) at pressures of up to 400 GPa in order to understand the possible crystal structures and stoichiometry of stable Fe-Si compounds. USPEX has successfully predicted a number of new crystalline phases of various materials, in particular at extreme conditions [*Oganov et al.*, 2006, 2008; *Li et al.*, 2009; *Ma et al.*, 2009; *Oganov et al.*, 2009].

2. Computational Methodology

[3] Using USPEX, 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). As a test, we successfully found the experimentally known non-trivial structure with space group $P2_13$ that FeSi adopts at ambient conditions. Importantly, no symmetry or experimental information was imposed in the calculations; this enables any space group to have a chance to be found and guarantees that the resulting structures are mechanically stable and do not have dynamical instabilities at the center of the Brillouin zone. Our structure prediction calculations were performed at 0 K; there is a possibility that some structures dynamically unstable at 0 K may be dynamically stabilized at high temperatures (as happens with bcc-Fe at high pressures).

[4] The first generation of structures was created randomly; the number of structures in each generation was up

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Table 1. Enthalpies of Formation (ΔH_f) of Fe Silicides

Chemical Formula	Space Group	ΔH_f (eV/atom)	
		400 GPa	300 GPa
Fe_3Si	*Cmcm*	−0.68	−0.66
Fe_2Si	*I4/mmm*	−0.99	−0.94
Fe_5Si_3	*Im3m*	−1.18	−1.12
FeSi	*Pm3m*	−1.80	−1.69
$FeSi_2$	*C2/m*	−0.98	−0.97
$FeSi_3$	*C2/c*	−0.77	−0.76

to 50. Each generated structure was locally optimized with the conjugate-gradients method using the VASP code [*Kresse and Furthmüller*, 1996]. The best 60% (i.e., lowest-enthalpy) structures of each generation were used to produce the next-generation structures by heredity (60% structures), lattice mutation (20% structures) and permutation (20% structures). Typically, our global optimization runs required not more than 20 generations to find the lowest-enthalpy structure. Ab initio VASP calculations were performed based on GGA [*Perdew et al.*, 1996] and the frozen-core all-electron PAW method [*Blöchl*, 1994; *Kresse and Joubert*, 1999]. The PAW potentials used here have $1s^2 2s^2 2p^6$ core (radius 1.5 a.u.) for Si and $1s^2 2s^2 2p^6 3s^2$ core (radius 2.2 a.u.) for Fe. In these calculations we used the plane-wave cut-off of 400 eV, which gives excellent convergence for energy differences and stress tensors. Table 1 lists space groups and enthalpies of formation (see also Figures 1 and 2) of the lowest-enthalpy structures for each Fe-Si compound composition. The enthalpies of formation were computed with respect to the ground states of pure elements - FM bcc-structure for Fe at 1 atm [*Wilburn and Bassett*, 1978], hcp-structure for Fe at high pressures [*Takahashi and Bassett*, 1964; *Oganov and Glass*, 2006], and fcc-structure for Si [*Duclos et al.*, 1987].

3. Results

[5] Our calculations find the unusual cubic iron mono-silicide, B20-FeSi, structure at 1 atm with the space group: $P2_13$ (Nr. 198), in which all atoms have sevenfold coordination. This result is consistent with the experimental findings [*Wever and Möller*, 1930]. Figure 1 shows the enthalpy of formation of Fe silicides as a function of composition at 1 atm, which is in very good agreement with the available experimental data [*de Boer et al.*, 1988] and previous Fe-Si compounds stability calculation [*Moroni et al.*, 1999]. At the pressures of 300 GPa and 400 GPa, our results suggest that FeSi with the CsCl-type B2 structure is the only stable iron silicide (Figure 2). From the calculation of relative enthalpies, we find that the CsCl-type phase is stable above 20 GPa. According to previous experimental and theoretical studies, FeSi undergoes a phase transition to the CsCl-type phase at 12 GPa [*Santamaría-Pérez and Boehler*, 2008], 24 GPa [*Dobson et al.*, 2002, 2003; *Dubrovinsky et al.*, 2003], 13 GPa [*Vočadlo et al.*, 1999], 15 GPa [*Moroni et al.*, 1999] and 30 − 40 GPa [*Caracas and Wentzcovitch*, 2004], respectively. *Vočadlo et al.* [2003] found that impurities of Si stabilize the bcc phase of Fe - a structure closely related to B2-FeSi. Our simulations, employing a novel global optimization method [*Glass et al.*, 2006; *Oganov and Glass*, 2006; *Oganov et al.*, 2006]

not only confirm the stability of B2-structured FeSi at conditions of the Earth's core [*Belonoshko et al.*, 2009], but also for the first time demonstrate that the B2-structured FeSi is more stable than any other Fe-Si compound (Fe_3Si, Fe_2Si, Fe_5Si_3, $FeSi_2$ and $FeSi_3$).

[6] Even though FeSi is the only stable iron silicide at high pressures, there is considerable interest in other meta-stable compositions. Fe_5Si_3 is experimentally known and two peculiar structures were studied − one with the space group $P6_3/mcm$ (unit cell parameters: a = 6.752 Å and c = 4.741 Å) [*Santamaría-Pérez et al.*, 2004] and another with the space group *Ia3d* (unit cell parameter 7.025 Å) and displaying the structure of the cation array in the garnet $Fe_5Si_3O_{12}$ [*Muñoz et al.*, 2005]. However, the structure found in our USPEX simulations (space group *Im3m*, unit cell parameter 4.761 Å at 300 GPa) is different and more stable than these two structures at all pressures (Figure 3).

4. Conclusions

[7] Silicon is likely to be a major component in the iron-based alloys of the Earth's core. Our work, based on a *ab initio* global optimization technique [*Glass et al.*, 2006; *Oganov and Glass*, 2006; *Oganov et al.*, 2006] establishes that at pressures of the Earth's core only one iron silicide is stable – FeSi with the CsCl-type structure. This has been previously [*Dubrovinsky et al.*, 2003] shown by experiments at pressures in the range of 85 GPa to140 GPa. Our work extends this conclusion to much higher pressures, which are directly relevant to the Earth's core. In fact, 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 [*Dobson et al.*, 2003], where it
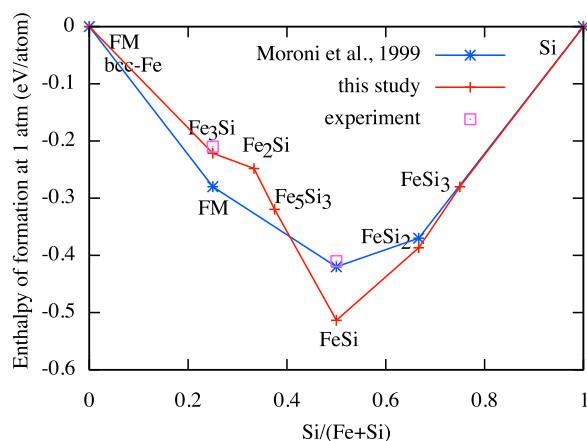

Figure 1. Enthalpy of formation of Fe silicides as a function of composition at 1 atm. Crosses (+) - this study; squares (□) - experimental data [*de Boer et al.*, 1988]; stars (*) - previous calculation [*Moroni et al.*, 1999]. We did not do magnetic calculations for Fe silicides in this study, whereas *Moroni et al.* [1999] took the hypothetical DO$_3$-type FM Fe_3Si and got a lower energy. Our results confirm stability of FeSi and $FeSi_2$ compounds at 1 atm. The lower enthalpy for FeSi in our calculation than that in the previous study is because of different potential used.
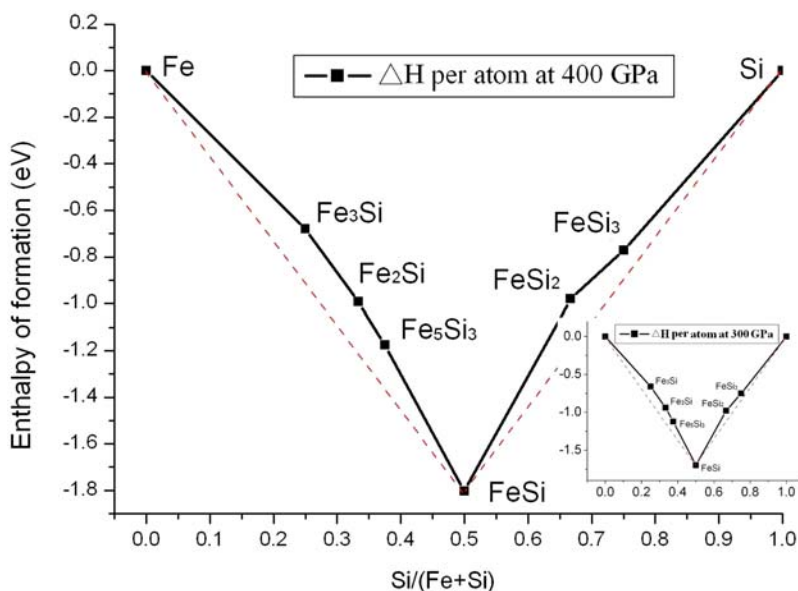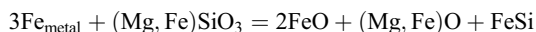
Figure 2. Compositional dependence of the enthalpy of formation of iron silicides at 400 GPa. The inset shows results at 300 GPa. Dashed lines show the enthalpies of mechanical mixtures (Fe + FeSi) and (FeSi + Si). The negative enthalpies of formation and the topology of this graph suggest that FeSi is the only stable compound. All other compounds are unstable with decomposition into (Fe + FeSi) or (FeSi + Si) mixtures at the Earth's core pressures.

may be formed by a reaction of the type [*Knittle and Jeanloz*, 1989]:

$$3\mathrm{Fe_{metal}} + (\mathrm{Mg,Fe})\mathrm{SiO_3} = 2\mathrm{FeO} + (\mathrm{Mg,Fe})\mathrm{O} + \mathrm{FeSi}$$

What are scenarios of the behavior of silicon in the Earth's inner core? The calculations [*Alfè et al.*, 2002] showed that

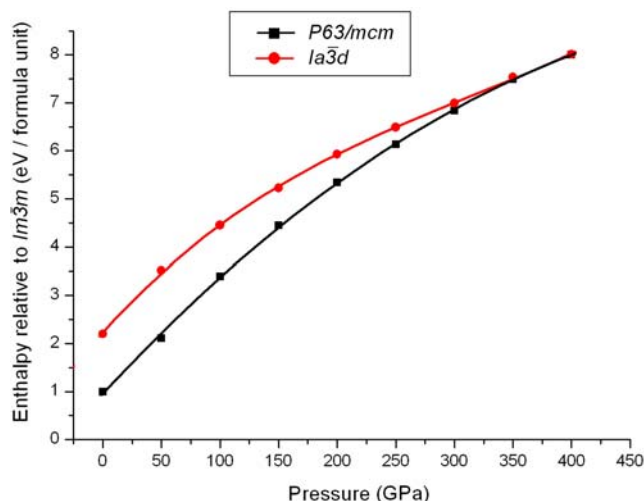**Figure 3.** Enthalpies of the *P6₃/mcm* and *Ia3d* phases of Fe₅Si₃ relative to the *Im3m* phase. Positive enthalpy differences means that both *P6₃/mcm* and *Ia3d* have a higher enthalpy and therefore less stable than *Im3m* Fe₅Si₃. Structural parameters of the Fe₅Si₃ phases: (a) *Ia3d*: Fe1 (0 0 0), Fe2 (1/8 0 1/4), Si (3/8 0 1/4); (b) *P6₃/mcm*: Fe1 (1/3 2/3 0), Fe2 (0.237 0 1/4), Si (0.605 0 1/4); (c) *Im3m*: Fe1 (0 0 0), Fe2 (3/4 3/4 3/4), Si (0 0 1/2).

the inner core may contain up to 8.5 mol.% Si. Our results imply that at low temperatures the stable assemblage would be Fe + FeSi, with a considerable (up to ~18 vol.%) abundance of FeSi. At higher temperatures, solubility of Si in iron will increase and the proportion of FeSi will decrease and may disappear completely at sufficiently high temperatures. It is an open question whether or not FeSi will exist as an individual mineral phase at high temperatures of the inner core. Recent laser-heated diamond anvil cell measurement [*Lin et al.*, 2002, 2009] indicated that at very high pressures (> 170 GPa) and temperatures below approximately 3000 K, the Fe-Si alloy with 15% Si will exist in the hcp (rather than bcc) structure; while lattice dynamics calculations [*Côté et al.*, 2010] gave the evidence of fcc Fe stability at the inner core conditions. Experimental results [*Dubrovinsky et al.*, 2007], confirming prediction [*Belonoshko et al.*, 2003], suggested that the (Fe,Ni) alloy adopts the bcc structure at pressures and temperatures of the inner core, although this has been challenged by other experiments [*Kuwayama et al.*, 2008]. The close similarity of the bcc and CsCl-type structures, and similar sizes of Fe and Si atoms at core pressures suggest easy miscibility between bcc-(Fe,Ni) alloy and FeSi. Furthermore, incorporation of Si impurities will further stabilize the bcc structure of the iron-based alloy [*Vočadlo et al.*, 2003]. This work should be further extended to high temperatures. The crystallography of Fe silicides in the Earth's inner core conditions may resolve some of the long-standing problems, such as the interpretation of the observed seismic anisotropy of the inner core.

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