Revision 2

Phase transition boundary between fcc and hcp structures in Fe-Si alloy and its implications for terrestrial planetary cores

Tetsuya Komabayashi[1*], Giacomo Pesce[1], Guillaume Morard[2], Daniele Antonangeli[2], Ryosuke Sinmyo[3†], Mohamed Mezouar[4]

[1]School of GeoSciences and Centre for Science at Extreme Conditions, University of Edinburgh EH9 3FE, UK

[2]Sorbonne Université, Muséum National d'Histoire Naturelle, UMR CNRS 7590, IRD, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, IMPMC, 75005 Paris, France

[3]Bayerisches Geoinstitut, Universitat Bayreuth, 95440 Bayreuth, Germany

[4]European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble Cedex, France

*corresponding author: Tetsuya Komabayashi
E-mail: tetsuya.komabayashi@ed.ac.uk

[†]Now at Department of Earth and Planetary Science, University of Tokyo, 7-3-1 Hongo, Bunkyo, Tokyo 113-0033, Japan

ABSTRACT

The phase transition between a face-centered cubic (fcc) and hexagonal close-packed (hcp) structures in Fe-4wt% Si alloy was examined in an internally resistive heated diamond anvil cell (DAC) under high-pressure (*P*) and -temperature (*T*) conditions to 71 GPa and 2000 K by *in-situ* synchrotron X-ray diffraction. Complementary laser-heated DAC experiments were performed in Fe-6.5wt% Si. The fcc-hcp phase transition boundaries in the Fe-Si alloys are located at higher temperatures than that in pure Fe, indicating that the addition of Si expands the hcp stability field. The dP/dT slope of the boundary of the entrant fcc phase in Fe-4wt% Si is similar to that of pure Fe, but the two-phases region is observed over a temperature range increasing with pressure, going from 50 K at 15 GPa to 150 K at 40 GPa. The triple point, where the fcc, hcp, and liquid phases coexist in Fe-4wt% Si, is placed at 90-105 GPa and 3300-3600 K with the melting curve same as in Fe is assumed. This supports the idea that the hcp phase is stable at Earth's inner core conditions. The stable structures of the inner cores of the other terrestrial planets are also discussed based on their P-T conditions relative to the triple point. In view of the reduced P-T conditions of the core of Mercury (well below the triple point), an Fe-Si alloy with a Si content up to 6.5 wt% would likely crystallize an inner core with an fcc structure. Both Venusian and Martian cores are believed to

currently be totally molten. Upon secular cooling, Venus is expected to crystallize an inner core with an hcp structure, as the pressures are similar to those of the Earth's core (far beyond the triple point). Martian inner core will take an hcp or fcc structure depending on the actual Si content and temperature.

Key words

Earth's core; high-pressure; diamond anvil cell; internal resistive heating; Fe-Si alloy

INTRODUCTION

Terrestrial core formation process has been discussed in relation to metal-silicate equilibration during accretion stage (Li and Agee 1996; Wade and Wood 2005; Siebert et al. 2013) although some recent models considered disequilibrium processes at a later stage (Rubie et al. 2011). The metal-silicate equilibration inevitably results in an impure iron rich metallic core (Wade and Wood; Siebert et al. 2013). The impurity includes nickel and several less dense elements which are also called light elements (Poirier 1994; Allègre et al. 1995).

Birch (1952) pointed out that the density of pure iron might be greater than the seismological determination for Earth's core. Such a density deficit has been associated with the presence of lighter element(s), and a recent internally consistent thermodynamic model of pure iron estimated the core density deficit to be 7% for the outer core and 4.5 % for the inner core (Komabayashi 2014). Other terrestrial planetary cores also likely contain light elements considering metal-silicate partitioning during their cores formation. In addition, the presence of a magnetic field found in some terrestrial planets may indicate the presence of a light element-bearing partially molten core (e.g., Sohl and Schubert 2007). Light elements would be expelled at the bottom of the liquid outer core as it is less partitioned in the solid inner core and this would drive convection in the outer core (Stevenson et al. 1983; Lister and Buffett 1995).

Among the potential light elements, silicon is considered a plausible candidate for the terrestrial planetary cores for various reasons: i) silicon is the second most abundant element in the mantle and series of high-pressure (P) and –temperature (T) experiments demonstrated that silicon and oxygen could be dissolved from mantle silicates to core melt (Takafuji et al. 2005; Ozawa et al. 2009), and then silicon is partitioned between solid and liquid during core crystallization; ii) silicon isotopic composition of stony meteorites is different from bulk silicate Earth (Georg et al. 2007; Fitoussi et al. 2009), implying that silicon might have been partitioned into the core during core-mantle differentiation (Shahar et al. 2011; Hin et al. 2014); iii) all the core formation models based on silicate-metal equilibration inevitably have silicon as a light element in the core (Wade and Wood 2005; Rubie et al. 2011; Siebert et al. 2013).

Phase relations and equations of state (EoS) of solid phases in the system Fe-(Fe)Si have been extensively studied by both experiment and theory (Alfe et al. 2002; Dobson et al. 2002; Lin et al. 2002; Kuwayama and Hirose 2004; Lin et al. 2009; Tateno et al. 2015; Ozawa et al. 2016). An important phase relation is the transition between face-centered cubic (fcc) and hexagonal close-packed (hcp) structures, as this is central to address the solid inner core structure (Uchida et al. 2001; Asanuma et al. 2008; Komabayashi et al. 2009), and the P-T location of the phase boundary can be used to deduce thermodynamic properties (Wood 1993; Komabayashi 2014). Notably, the triple point P-T location where the hcp, fcc, and liquid phases coexist can be constrained from the fcc-hcp boundary and melting curve (Zhang et al. 2016). An experimental study in a laser-heated diamond anvil cell (DAC) reported that the transition temperature was greatly reduced when 3.4 wt%Si was added to Fe (Asanuma et al. 2008). In contrast, phase relations inferred by Fischer et al. (2013) suggested that addition of silicon should increase the transition temperature. Tateno et al. (2015) experimentally demonstrated that the transition temperature was increased by the addition of 6.5 wt%Si to iron. As such the effect of Si on the transition temperature has been a controversy and the P-T conditions of the actual boundaries in the system Fe-Si are not unanimous.

In this study, we present the investigation of the P-T locations of the fcc-hcp transition boundaries in Fe-Si alloys in an internally resistive heated DAC. The internally heated DAC heats the sample by its resistance, with an improved accuracy in temperature with respect to conventional laser heated DAC (Komabayashi et al. 2009; 2012). Based on these experimental results, we will discuss the effect of Si on the Fe properties under high P-T condition and address the stable structure of a solid Fe-Si alloy at the conditions of the inner cores of the terrestrial planets of the solar system.

EXPERIMENTAL PROCEDURE

We conducted high-P-T in-situ X-ray diffraction (XRD) experiments on Fe-Si samples at the beamline ID27, European Synchrotron Radiation Facility (ESRF). X-rays with a wavelength of 0.3738Å were focused to a 3x3 μm^2 spot at sample position and the diffracted X-rays were collected on a two dimensional detector (mar345 Image Plate Detector). The collection time was 10 seconds for each measurement. Using the fit-2D program (Hammersley 1996), the obtained data were converted to the conventional one-dimensional XRD pattern.

High pressure was generated in a DAC with a pair of diamond anvils with a culet size of 300 μm or 150-450 μm beveled depending on the pressure range. The starting material was a 5-7 μm thick Fe-Si alloy with 4 wt% Si (Rare Metallic. Co., hereafter Fe-4Si), placed in the sample chamber and connected to platinum leads. The junction between the Fe sample and Pt leads was outside the sample chamber (see Komabayashi et al. (2009) for the sample geometry). SiO_2 glass layers served as a pressure transmitting medium and thermal insulator. High temperature was achieved with an internal resistive system (Komabayashi et al. 2009; 2012; Antonangeli et al. 2012). The sample was resistively heated by directly applying a DC voltage by an external power supply. The temperature was measured by a spectral radiometric system as conventional in laser heating experiments. Noteworthy, thanks to the improved time and spatial stability of the hotspot and the reduced thermal gradients, resulting uncertainties in temperature were about 50 K (Komabayashi et al., 2012)

Complementary laser heating experiments were conducted on an Fe-6.5Si sample (Rare Metallic. Co.) at ID27, ESRF (see Morard et al. (2011) for details of the laser heating experimental set up). The internal heating system was not applied because this alloy is so brittle that it was not possible to make it into thin foil. Irrespectively of the use of low numerical aperture and reflecting objectives which effectively minimize

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the chromatic aberration and improve reliability of temperature determination (Mezouar et al. 2017), the laser heating experiments show larger temperature uncertainty due to large temperature gradient across the sample and laser fluctuations. The two microns diameter pinhole at the entrance of the spectrometer allows for a collection of signal only coming from the very central part of the hotspot and an optimal alignment of lasers and X-ray beam. Morard et al. (2011) discussed that the possible uncertainty in the temperature in this experimental setup might be 150 K at 3000 K. In the present study, we assumed a more conservative number, 10% of the generated temperature.

In all the runs, the pressure at any given temperature was calculated with a thermal EoS for Fe-4Si or Fe-6.5Si with the hcp structure that was assessed based on pure iron (Dewaele et al. 2006) and Fe-9wt%Si (Tateno et al. 2015). The room temperature parameters for the Vinet EoS were obtained by averaging on the basis of mole fraction between the two compositions: for Fe-4Si, V_0 = 22.56Å^3, K_0 = 166 GPa, K' = 5.4, and for Fe-6.5Si, V_0 = 22.63 Å^3, K_0 = 167 GPa, K' = 5.5, where V_0, K_0, K' are the unit-cell volume, bulk modulus, and its pressure derivative at 300 K and 1 bar, respectively. We assumed the same thermal parameters as for pure iron (Dewaele et al. 2006; Tateno et al. 2015).

The thermal pressure effect on the sample pressure was checked against the pressure for the SiO_2 pressure medium. The EoS for stishovite by Wang et al (2012) was used to calculate the pressure for SiO_2. As the precise temperature for the pressure medium was unknown, we calculated the pressure for SiO_2 at the sample temperature and 300 K. At 42.8 GPa and 1940 K for the sample, the pressure for SiO_2 were 44.9 GPa and 34.1 GPa at 1940 K and 300 K respectively. Since the crystallized portion of the pressure medium should be at the same (or slightly lower) temperature of the sample, the above calculation independently supports our pressure determination for the iron alloy. Also, after quench, the pressure for SiO_2 is 37.6 ± 1.0 GPa, which is consistent with the sample pressure of 36.6 ± 0.4 GPa. Therefore, we can conclude that the pressure estimation at high temperatures is reasonable.

The use of the unit-cell volume of the hcp phase in the pressure calculation may introduce an uncertainty when the experimental condition is near the completion of the hcp-fcc reaction. Based on a binary temperature-composition (T-X) phase loop detailed below, the pressure could have been underestimated by less than 1.3 GPa at 40 GPa and 1870K. When the unit-cell volume for the hcp phase was not obtained, due to either grain growth or complete transition to the fcc phase, we assumed constant pressure upon further heating.

RESULTS

Fe-4Si

Six separate in-situ XRD experiments were carried out on the Fe-4Si sample in the internally heated DAC. The results are illustrated in Fig. 1a and summarized in Table 1.

In the first run, the sample was compressed to 16.4 GPa and the XRD pattern shows coexistence of the bcc and hcp phases. Then the sample was heated to 1060 K and the fcc phase, with a minor amount of hcp phase, was observed. The hcp phase disappeared in the following XRD pattern at a similar temperature of 1050 K. Temperature slightly increased with time to 1080 K at steady power from the DC power supply without further changes in the pattern. Then, we tried to reverse the reaction. As the spectroradiometric method could not reliably measure temperatures below 1000 K, the temperature was estimated based on the linear power-temperature relationship established at 1060 K. During the cooling path, the reversal reaction started at 860 K, 200 K lower than the reaction in the forward heating cycle. Further decreasing temperature to 770 K only slightly promoted the reaction, which suggests that nucleation of the hcp phase is very sluggish and implies that the width of the reaction in the backward cycle is much wider than the forward cycle. Accordingly, we constrained

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the P-T conditions of the reaction in the forward cycle only and the results of the backward cycle are not listed in Table 1 to avoid confusion.

In the following runs, we only employed heating cycles which started from the hcp phase towards the fcc stability field. In the runs 2, 3, and 4, we observed a transition sequence from hcp to hcp+fcc and to fcc with increasing temperature. Figure 2 shows a series of XRD patterns collected during the run 2 for increasing temperature at about 24 GPa. The temperature was first held at 1120 K for 4 minutes, observing only the hcp phase. Then we increased the temperature to 1230 K and fcc peaks appeared. No further changes in the XRD pattern were recognized during the following 40 minutes, during which the temperature was kept constant. We further increased the temperature to 1260 K, which instantaneously increased the intensity of the fcc peaks. During the following 30 minutes at constant temperature, the XRD patterns did not show significant changes. The transition was completed at 1330 K. In summary, the drastic changes in XRD were observed only upon temperature increase. The transition from the hcp to fcc phase seems to be very fast, with minimal kinetic effects.

In the runs 5 and 6, we observed no structural change to the highest temperatures and confirmed stability of the hcp phase to 71.0 GPa and 2020 K.

Overall, thanks to the performances of the internal heating system, we have

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been able to place tight constraints on the P-T location of the transition boundaries. In particular, the width of the phase loop was accurately constrained. The dP/dT slope of the boundary of the entrant fcc phase in Fe-4wt% Si is similar to that of pure Fe, while the temperature interval of the two-phase region expands with increasing pressure from 50 K at 15 GPa to 150 K at 40 GPa (Fig. 1a).

Fe-6.5Si

Two separate laser-heating runs were conducted on the Fe-6.5Si sample (Fig. 1b). Same as for the internal-heating runs, we increased the temperature under high pressures. In the first run, we compressed the sample to 24.0 GPa at room temperature and then heated it by laser, reporting the appearance of fcc peaks at 1850 K in coexistence with hcp peaks. In the second run, we observed a complete transition to the fcc phase at 2340 K and 56.6 GPa. Considering the uncertainty in temperature in the laser heating experiment (i.e., ±10%), the present experimental data are consistent with results by Tateno et al. (2015) (Fig. 1b).

DISCUSSION

Effect of Si on the fcc-hcp transition

The present experiments confirmed the enlarged high temperature stability of the hcp phase in Fe-4Si and Fe-6.5Si with respect to the case in pure Fe (Fig. 1), in agreement with Fischer et al. (2013) and Tateno et al. (2015) but in contrast to Asanuma et al. (2008). Dissecting the XRD patterns in Asanuma et al. (2008), we noted that they assigned tiny shallow rises as peaks from the fcc phase, while the appearance of the fcc phase is clearly marked by the presence of the (200) peak (Fig. 2) (Komabayashi et al. 2009; 2012). We conclude that the transition temperature between the hcp and fcc phases increases with Si content.

Figure 3 shows a T-X diagram at 40 GPa based on the present data on Fe-4Si and Fe-6.5Si and existing experimental data on pure Fe and Fe-9Si (Komabayashi et al. 2009; Tateno et al. 2015). The fcc-hcp transition temperature increases with Si content. The P-T conditions for a reaction hcp = hcp + B2 phase (Tateno et al. 2015) placed additional constraint on the phase diagram (Fig. 3). The maximum solubility of Si into the fcc phase should be about 7 wt%. A thermodynamic model will be made to fit the data in the near future.

IMPLICATIONS

Figure 4 shows a phase diagram of iron alloys reporting the fcc-hcp boundaries in Fe, Fe-4Si, and Fe-6.5Si, together with the P-T ranges for the cores of Mars and Mercury. Addition of Si to Fe expands the stability of the hcp phase as confirmed by the P-T locations of the fcc-hcp transitions observed in this study, which are consistent with Tateno et al. (2015) based on a laser-heated DAC experiments (Fig. 1b). The triple point where the fcc, hcp, and liquid phases coexist in Fe-4wt% Si is placed at 90-105 GPa and 3300-3600 K (the melting curve is assumed to be the same as in Fe as Si inclusion at 4wt% level should not significantly affect the melting temperature (Morard et al. 2011)), supporting the idea that Earth's inner core at 330-364 GPa is made up with the hcp phase. Tateno et al. (2015) similarly proposed that the inner core would be made of a sole hcp alloy if the Si content is up to 7 wt.%.

More complex can be the cases for the other terrestrial planets of the solar system, namely, Venus, Mercury, and Mars. Due to the lack of seismic data, information about their internal structures heavily depends on the average density. As such, the core density deficit cannot be pertinently discussed. Nevertheless geophysical modelling studies argued for the presence of light elements in the cores and kept this into consideration when simulating planetary core, and in particular when discussing their molten/solid state (Stevenson et al. 1983; Williams and Nimmo 2004; Rivoldini et al. 2011; Dumberry and Rivoldini 2015; Knibbe and van Westrenen 2018). In the

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following, we will limit our discussion to the Fe-Si-S system. Tsujino et al. (2013) summarized existing thermal models for terrestrial core-mantle boundaries in the system Fe-S (Stevenson et al. 1983; Sohl and Spohn 1997; Fei et al. 2000; Williams and Nimmo 2004) and assessed the adiabats across the cores on the basis of the Grüneisen parameter for pure fcc iron (Fig. 4). The known reduction of the crystallizing temperature of iron by addition of silicon (Kubaschewski 1993; Kuwayama and Hirose 2004) implies that the thermal profiles in Fig. 4, which are based on the liquidus of the system Fe-S, can be considered as the maximum estimates for the system Fe-Si-S.

Venus' similar size to the Earth implies that its internal structure is differentiated into crust, mantle, and core (Sohl and Schubert 2007). However, contrarily to the Earth, Venus does not have a global magnetic field .The pressure at the center of the planet was estimated to be 295 GPa which is slightly lower than of the Earth and crystallization of the liquid core might have not yet started (Stevenson et al. 1983). Since the core pressure is far greater than the triple point pressure in the system Fe-4Si (Fig. 4), when upon secular cooling the inner core will start crystallizing, likewise the Earth, it should take an hcp phase.

It is suggested that Mercury has a partially molten iron core as it shows a dipole magnetic field from a spacecraft observation (Ness 1979). Further support of the

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presence of a liquid portion of the core comes from and the amplitude of its librations (Margot et al. 2005). The suggested thermal structure of Mercurian core modeled on the basis of the system Fe-S argues for a temperature much higher than the fcc-hcp transition in Fe-6.5Si (Fig. 4). Recently proposed thermal models of Fe-Si cores showed a similar temperature range as in Fig. 4 (Knibbe and van Westrenen 2018). Hence Mercurian inner core is expected to take an fcc structure if the Si content is less than 6.5 wt%. Only upon further cooling, the fcc-structured alloy in Mercurian inner core, will be transformed to the hcp phase.

Mars currently does not have an active global magnetic field, although it has a metallic core in view of its average density and moment of inertia (Yoder et al. 2003). However, the presence of magnetized rock records found in southern highland area indicates that the planet should have had a magnetic field in the past. Stevenson et al. (1983) suggested that present Martian core should still be totally molten to account for the absence of the magnetic field and the rocks were magnetized by a field produced by a past, now extinct, thermal convection of the liquid core. The inferred thermal profiles of the core partially overlap with the fcc-hcp transition in Fe-4Si (Fig. 4). As such the first iron alloy crystal that will crystallize in the future will be either fcc or hcp phase depending on the actual Si content and exact temperature. In the case of the fcc phase, it will be transformed to the hcp phase as the core further cools down.

In summary, the inner core structure of the terrestrial planets can be discussed based on the phase relations in Fig. 4. The hcp core would show more anisotropic seismic properties (Steinle-Neumann et al., 2001) than the fcc core because of the anisotropic crystal structure. Also the hcp core would be denser than the fcc core as the fcc-hcp transition in Fe-4Si shows about 0.8% density jump. Those changes are important in future attempts to construct a precise density model for the planetary interior.

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Figure captions

Figure 1. Results of the experiments in (a) Fe-4Si and (b) Fe-6.5Si. The phases observed in XRD patterns are plotted: inversed triangle, hcp+bcc; square, hcp; normal triangle, fcc+hcp; circle, fcc. In (a), the boundaries between the fcc and hcp phases in pure iron (Komabayashi et al. 2009) and Fe-3.4Si (Asanuma et al. 2008) are also plotted. The data with asterisk have larger temperature uncertainty. In (b), our data are shown together with experimental data by Tateno et al. (2015). The typical uncertainty (2.5 GPa and 200 K) is shown for a guide to the eye, see Table 1 for the uncertainty for each data point. The two datasets are fairly consistent considering the uncertainty in the laser heating experiments.

Figure 2. Series of XRD patterns collected in the run 2 for increasing temperature. The presence of the fcc phase was unambiguously marked by the appearance of (200) peak.

Figure 3. Temperature-composition diagram for the fcc-hcp transition. The open circle denotes the transition temperature in pure Fe (Komabayashi et al. 2009); the star symbols are the fcc-hcp reactions constrained by the present experiments; the filled circle is the P-T condition for a reaction of hcp = hcp + B2 phase observed in Tateno et

al. (2015). The stability fields of fcc+B2 and hcp+B2 were constrained by phase relations. In particular: (i) the boundary hcp = hcp+B2 should have a negative slope (Tateno et al. 2015) and (ii) the invariant boundary where the fcc, hcp, and B2 phases coexist should be placed at a temperature higher than the upper star at Fe-6.5Si.

Figure 4. The fcc-hcp boundaries in Fe-4Si and Fe-6.5Si (this study) with phase relations of pure iron (black lines) (Komabayashi et al. 2009; Komabayashi 2014). Thermal profiles of Mercurian and Martian cores in the system Fe-S are also shown (Tsujino et al. 2013).

Table 1. Experimental conditions and results

Run	P, GPa	T, K*	Phase	V(hcp), Å^3	a (hcp), Å	c (hcp), Å	V(fcc), Å^3	Remarks
Fe-4Si (internal resistive heating)								
1	16.4(6)	300	bcc+hcp	20.823(53)	2.4640(18)	3.9604(83)		
	13.1(4)	1060	fcc+hcp(small)	21.660(0)	2.4855(0)	4.04853(0)	43.643(14)	
	13.1(4)	1050	fcc				43.615(19)	
	13.1(4)	1080	fcc				43.683(19)	
2	23.6(4)	300	hcp	20.265(27)	2.4394(14)	3.9323(24)		
	22.6(4)	1120	hcp	20.816(3)	2.4554(2)	3.9866(3)		
	21.9(5)	1230	hcp+fcc	20.955(3)	2.4596(2)	3.9998(3)	42.352(0)	
	21.2(4)	1260	hcp+fcc	21.036(0)	2.4596(0)	4.0152(0)	42.343(38)	
	21.2	1260	hcp+fcc	-	-	-	42.330(5)	one peak for hcp
	21.2	1270	hcp+fcc	-	-	-	42.370(4)	one peak for hcp
	21.2	1330	fcc				42.475(15)	
	21.2	1360	fcc				42.520(12)	
	21.2	1430	fcc				42.720(21)	
	21.2	1450	fcc				42.854(69)	
3	33.3(2)	300	hcp	19.629(11)	2.4193(6)	3.8725(11)		
	32.7(5)	1030	hcp	20.016(10)	2.4280(5)	3.9206(10)		
	30.6(5)	1190	hcp	20.247(7)	2.4342(4)	3.9456(7)		
	30.2(5)	1240	hcp	20.312(9)	2.4361(5)	3.9521(9)		
	29.3(1.0)	1300**	hcp+fcc	20.411(13)	2.4399(7)	3.9592(13)	41.463(0)	
	29.3(1.1)	1370**	hcp+fcc	20.453(18)	2.4417(9)	3.9611(18)	41.392(0)	
	29.0(6)	1440	hcp+fcc	20.524(14)	2.4434(7)	3.9696(14)	41.285(0)	
	28.4(1)	1470	hcp+fcc	20.559(5)	2.4465(3)	3.9663(3)	41.344(51)	
	28.6(8)	1500	hcp+fcc	20.595(25)	2.4472(14)	3.9710(16)	41.480(37)	
	28.6	1580	fcc				41.652(23)	
	28.6	1620	fcc				41.650(19)	
4	41.0(5)	300	hcp	19.198(26)	2.3956(14)	3.8626(24)		
	43.7(6)	1130	hcp	19.392(13)	2.4019(7)	3.8813(12)		
	43.6(6)	1190	hcp	19.426(13)	2.4028(7)	3.8852(12)		
	43.3(6)	1250	hcp	19.473(10)	2.4043(5)	3.8899(9)		
	42.8(6)	1310	hcp	19.527(9)	2.4060(5)	3.8949(8)		
	42.3(5)	1380	hcp	19.592(7)	2.4081(4)	3.9011(6)		
	41.9(5)	1460	hcp	19.659(7)	2.4103(4)	3.9074(7)		
	41.8(7)	1410	hcp	19.637(14)	2.4106(8)	3.9021(13)		
	41.4(7)	1450	hcp	19.686(13)	2.4125(7)	3.9056(12)		
	41.5(7)	1560	hcp	19.736(13)	2.4139(7)	3.9111(12)		
	41.2(7)	1600	hcp	19.777(17)	2.4157(9)	3.9133(15)		
	41.5(8)	1680	hcp	19.799(25)	2.4158(13)	3.9173(23)		
	41.6(6)	1740	hcp+fcc	19.833(11)	2.4160(6)	3.9234(10)	39.934(0)	
	42.0(8)	1800	hcp+fcc	19.841(24)	2.4161(13)	3.9247(22)	40.055(0)	
	42.1(9)	1870	hcp+fcc	19.868(28)	2.4175(15)	3.9253(26)	40.080(0)	
	42.8(5)	1940	hcp+fcc	19.868(0)	2.4149(0)	3.9338(0)	40.133(10)	
	42.8	2050	fcc				40.204(13)	
	42.8	2090	fcc				40.216(36)	
	42.8	2160	fcc				40.315(44)	
	42.8	2230	fcc				40.344(43)	
	42.8	2260	fcc				40.340(48)	

5	46.0(3)	300	hcp	18.938(15)	2.3856(9)	3.8426(15)		
	50.0(6)	1050	hcp	19.020(12)	2.3882(7)	3.8507(11)		
	50.3(6)	1120	hcp	19.036(10)	2.3885(5)	3.8530(9)		
	50.6(5)	1230	hcp	19.068(7)	2.3890(4)	3.8579(6)		
	50.9(5)	1350	hcp	19.108(4)	2.3897(2)	3.8637(4)		
	52.0(5)	1530	hcp	19.124(5)	2.3901(3)	3.8657(5)		
	52.6(8)	1620	hcp	19.139(17)	2.3904(9)	3.8676(16)		
	52.8(1.3)	1750	hcp	19.186(44)	2.3914(24)	3.8739(41)		
6	75.8(1.2)	300	hcp	17.705(43)	2.3355(25)	3.7481(42)		
	70.1(1.6)	1080	hcp	18.135(48)	2.3563(22)	3.7716(72)		
	70.7(1.5)	1140	hcp	18.133(42)	2.3553(19)	3.7745(62)		
	70.8(1.3)	1200	hcp	18.151(35)	2.3551(16)	3.7789(53)		
	70.5(8)	1300	hcp	18.194(16)	2.3549(7)	3.7886(24)		
	68.7(7)	1460	hcp	18.323(10)	2.3596(5)	3.8000(16)		
	71.0(8)	1510	hcp	18.247(14)	2.3540(6)	3.8025(22)		
	71.0(1.0)	1650	hcp	18.301(21)	2.3552(8)	3.8096(36)		
	70.8(1.0)	1760	hcp	18.347(24)	2.3570(9)	3.8134(42)		
	70.6(1.1)	1840	hcp	18.387(25)	2.3585(9)	3.8169(43)		
	70.6(9)	1910	hcp	18.415(21)	2.3595(8)	3.8193(36)		
	71.2(9)	1960	hcp	18.410(17)	2.3600(8)	3.8169(26)		
	71.0(7)	2020	hcp	18.444(9)	2.3616(4)	3.8187(14)		
Fe-6.5Si (laser heating)								
1	24.0(1.3)	300	hcp	20.321(14)	2.4382(8)	3.9471(14)		
	28.8(2.3)	1320	hcp	20.539(10)	2.4438(5)	3.9713(9)		
	30.5(2.5)	1520	hcp	20.544(10)	2.4440(5)	3.9717(9)		
	29.6(2.4)	1500	hcp	20.602(9)	2.4457(5)	3.9773(8)		
	28.2(2.3)	1360	hcp	20.612(9)	2.4459(5)	3.9784(9)		
	28.0(2.3)	1430	hcp	20.671(9)	2.4473(3)	3.9854(12)		
	29.5(2.8)	1610	hcp	20.683(36)	2.4465(15)	3.9900(51)		
	29.5(3.1)	1640	hcp	20.695(60)	2.4507(25)	3.9788(82)		
	29.5(2.8)	1750	hcp	20.777(29)	2.4513(10)	3.9927(44)		
	29.5	1850	hcp+fcc	-	-	-	42.569(51)	one peak for hcp
2	62.1(3.5)	300	hcp	18.308(55)	2.3616(21)	3.7904(93)		
	64.0(3.9)	1480	hcp	18.620(32)	2.3702(10)	3.8271(57)		
	64.0(3.7)	1600	hcp	18.664(20)	2.3702(6)	3.8364(37)		
	63.7(3.6)	1690	hcp	18.717(11)	2.3703(3)	3.8468(19)		
	66.0(5.3)	1930	hcp	18.711(77)	2.3733(8)	3.8360(157)		
	59.5(6.6)	2040	hcp	19.064(158	2.3848(13)	3.8706(318)		
	53.0(3.5)	2140	hcp	19.456(0)	2.3960(0)	3.9134(0)		
	56.6(3.6)	2240	hcp	19.309(0)	2.3859(0)	3.9169(0)		
	56.6(3.6)	2340	fcc	-	-	-	39.548(156)	

[*] The uncertainty in temperature in the resistive and laser heating are typically 50 K and 10%, respectively.

[**] Temperature uncertainty is as large as ±100 K.

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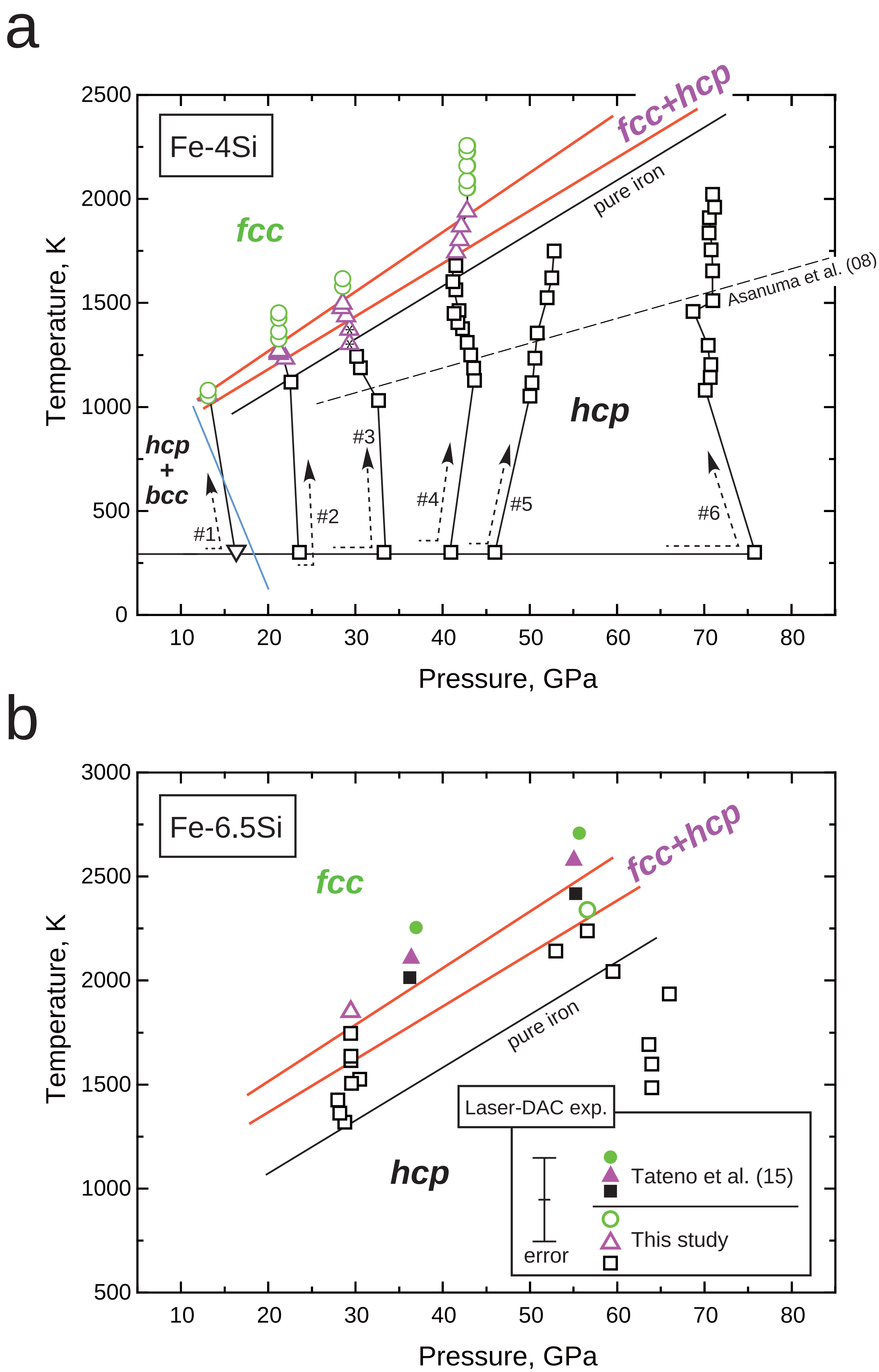

figure 1

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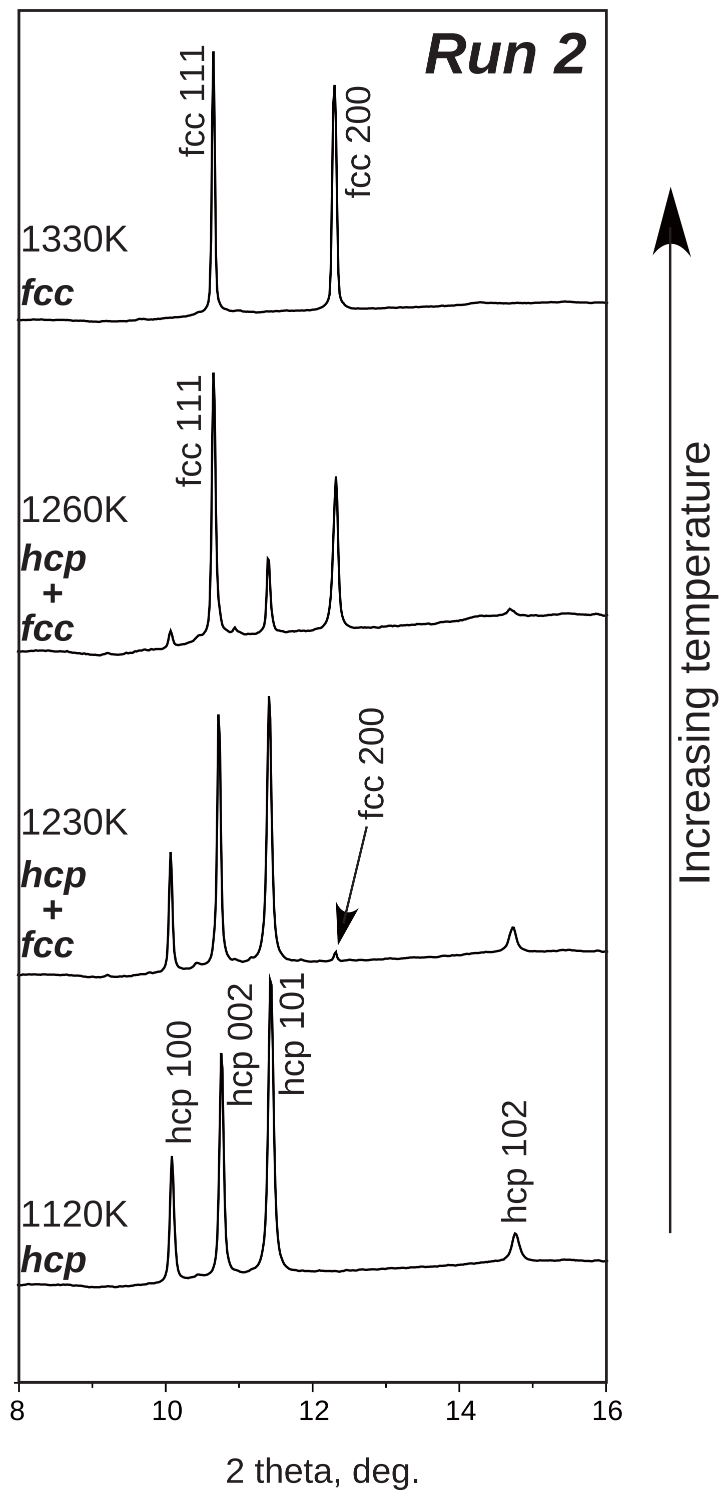

figure 2

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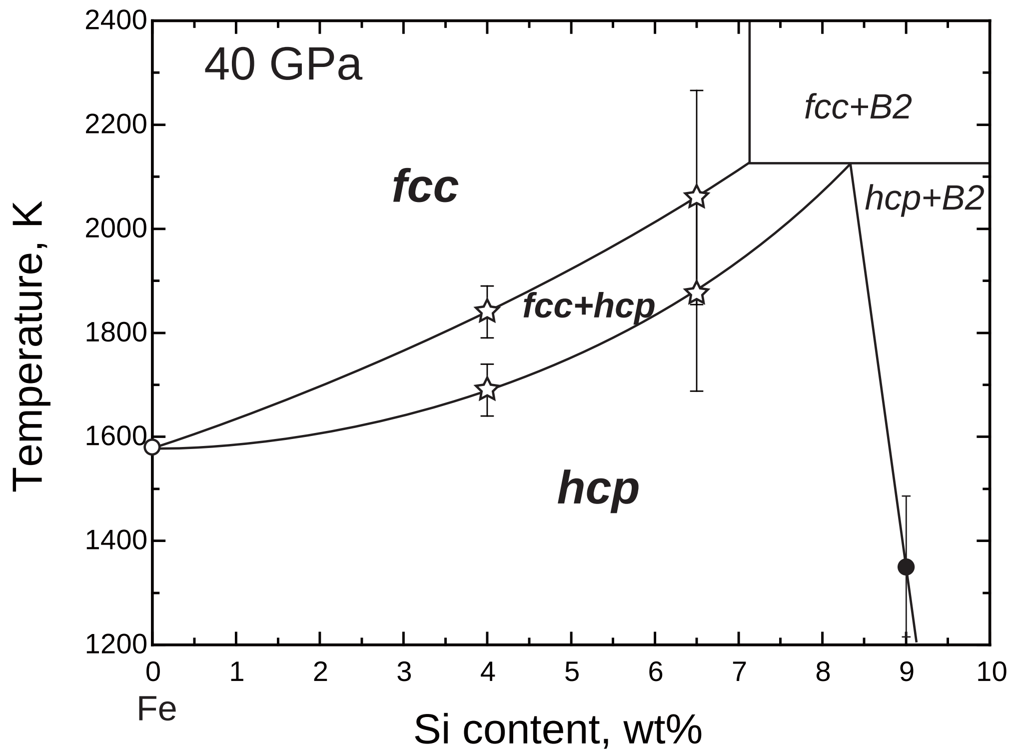

figure 3

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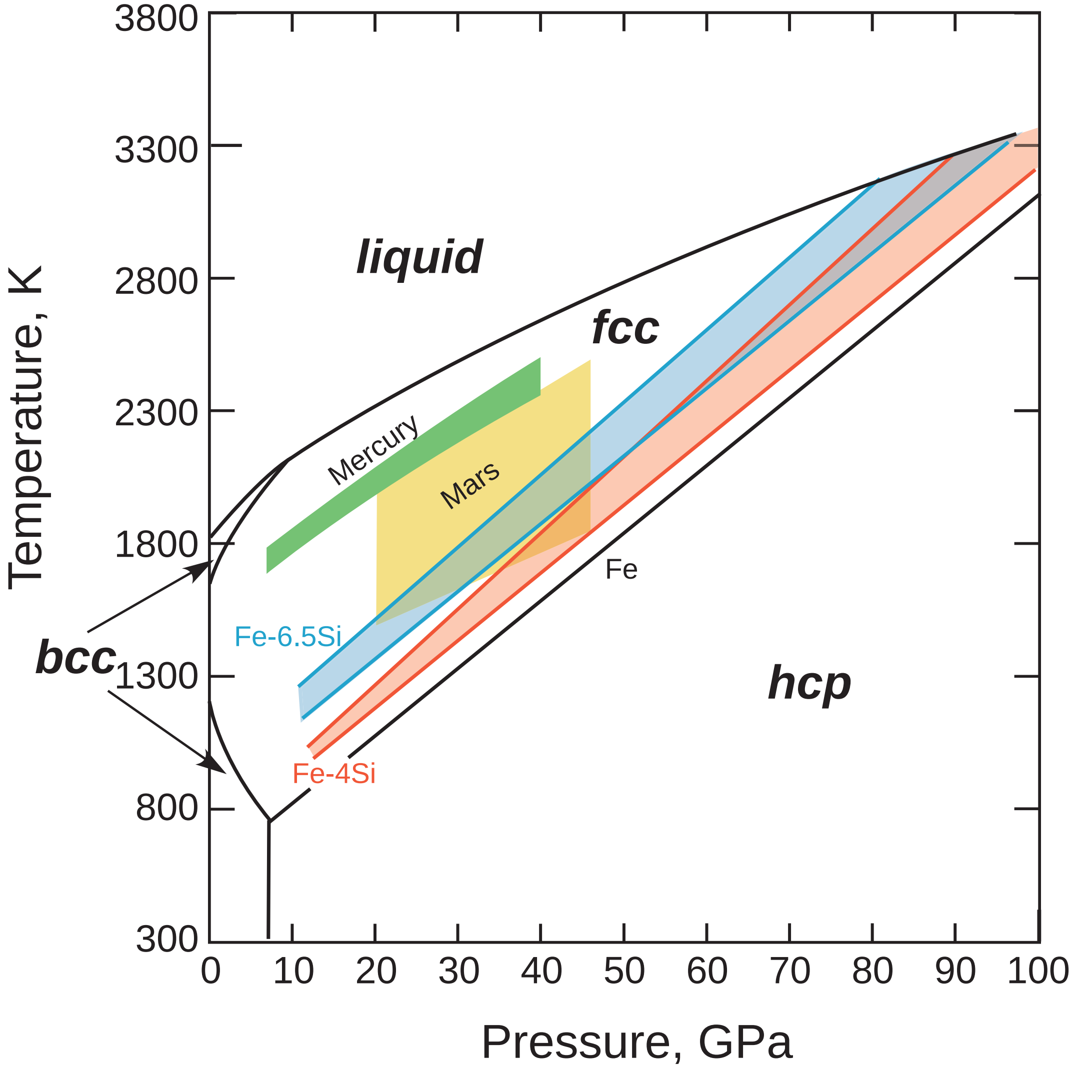

figure 4