



Phase diagram of Fe-C-S ternary system under planetary core conditions

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ABSTRACT

High-pressure, high-temperature experiments were conducted to investigate melting relations and phase assemblages in the Fe-C-S ternary system at 5 and 15 GPa, covering a temperature range of 1300–1900 K, conditions directly relevant to the Moon's and Mercury's cores. At 1300 K, the system is primarily governed by Fe-S eutectic melting, exhibiting notable complexity in the carbon-rich and sulfur-poor regions. With increasing temperature, the phase diagram simplifies: at 5 GPa and 1700 K, the Fe-Fe₃C-FeS system features three regions (Fe+L, C+L, and L). Similar phase assemblages are observed at 15 GPa, with Fe₇C₃ and diamond replacing Fe₃C and graphite, respectively. Extensive Fe+L, C+L, and L regions are observed at 1900 K.

For a Moon's core composed of a Fe-C-S alloy, nearly pure Fe is the only viable inner core phase above 1700 K. Below this temperature, both Fe and Fe₃C are potential solid inner core phases, depending on carbon content; a two-phase solid inner core is also theoretically possible. The inferred compositions of the outer core suggest densities of 6200–7300 kg/m³, with tighter constraints for models featuring an Fe₃C core.

At Mercury-relevant pressures, either Fe or Fe₇C₃ may form the solid inner core, again depending on carbon content. If the inner core is nearly pure Fe, the liquid outer core density ranges from 7300 to 7900 kg/m³. In both scenarios, a “snow” regime is plausible, though with distinct settling times. The ternary phase diagram indicates that Mercury is likely to develop a structurally layered inner core during secular cooling.

1. Introduction

Carbon (C) and sulfur (S) are commonly considered as two plausible light elements in the core of terrestrial planets as the most abundant light elements in the core of differentiated iron meteorites (Buchwald, 1975).

Sulfur was often regarded as a main light element in the models of Mercury's core due to its cosmochemical abundance and siderophile property at high pressures (Harder and Schubert, 2001; Rivoldini et al., 2009). MESSENGER's Gamma-ray spectral data enabled the estimation of the average C content on Mercury's surface (e.g., ~1.4 wt %, Peplowski et al., 2015), which is much higher than that of other terrestrial planets in the solar system. Lark et al. (2023) estimated the total mass of C within Mercury's shallow interior and proposed that it would have been C-saturated during the core-mantle differentiation. Most of the C was considered to have precipitated as graphite and

floated up to the surface of the magma ocean during this stage, with the remainder incorporated into the metallic core due to its siderophile properties (Dasgupta and Walker, 2008; Dasgupta et al., 2013; Keppler and Golabek, 2019). At Mercury's reducing conditions, between IW-2.6 and IW-7.3 (McCubbin et al., 2012; Zolotov et al., 2013), silicon (Si) would have also efficiently partitioned into the metallic core (Chabot et al., 2014), so that Si, C, and S are all considered as potential candidates when establishing the model of Mercury's core (e.g., Chabot et al., 2014; Namur et al., 2016; Vander Kaaden et al., 2020). However, due to lack of constraints on the properties of multi-component systems, core models have often been developed based on binary or pseud-binary iron systems and neglecting C (e.g. Rivoldini et al., 2009; Hauck et al., 2013; Dumberry and Rivoldini, 2015; Edmund et al., 2022; Davies et al., 2024). A Fe-C-S core model, while still likely a simplification, is a further step toward more complex systems.

Earlier assumptions suggested that the Moon was volatile-poor due

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to the tremendous heat generated during the giant impact (Hartmann and Davis, 1975; Canup, 2004). However, this notion has been challenged by analyses of lunar samples and high-temperature, high-pressure experiments conducted in the past decade (Hauri et al., 2011; Wetzel et al., 2015; Lin et al., 2017), which indicated that the water content in the primitive Moon is comparable to that of the Earth's mantle. The redox conditions of the Moon are more oxidizing compared to Mercury (ranging between IW-2 and IW, Wadhwa, 2008), and thus Si is not favored in the core (Kilburn and Wood, 1997). Based on metal-silicate partitioning and estimated C and S abundance in the bulk silicate Moon (BSM), the Moon's core could contain up to 4.8 wt % C (Steenstra et al., 2017). The presence of other light elements (such as P, H) is also possible, though their overall abundances remain poorly constrained due to the lack of geochemical data. As such, most current lunar models consider S to be the dominant light element in the core, due to its cosmochemical abundance, siderophile properties, and its ability to lower the melting point and density of iron (e.g., Weber et al., 2011; Antonangeli et al., 2015). Once again, a Fe-C-S core model would provide a more realistic scenario.

Given its importance, we constrain the ternary Fe-C-S phase diagram across a range of *P-T* conditions to refine constraints on and model the core properties of small to mid-sized telluric bodies. Our approach spans early differentiation to present-day melting state and composition. To this end, we experimentally determined the phase diagram within the ternary Fe-FeS-Fe₃C/Fe₇C₃ system, from subsolidus to superliquidus temperatures, using multi-anvil presses at 5 and 15 GPa. The results are then applied to address the cooling process of the Moon's and Mercury's cores.

2. Experimental methods

Experiments were performed using either a 1000-ton or 5000-ton Kawai-type multi-anvil press at the Institute for Planetary Materials, Okayama University. Experiments at 5 GPa used 18/11 cell assemblies, while those at 15 GPa 14/8 assemblies. The relationship between oil load (tons) and pressure (GPa) was established via well-documented phase transition boundaries: at 1700 K for 18/11 assemblies (quartz-coesite and fayalite-spinel), and at 1600 K for 14/8 assemblies (quartz-coesite, coesite-stishovite, olivine-wadsleyite, and wadsleyite-ringwoodite). The estimated pressure uncertainty is ± 0.5 GPa. Starting materials consisted of mixtures of pure iron powder (Macklin, 99.99 %), FeS powder (Alfa Aesar, 99.99 %), and graphite powder (Alfa Aesar, 99 %). The stoichiometric bulk composition was within the Fe-Fe₇C₃-FeS system ($C < 8.44$ wt % and $S < 36.5$ wt %). The powders were mixed and ground in an agate mortar for 30 min to achieve uniform texture and composition, then stored in a vacuum box. 19 compositions (see Table 1) were used to constrain the phase diagram. Powders were loaded into Al₂O₃ capsules (outer diameter: 2 mm; inner diameter: 1 mm; height: 0.8 mm). For 5 GPa experiments, 4 capsules were loaded simultaneously in 18/11 assemblies, while 2 capsules were used in 14/8 assemblies for 15 GPa experiments. The capsules were separated by 0.3 mm-thick MgO disks. Experiments were conducted at temperatures ranging from 1300 K to 1700 K (5 GPa) and 1300 K to 1900 K (15 GPa). Temperature was monitored using a W3 %Re-W25 %Re thermocouple, with the junction placed at the center of the cell. Schematics of the used cell assemblies are provided in Supplementary Materials Figure S1. A dedicated run estimated the temperature gradient in the 4-capsule setup using two sets of thermocouples: one at the center and another 2 mm away. The temperature difference was less than 60 degrees at ~ 1800 K.

For all the experiments, the cell assembly was first compressed to the target hydraulic load and then heated at a rate of 100 K/min to 1900 K. The cell was subsequently slowly cooled over 3 h and maintained at the target temperature for approximately 1 hour before quenching. Although the cooling process may lead to a slight drop in pressure, this step was considered necessary to facilitate the equilibration of the sample (see Results section). The recovered samples were mounted in

epoxy and polished for analysis. The texture of all samples was examined using a field-emission scanning electron microscope (FE-SEM; JEOL JSM-7001F). Chemical composition was analyzed by a field-emission electron microprobe analyzer (FE-EPMA, JEOL JXA-IHP200F) at the Institute for Planetary Materials, Okayama University. For EPMA analyses, the operating conditions were set to 15 kV/100 nA for C and 15 kV/10 nA for the other elements. A defocused beam of 10 μ m was used to minimize scattering in the liquid composition caused by the quench texture. Each phase of all samples was probed at 8–10 points. To determine C content, a calibration curve (Supplementary material Figure S2) was developed based on the K α line intensity of C in pure Fe (Nilaco, 99.999 %) and multiple C-bearing standards: Fe-0.295wt %C and Fe-1.44wt %C (manufactured by The Japan Iron and Steel Federation), and synthesized Fe₇C₃.

3. Results

Representative textures of the recovered samples, as observed by backscattered electrons (BSE) imaging, are presented in Fig. 1. Below the liquidus, one or two solid phases typically co-exist with liquid, including Fe, Fe-C compounds (either Fe₃C or Fe₇C₃, depending on pressure), and/or C (graphite or diamond, also depending on pressure). Carbon is minorly dissolved in solid iron in all the runs, with the solubility limit being dependent on the specific *P-T* conditions (Fei and Brosh, 2014). Once carbide phases appear, the Fe phase can be considered as C-saturated. The measured C content in the C-saturated Fe is well consistent with the results reported by Fei and Brosh (2014) except one outlier, the Fe-4C-2S run, quenched from 5 GPa and 1300 K, with 2.46 wt % of C in the Fe, much higher than the suggested value of ~ 1.1 wt %. The larger uncertainty in the analyzed C content of this sample could indicate a partial contribution from the carbide phase, potentially due to the use of a defocused beam. Solid FeS co-existing with the liquid was observed only in S-rich, C-poor samples at relative low temperature. This is primarily due to the higher melting temperature of Fe-C phases compared to Fe-S components under similar *P-T* conditions (Morard et al., 2007; Nakajima et al., 2009; Fei and Brosh, 2014). Iron carbide Fe₇C₃ formed exclusively in the 15 GPa experiments, consistent with the Fe₇C₃ stability field (Nakajima et al., 2009; Deng et al., 2013; Gromilov et al., 2019). Notably, at 5 GPa solid phases tend to accumulate at the sides of the samples, whereas at 15 GPa, suspended Fe₇C₃ grains indicate density equilibrium with in the surrounding liquid, as evidenced by the dendritic texture observed in quenched samples. The high compressibility of the S-rich liquid (e.g., Knibbe et al., 2021) suggests that the density contrast between liquid and solid phases decreases markedly with pressure. A comprehensive discussion is presented in Section 4.3.

The phase assemblage and chemical composition of each phase of the run products are listed in Table 1. Compared to Fe-C binary system (e.g., Fei and Brosh, 2014), partial melting is already identified at 1300 K in all the ternary samples, indicating that the onset of melting is dominated by Fe-S eutectic melting. Minor oxygen contamination, duly reported, likely results from interaction with the MgO disks sealing the liquid at high temperature. Limited diffusion of oxygen into the metallic liquid has been widely documented in similar experiments (Corgne et al., 2008; Deng et al., 2013; Zhao et al., 2023). The scattering in Fe and S content in the liquid phase arises from difficulties in analyzing samples with quench texture at a small spatial scale. In carbon-saturated samples, graphite (at 5 GPa) and diamond (at 15 GPa) grains are easily identifiable in the BSE images, though some grains were lost during polishing. The composition of C-saturated liquids aligns with results reported in earlier studies (Zhang et al., 2018).

Based on the experimentally determined phase assemblages, the liquid compositions in fully-molten and partially-molten samples, and the binary phase assemblages reported in the literature, the ternary phase diagrams were constructed and are presented in Fig. 2.

At 5 GPa, the solidus of Fe-C system is significantly lowered by the incorporation of S. At 1300 K, at least partial melting is observed in all

Table 1

Phase assemblage and chemical composition of the run products.

Starting composition	Phase assemblage	Phase	Concentration (wt %)				
			Fe	C ^d	S	O	Total
5 GPa, 1300 K							
Fe-0.4C-5S	Fe+L	Fe	101.15(40)	0.43(4)	0.06(1)	0.02(2)	101.66
		L	84.14(347)	0.42(8)	15.98(330)	0.05(6)	100.59
Fe-0.4C-10S	Fe+L	Fe	101.02(41)	0.47(3)	0.09(1)	0.01(2)	101.59
		L	86.55(314)	0.66(9)	13.27(300)	0.06(5)	100.54
Fe-0.4C-20S	L	L	80.84(50)	0.13(4)	19.87(37)	0.10(8)	100.87
Fe-1C-2S	Fe+L	Fe	101.37(41)	0.65(7)	0.05(1)	0.07(5)	102.14
		L	93.76(163)	1.44(8)	5.75(110)	0.05(7)	101.00
Fe-1C-10S	L	L	90.31(235)	1.07(9)	10.10(232)	0.06(7)	101.54
Fe-1C-30S	FeS+ Gr+L	FeS	62.58(20)	-	36.98(13)	0.05(5)	99.61
		L	67.92(244)	0.95(96)	31.81(267)	0.42(28)	101.10
Fe-1.5C-15S	L	L	78.94(207)	1.37(23)	17.15(196)	0.36(17)	97.82
Fe-1.5C-20S	Gr+L	L	77.25(181)	0.39(9)	21.97(89)	0.42(13)	100.03
Fe-1.5C-28S	FeS+ Gr+L	FeS	64.43(34)	0.33(24)	36.56(22)	0.10(12)	101.41
		L	74.66(288)	0.55(30)	24.81(282)	0.18(15)	100.20
Fe-2.5C-10S	L	L	84.25(557)	1.82(176)	12.77(603)	0.19(11)	99.03
Fe-2.5C-22S	Gr+L	L	75.83(50)	0.22(8)	24.13(52)	0.53(14)	100.71
Fe-4C-2S	Fe+	Fe	97.81(85)	2.46(169)	0.02(1)	0.08(4)	100.37
	Fe ₃ C+L	Fe ₃ C	91.85(38)	6.83(40)	0.01(1)	0.06(6)	98.75
		L	87.17(349)	4.53(175)	10.03(376)	0.19(11)	101.92
		L	82.39(182)	1.47(21)	16.27(171)	0.17(8)	100.30
5 GPa, 1500 K							
Fe-0.4C-5S	Fe+L	Fe	100.77(56)	0.31(4)	0.07(1)	0.02(2)	101.16
		L	85.78(336)	0.32(11)	14.54(315)	0.08(5)	100.73
Fe-0.4C-10S ^a	Fe+L	Fe	/	/	/	/	/
		L	87.78(200)	0.36(7)	12.21(184)	0.1(11)	100.46
Fe-0.4C-20S	L	L	80.07(60)	0.67(16)	20.48(24)	0.14(8)	101.36
Fe-0.4C-30S	Gr+L	L	69.61(288)	0.45(22)	31.14(295)	0.28(16)	101.47
Fe-1C-2S	Fe+L	Fe	100.58(126)	0.83(12)	0.05(2)	0.11(7)	101.57
		L	92.47(313)	1.69(20)	7.63(282)	0.03(6)	101.82
Fe-1C-10S	L	L	89.91(281)	1.06(18)	11.22(278)	0.11(8)	102.29
Fe-1C-30S	Gr+L	L	69.24(213)	0.26(12)	30.52(286)	0.17(18)	100.19
Fe-1.5C-20S	Gr+L	L	79.17(267)	0.76(8)	21.41(263)	0.22(12)	101.56
Fe-2C-1S	Fe+L	Fe	98.65(38)	1.36(6)	0.03(1)	0.04(5)	100.07
		L	93.38(71)	2.98(23)	2.91(57)	0.03(5)	99.29
		L	86.70(325)	3.19(128)	10.42(393)	0.17(8)	100.48
		Fe	98.83(45)	1.42(10)	0.03(1)	0.04(7)	100.32
Fe-2.5C-10S	L	Fe ₃ C	93.06(55)	6.45(11)	0.02(4)	0.02(3)	99.55
		L	91.95(103)	2.79(102)	5.03(95)	0.03(3)	99.80
		L	93.79(192)	3.71(81)	2.88(173)	0.07(4)	100.44
		L	85.68(74)	3.01(23)	11.47(63)	0.11(7)	100.28
Fe-4C-2S	L	L	92.46(51)	5.97(10)	0.01(1)	0.02(3)	98.45
Fe-4C-10S	Gr+L	L	93.43(132)	2.95(68)	2.10(141)	0.03(1)	98.52
		Fe ₃ C	92.11(68)	6.24(8)	0.01(2)	0.02(4)	98.39
Fe-6C-2S	Fe ₃ C+L	L	90.94(182)	3.20(38)	3.54(240)	0.06(8)	97.74
5 GPa, 1700 K							
Fe-0.4C-10S	L	L	85.84(399)	0.56(9)	12.19(409)	0.40(30)	98.99
Fe-1.5C-20S	S-L + C-L	S-L	74.78(120)	0.66(22)	22.70(124)	0.37(21)	98.51
		C-L	88.99(200)	2.44(60)	4.74(132)	0.12(10)	96.29
Fe-2C-1S	L	L	94.57(147)	1.92(30)	1.47(100)	0.15(13)	98.11
Fe-3C-1S	L	L	94.23(127)	2.56(96)	1.33(67)	0.13(7)	98.25
15 GPa, 1300 K							
Fe-0.4C-5S	Fe+L	Fe	98.34(61)	0.27(5)	0.20(5)	0.23(7)	99.04
		L	89.65(178)	0.43(2)	7.97(170)	0.37(9)	98.42
Fe-0.4C-10S	L	L	86.21(164)	0.45(5)	11.57(159)	0.42(15)	98.66
Fe-1C-10S	L	L	86.71(129)	0.71(7)	10.68(139)	0.37(10)	98.46
Fe-1.5C-15S	L	L	80.69(29)	1.51(39)	14.83(65)	0.59(26)	97.60
Fe-1.5C-28S	Dia+L	L	69.21(342)	-	29.55(331)	0.79(52)	99.55
Fe-2.5C-22S ^b	Fe ₇ C ₃ + Dia+L	Fe ₇ C ₃	\	\	\	\	\
		L	75.54(356)	0.18(16)	24.86(347)	0.25(27)	100.83
Fe-4C-2S ^c	Fe+ Fe ₃ C+L	Fe	100.47(298)	0.69(34)	0.26(22)	0.22(27)	101.63
		Fe ₃ C	94.64(77)	6.65(48)	0.07(7)	0.15(14)	101.51
		L	\	\	\	\	\
Fe-4C-10S	Fe ₃ C+ Fe ₇ C ₃ +L	Fe ₃ C	92.11(86)	8.49(57)	0.09(2)	0.27(13)	100.97
		Fe ₇ C ₃	94.43(25)	6.50(44)	0.06(1)	0.07(7)	101.06
		L	77.93(233)	1.09(91)	20.70(252)	0.13(13)	99.85
		Fe ₇ C ₃	90.59(47)	8.91(21)	0.15(20)	0.14(14)	99.79
Fe-5C-12S	+Dia+L	L	75.86(643)	0.24(65)	23.99(673)	0.18(11)	100.26
15 GPa, 1500 K							
Fe-1C-2S	Fe+L	Fe	97.63(183)	0.63(5)	0.06(1)	0.13(14)	98.45
		L	87.75(251)	1.50(31)	7.78(227)	0.17(2)	97.20
Fe-2C-1S	Fe+L	Fe	96.30(39)	0.99(9)	0.05(1)	0.05(5)	97.39

(continued on next page)

Table 1 (continued)

Starting composition	Phase assemblage	Phase	Concentration (wt %)				
			Fe	C ^d	S	O	Total
Fe-2.5C-10S	L	L	89.92(99)	2.54(26)	4.17(65)	0.04(5)	96.67
Fe-2.5C-22S	Dia+L	L	86.21(80)	2.80(24)	11.13(108)	0.15(8)	100.29
Fe-4C-2S	Fe+	Fe	73.61(392)	0.01(15)	24.42(413)	0.17(13)	98.21
	Fe ₃ C+L	Fe ₃ C	98.16(61)	0.62(10)	0.04(2)	0.08(8)	98.90
		L	90.65(125)	6.34(18)	0.01(1)	0.03(2)	97.03
Fe-4C-10S	Fe ₃ C+Fe ₇ C ₃ +L	L	90.51(184)	3.08(41)	5.81(204)	0.10(5)	99.50
		Fe ₃ C	91.60(38)	6.61(29)	0.02(1)	0.02(1)	98.23
		Fe ₇ C ₃	89.77(13)	7.82(20)	0.02(1)	0.14(11)	97.75
		L	80.76(72)	2.09(12)	17.32(72)	0.23(8)	100.40
Fe-5C-12S	Fe ₇ C ₃	Fe ₇ C ₃	88.74(24)	7.79(4)	0.03(1)	0.06(8)	96.62
	+Dia+L	L	77.60(51)	1.99(17)	20.32(81)	0.03(5)	99.94
15 GPa, 1700 K							
Fe-2.5C-10S	L	L	86.45(143)	1.89(33)	9.99(153)	0.34(7)	98.67
Fe-4C-2S	Fe+	Fe	98.66(37)	0.71(11)	0.04(1)	0.32(8)	99.73
	Fe ₃ C+L	Fe ₃ C	92.00(43)	6.23(6)	0.01(1)	0.27(10)	98.51
		L	90.01(262)	1.54(112)	6.22(301)	0.42(12)	98.19
Fe-4C-14S	Fe ₇ C ₃	Fe ₇ C ₃	88.82(43)	8.19(12)	0.03(1)	0.19(8)	97.23
	+Dia+L	L	78.11(141)	2.57(147)	17.51(140)	0.42(10)	98.61
Fe-6C-2S	L	L	91.50(89)	6.24(60)	2.58(129)	0.17(20)	100.49
15 GPa, 1900 K							
Fe-6C-2S	L	L	90.58(58)	5.36(64)	1.57(159)	0.23(32)	97.74
Fe-5C-12S	Dia+L	L	82.28(97)	2.41(43)	16.60(126)	0.11(8)	101.39

^a A solid phase is expected on the basis of mass balance but is not observed on the polished surface.

^b The grain sizes of the Fe₇C₃ phase are too small to be analyzed.

^c The degree of melting is too small to produce a quenched phase that can be analyzed.

^d C content below detection limit is marked with ‘-’.

runs, extending across the entire Fe-Fe₃C-FeS ternary diagram. The degree of melting is clearly correlated with the S bulk concentration. The liquidus surface steadily expanded from 1300 K to 1700 K, with the 3-phase regions located far from the Fe corner drastically shrinking until they are fully replaced by 2-phase areas or solely liquid, similar to the evolution reported for the Fe-C-Si system (Miozzi et al., 2022). Notably, the liquidus on ‘Gr+L’ side evolves only mildly with temperature. We attribute this behavior to the low carbon solubility in S-rich liquid up to 2273 K (Corgne et al., 2008; Zhang et al., 2018). Additionally, no immiscibility was observed in the fully molten samples, in contrast to observations at lower pressures (Corgne et al., 2008).

It should be noted that, based on the phase rule, at fixed *P-T* conditions, the liquid in each 3-phase-assemblage is unique (Fe+Fe₃C+L, FeS+graphite+L, etc.). However, achieving chemical equilibrium in these 3-phase systems proved extremely challenging, even after dedicating 4 h to slow cooling from 1900 K to the target temperature and annealing. The deviations in the liquid composition due to quasi-equilibrium conditions (e.g., the liquid coexisting with FeS and graphite at 5 GPa and 1300 K), along with the scattering in the EPMA results caused by quench textures, introduce significant uncertainties in defining the boundaries of the 3-phase domains. In contrast, the 2-phase systems appear to have rapidly reached equilibrium, as evidenced by the clear trend in the liquid compositions, which define the liquidus curves. The curvature of the liquidus on the Fe-rich and C-rich sides is consistent with the non-ideality of the liquid chemical potential when both C and S are incorporated simultaneously (Zhao et al., 2023).

Compared to 5 GPa, the negative slope of the Fe-S eutectic melting temperature with respect to pressure (Morard et al., 2007) results in an even greater degree of melting on the C-depleted side of the Fe-C-S system at 15 GPa and 1300 K. However, this area does not extend as far toward the C-rich side as it does at 5 GPa, due to the increases in melting temperature caused by the high eutectic temperature of Fe-C alloys. The 3-phase region diminishes with increasing temperature and nearly disappears at 1900 K, remaining confined to a very small area near the C-rich corner. The stabilization of the more C-rich phase, Fe₇C₃, adds complexity to the phase diagram, suggesting a distinct crystallization pathway for the planetary cores of larger bodies. The evolution of liquidus with temperature is illustrated in the Cartesian plane in

Supplementary materials Figure S3, along with the experimentally determined composition of the liquidus.

For comparison, literature data at 5 GPa, spanning temperatures from 1473 K to 1623 K (Deng et al. 2013), are plotted in our ternary diagram at 5 GPa and 1500 K (crosses in the second graph from the top on the left). The liquid compositions reported in Deng et al. (2013) are anomalously carbon-depleted compared to our experimental results under similar conditions, both for liquids coexisting with Fe+Fe₃C (yellow cross) and with Fe₃C alone (brown cross). Similar carbon-depleted liquid compositions were observed during our preliminary experiments, where the samples were directly heated to the target temperature and annealed for about 1 hour. However, we recognized that achieving chemical equilibrium in partially-molten samples was challenging under these conditions. When three phases coexist (e.g., Fe+Fe₃C+L), the initial mixture of Fe and graphite powder tend to form Fe₃C inclusions within large Fe grains prior to melting. Upon heating, a Fe-S liquid of eutectic composition forms, but equilibrium between this liquid and large Fe₃C grains is kinetically hindered. Consequently, the liquid remains carbon-poor, failing to reach equilibrium at these temperatures within 1 hour annealing time. Additionally, in the Fe+L phase field, one of the liquid compositions reported by Deng et al. (2013) exhibits a significantly higher S content, approaching the composition of Fe-S eutectic (Buono and Walker, 2011).

To mitigate the risk of disequilibrium, we adopted the experimental protocol described in Section 2: all samples were first heated to 1900 K to ensure extensive melting, then slowly cooled over 3 h to the target temperature, followed by a 1-hour annealing step prior to quenching. While this protocol was designed to promote equilibrium and minimize kinetic barriers to phase homogenization, defining a generalized compositional uncertainty for all the phase boundaries remains challenging. In particular, the degree of equilibrium varies with the complexity of the phase assemblages. To ensure a consistent reconstruction of the phase diagram and its evolution with temperature, we relied not only on the liquid composition of the run products, but also on guiding principles. Specifically, three-phase regions should shrink and evolve into two-phase regions, and two-phase regions should evolve into single-phase (L) regions with increasing temperature. By combining these principles with literature data on binary phase assemblages, we

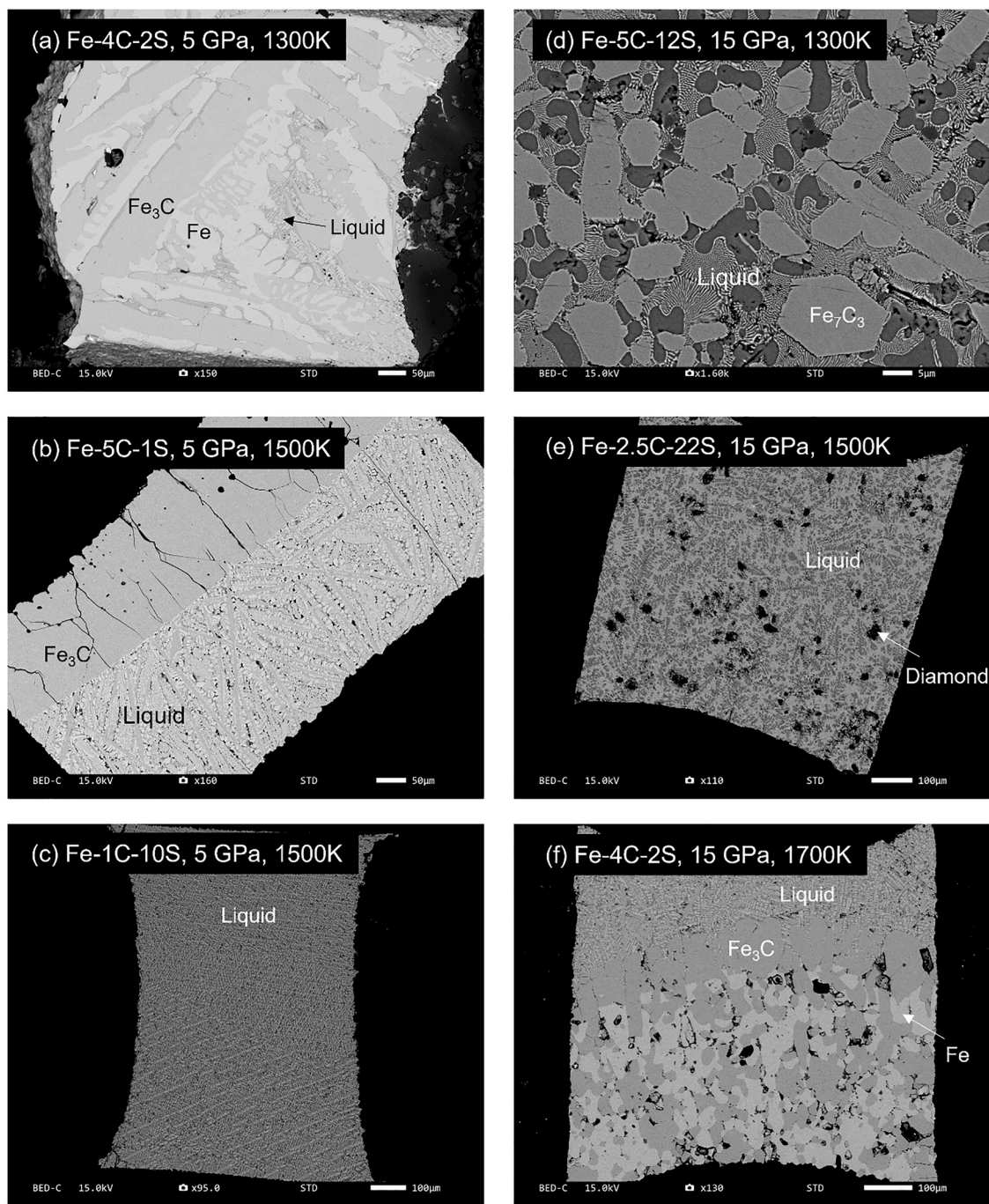


Fig. 1. Back-scattered electrons images illustrating the representative textures of the recovered samples. Left and right columns show samples recovered from 5 to 15 GPa experiments, respectively. During quenching, the liquid phase typically undergoes phase segregation (e.g., forming a moderate S-rich phase in lamellar shape and a more S-rich phase appearing darker, panel d). This behavior arises due to the incongruent melting of the system. Pores, commonly observed in polished samples quenched from C-rich liquids (panels d and e), are interpreted as detached graphite nanograins (for 5 GPa runs) or diamond nanograins (for 15 GPa runs). This interpretation is based on mass balance considerations and the high-pressure phase diagram of the Fe-C system. The dark regions in panel f are voids associated with detached grains. These voids result from the poor bonding between Fe and Fe₃C after quenching, which is attributed to their divergent thermal expansivities.

were able to construct a well-constrained ternary diagram from our experimental results.

4. Discussion

4.1. The phase assemblages of a partially-molten Moon's core

For planetary bodies with a partially-molten core, as likely the case of the Moon, the composition of the liquid outer core and that of the

coexisting solid inner core are intrinsically linked. The core composition is typically constrained through either geochemical or geophysical approaches. In the geochemical approach, high-temperature and high-pressure metal-silicate partitioning experiments serve as the foundation for modeling the early differentiation of the terrestrial planetary bodies (e.g., [Steenstra et al., 2016; 2017](#)). In the geophysical approach, the thermos-elastic properties of candidate materials are used to interpret seismological and/or geodetic observations (e.g., [Weber et al., 2011; Garcia et al., 2019; Viswanathan et al., 2019; Briaud et al., 2023](#)).

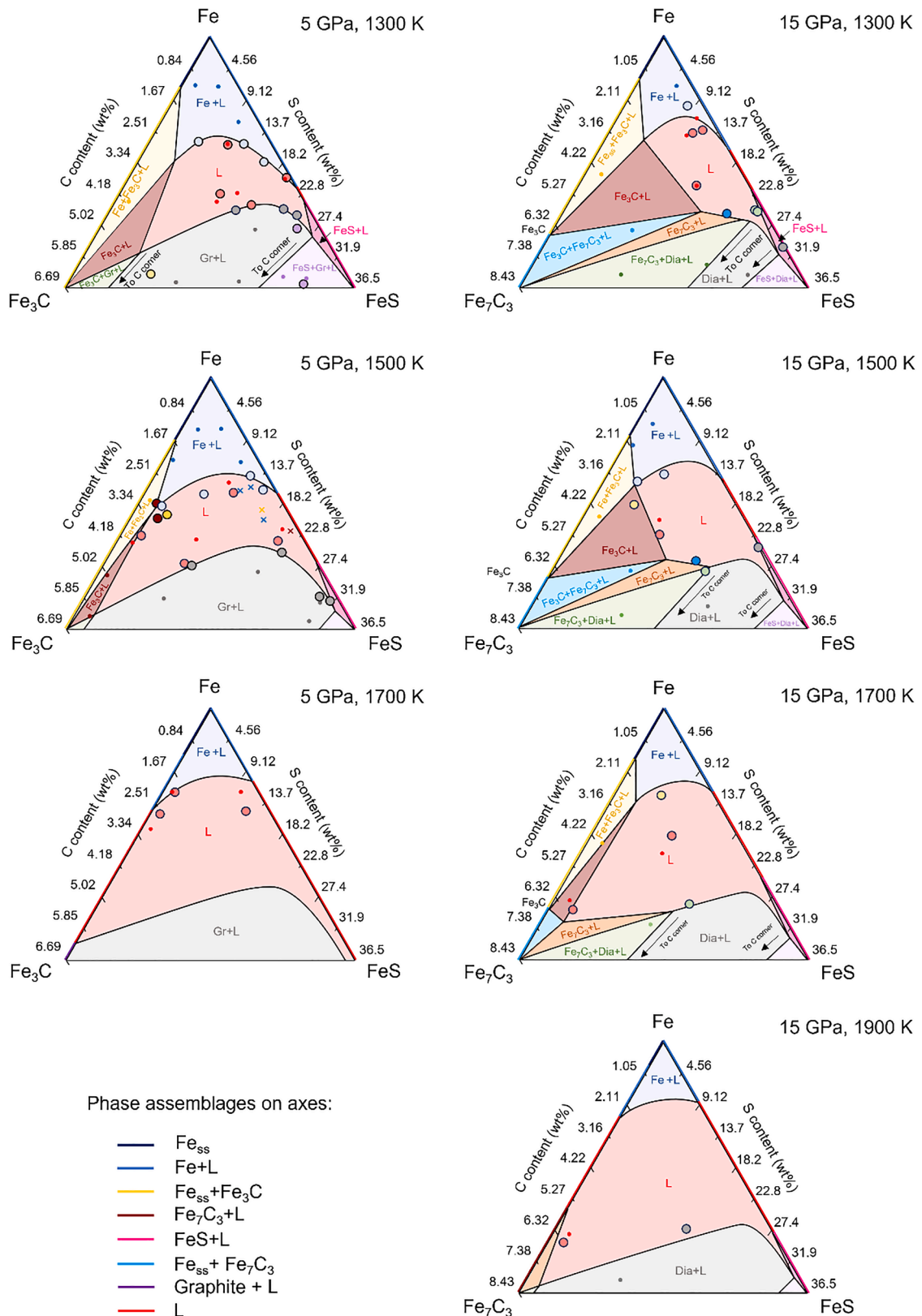


Fig. 2. Phase diagram of the Fe-C-S system at 5 (left) and 15 GPa (right). Small red circles represent the starting compositions and liquid compositions in the products, respectively. For comparison, data at 5 GPa from 1473 K to 1623 K from [Deng et al. \(2013\)](#) are plotted as crosses in the phase diagram at 5 GPa and 1500 K (second from the top on the left). The color of all the symbols follows that of the ternary zones. Phase boundaries were determined using the starting composition, liquid compositions in the products, and binary phase assemblages of binary alloys along the axes (Fe-FeS: [Buono and Walker, 2011](#); Fe-Fe₃C-Fe₇C₃: [Fei and Brosh, 2014](#)). The arrows “To C corner” indicate that “Gr/dia+L” areas originate from the C corner of the Fe-C-S phase diagram, of which the present diagram is a section. Abbreviations: Gr: graphite; Dia: diamond; L: liquid.

Within the framework of the geophysical approach, current structural and compositional models of the lunar core are primarily based on laboratory-measured physical properties of phases in the simple eutectic Fe-S binary system (Jing et al., 2014; Antonangeli et al., 2015; Morard et al., 2018; Nishida et al., 2020). However, the likely presence of multiple light elements renders the crystallization paths highly dependent on bulk compositions and extremely complex to predict without tight constraints on the relevant phase diagrams. Without a clear understanding of the possible crystallization paths, even well-constrained physical properties of Fe-C-S ternary liquids (Zhao et al., 2023) have limited applicability, essentially restricting their use to the case of a homogeneous liquid core.

Although some studies suggest the Moon may have a solid inner core (e.g. Briaud et al., 2023), its presence remains uncertain due to limited seismic data. Both models with and without a solid inner core can explain geodetic, geochemical, and tidal observations (e.g. Garcia et al., 2019; Viswanathan et al., 2019; Kuskov et al., 2021). Assuming an inner core exists, the ternary phase diagram for the Fe – Fe₃C – FeS system, established here under *P-T* conditions relevant to the Moon's interior, offer a robust framework for identifying stable phase assemblages and constraining the composition of the liquid outer core. Fig. 3 shows the temperature-dependent evolution (1300–1700 K) of the liquid composition along the liquidus (raw experimental data are provided in Supplementary Materials Figure S3).

The expected temperature range for the Moon's core spans 1300 K to 2100 K, depending on the model, with most estimates placing the core-mantle boundary temperature above 1650 K (Dyal et al., 1974; Kuskov and Kronrod, 1998; Khan et al., 2006; Antonangeli et al., 2015). For a partially-molten lunar core with an inner-core boundary at 1700 K, the phase diagram reveals that the only phase coexisting with the liquid, and thus the sole candidate for the inner core, is iron, likely containing minor carbon. While a 'graphite + liquid' phase assemblage could theoretically stabilize if the bulk C content exceeds its solubility limit, this scenario is

unlikely for the inner core. Indeed, graphite, being lighter, would float to form a layer at the core-mantle boundary. Furthermore, no seismic or geodetic evidence support the presence of such a layer.

By integrating the Fe-C-S density model derived from combined X-ray diffraction and absorption measurements (Zhao et al., 2023), the density of the liquid outer core coexisting with an Fe-rich inner core is constrained to 6600–7300 kg/m³ (as determined by the intersections of density contours and liquidus lines). This estimate significantly exceeds the density proposed by Briaud et al. (2023) (~5000 kg/m³) and aligns closely with the upper bound (7000 kg/m³) suggested by Kuskov et al. (2021). In this case, the sulfur content in the outer core is likely below 10 wt % S, and the entire core is relatively depleted in carbon.

Assuming a core at lower temperature expands the range of possible inner core compositions. At 1500 K, a core with a bulk composition in the 'Fe₃C+L' region (Fig. 2) would crystallize an Fe₃C inner core, resulting in an outer core enriched in C but relatively depleted in S, with a density bounded between 7000 and 7200 kg/m³. Although its occurrence is very limited in the compositional space, it is also theoretically possible to crystallize a two-phase inner core composed of both Fe and Fe₃C. In this scenario, the outer core density would be very close to 7200 kg/m³. For a more carbon-depleted bulk composition, an Fe inner core would crystallize, with the liquid outer core density ranging from 6200 to 7200 kg/m³. This estimate is in good agreement with the model by Kuskov et al. (2021) (6200–7000 kg/m³) and higher than the model by Briaud et al. (2023) (~5000 kg/m³). Notably, at 1500 K, the 'Fe + L', 'Fe + Fe₃C + L', and 'Fe₃C + L' phase assemblages all converge to the same upper density limit for the liquid: 7200 kg/m³. Conversely, if the bulk lunar core is S-rich, and thus C-poor due to the limited solubility of C in S-rich liquid Fe-alloys (Corgne et al., 2008; Zhang et al., 2018), an FeS inner core would crystallize. The resulting Fe-C-S liquid outer core would have a density ranging from 4900 to 5300 kg/m³. This range is significantly lower than the Kuskov et al. (2021) model but falls within the range proposed by Briaud et al. (2023) (~5000 kg/m³), although

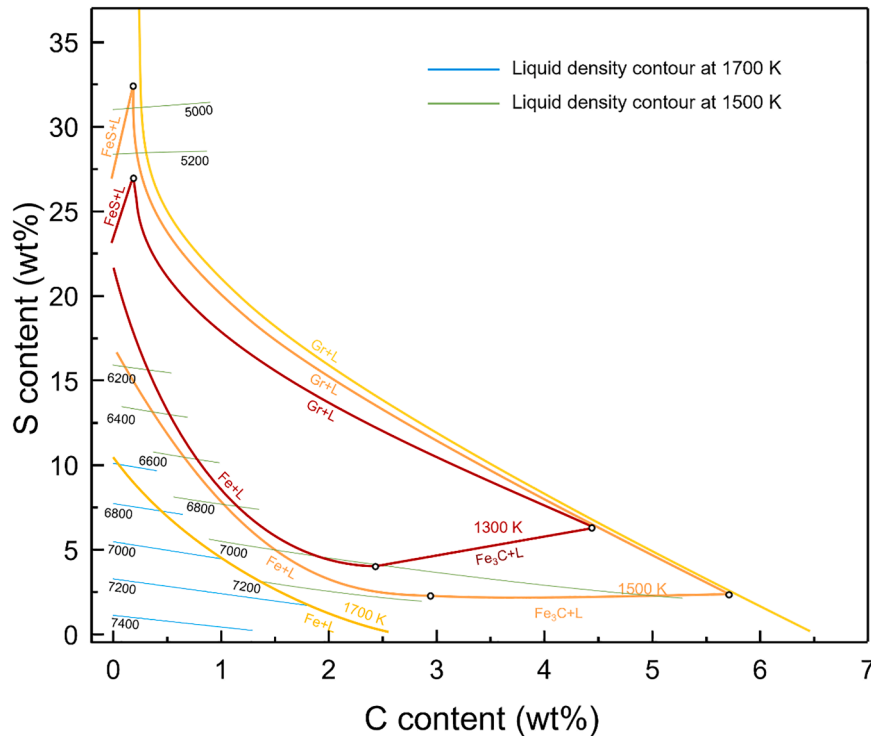


Fig. 3. Sulfur and carbon content in the ternary Fe-C-S liquid phase at liquidus, at 5 GPa and temperatures of 1300 K (red lines), 1500 K (orange lines), and 1700 K (yellow lines). The diagram also indicates the different phase assemblages along the liquidus within the Fe-FeS-Fe₃C domain. Open circles mark the inflection points between these phase assemblages. Density contours for Fe-C-S liquids are shown as blue lines (1700 K) and green lines (1500 K), modelled after Zhao et al. (2023). The numbers adjacent to the contours represent the density in kg/m³.

their model had an inner core density of $\sim 7800 \text{ kg/m}^3$, consistent with fcc-Fe under lunar core conditions rather than FeS. It is important to note that this crystallization scenario requires a bulk sulfur content exceeding 27 wt %, which is considerably higher than the estimates from geochemical studies (e.g. Steenstra et al., 2016; 2017).

The scenario for an even colder core, at approximately 1300 K, is qualitatively similar to that described for 1500 K. However, the compositional spaces for an Fe_3C inner core (including the potential formation of a graphitic layer at the core-mantle boundary) are slightly expanded. Similarly, the compositional range for a two-phase inner core, composed of both Fe and Fe_3C , is also broader at this lower temperature.

4.2. The phase assemblages of a partially-molten Mercury's core

Geodetic data and magnetic observations from the MESSENGER mission have independently constrained the radius of Mercury's liquid outer core to approximately 2000 km (Genova et al., 2019; Wardinski et al., 2019 and 2021). While the existence of a solid inner core is widely assumed, its size remains poorly constrained, with estimates ranging from 0.3 to 0.7 of the total core, depending on the model (Genova et al., 2019; Dumberry and Rivoldini, 2015; Wardinski et al., 2021; Davies et al., 2024). Most previous studies have assumed an Fe-FeS binary system to discuss the crystallization regime and outer core composition, according to which the inner core is composed of pure iron (Hauck et al., 2013; Dumberry and Rivoldini, 2015). Recently, alternative scenarios based on the Fe-FeSi phase diagram have been proposed (Edmund et al., 2022). These include a layered core structure, with an innermost fcc phase and an outer bcc shell for Si-poor models, as well as the formation of a solid B2 phase that, being less dense than the corresponding liquid, would rise and melt, driving convection without a solid inner core in Si-rich models. However, this work did not extensively address properties of the outer core, which are closely linked to its sulfur content.

More generally, an 'iron snow' crystallization regime, which is

strongly correlated with inner core growth, is a widely invoked mechanism to sustain the dynamo in small to mid-sized terrestrial planets and moons (e.g., Dumberry and Rivoldini, 2015; Breuer et al., 2015), which in turn is considered responsible for magnetic field generation (Cao et al., 2014). For 'iron snow' to occur over an extended period, the snowing iron must coexist with the surrounding outer core over a broad compositional field. Our phase diagram provides insights into the composition and density of the outer core under these constraints.

Thermal evolution models suggest that temperatures at Mercury's core-mantle boundary range from 1650 to 2050 K (e.g., Davies et al., 2024), with the upper range favored for dynamo generation. At a temperature of 1900 K, the phase diagram indicates that a liquid coexisting with Fe contains less than $\sim 9 \text{ wt } \% \text{ S}$ and $2.6 \text{ wt } \% \text{ C}$ (Fig. 4). Using the density model from Zhao et al. (2023), the density of the liquid outer core is predicted to be between 7300 and 7900 kg/m^3 . This estimate is 1–10 % higher than previous assessments of the liquid density just below the core-mantle boundary (7211 kg/m^3), which assumed a bulk composition on the S-poor side of the Fe-S binary system (Hauck et al., 2013). The higher density indicated in this study primarily results from variations in S content and improved accuracy of the equation of state. If Mercury's core has a C-rich composition, an alternative crystallization regime involving the ' Fe_7C_3 snow' could occur. Similar to the "Fe snow" scenario, this regime could sustain compositional and thermal-driven core convection, thereby supporting the dynamo. However, due to the lack of a suitable equation of state for C-rich ternary liquid (with C content $> 6.69 \text{ wt } \%$), the density cannot be constrained. Generally, C content in Mercury's core remains contentious. Xu et al. (2024) postulated that the core is C-saturated based on crustal graphite abundance. In contrast other studies suggest that most C either exsolved as graphite or degassed as CH_4 and CO_2 during the magma ocean stage (Peplowski et al., 2016; Li et al., 2017).

With an inner core composed of Fe or Fe_7C_3 , it is expected that, as the core cools over time, the liquid outer core will gradually become enriched in S while the inner core grows. Additionally, the inner core

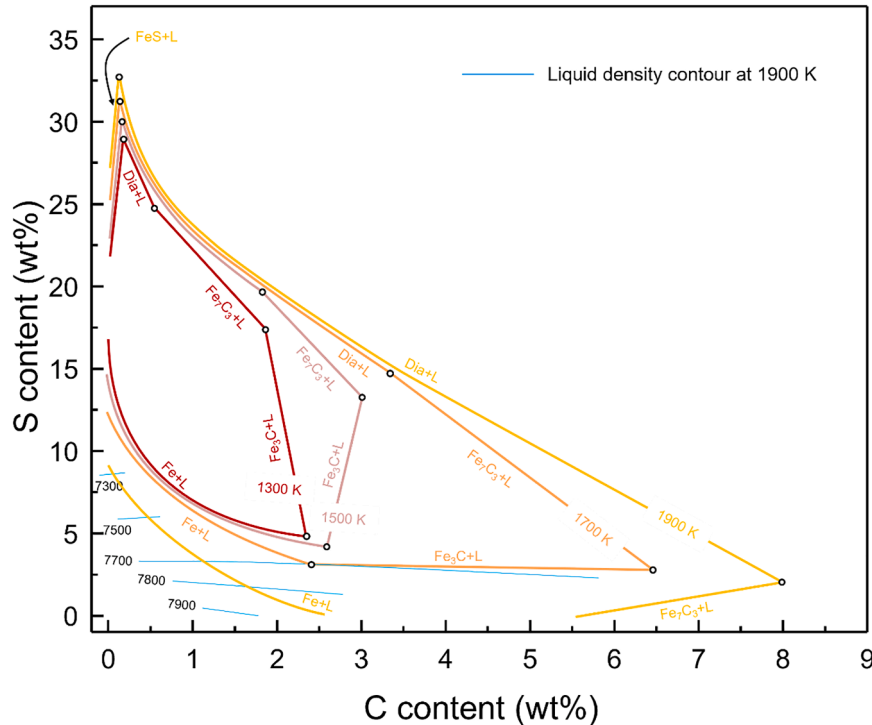


Fig. 4. Sulfur and carbon content in the ternary Fe-C-S liquid phase at liquidus, at 15 GPa and temperatures of 1300 K (red lines), 1500 K (pink lines), 1700 K (orange lines) and 1900 K (yellow lines). The diagram also indicates the different phase assemblages along the liquidus within the Fe-FeS- Fe_7C_3 domain. Open circles mark the inflection points between these phase assemblages. Density contours for Fe-C-S liquids at 1900 K extrapolated after Zhao et al. (2023), are shown as blue lines. The numbers adjacent to the contours represent the density in kg/m^3 .

could potentially develop multiple layers due to the complexity of the ternary phase diagram. The large pressure and temperature range within a large core may further increase this probability. The possible phases comprising the inner core include Fe, Fe_3C , and Fe_7C_3 , depending on the initial C budget in the early differentiated core and how the core geotherm intersect the ternary phase diagram over geological time.

4.3. An inner-core settling model for Mercury

The settling rates of crystals “snowing” through the liquid core directly affect the convective efficiency within Mercury’s core, with significant implications for the generation and sustainability of a global

magnetic field. Interestingly, analysis of the quenched samples reveals markedly different settling rates for Fe and Fe_7C_3 in liquid Fe-C-S alloys (Fig. 1d and f). To explore this further, we modeled the crystal residence time of Fe and Fe_7C_3 in a 100-km thick layer at 15 GPa as a function of liquid density, using the hindered-settling framework proposed by Faroughi and Huber (2015). We note that the precise depth at which “snow” formation begins remains highly uncertain. Additionally, “snow” originating at greater depths could potentially re-dissolve into the outer core at shallower depths. Our model at 15 GPa provides insight into the contrasting behavior of Fe and Fe_7C_3 . The results are presented in Fig. 5 (see Supplementary Material for the detailed methodology).

Both the particle size and the crystal fraction have a large impact on

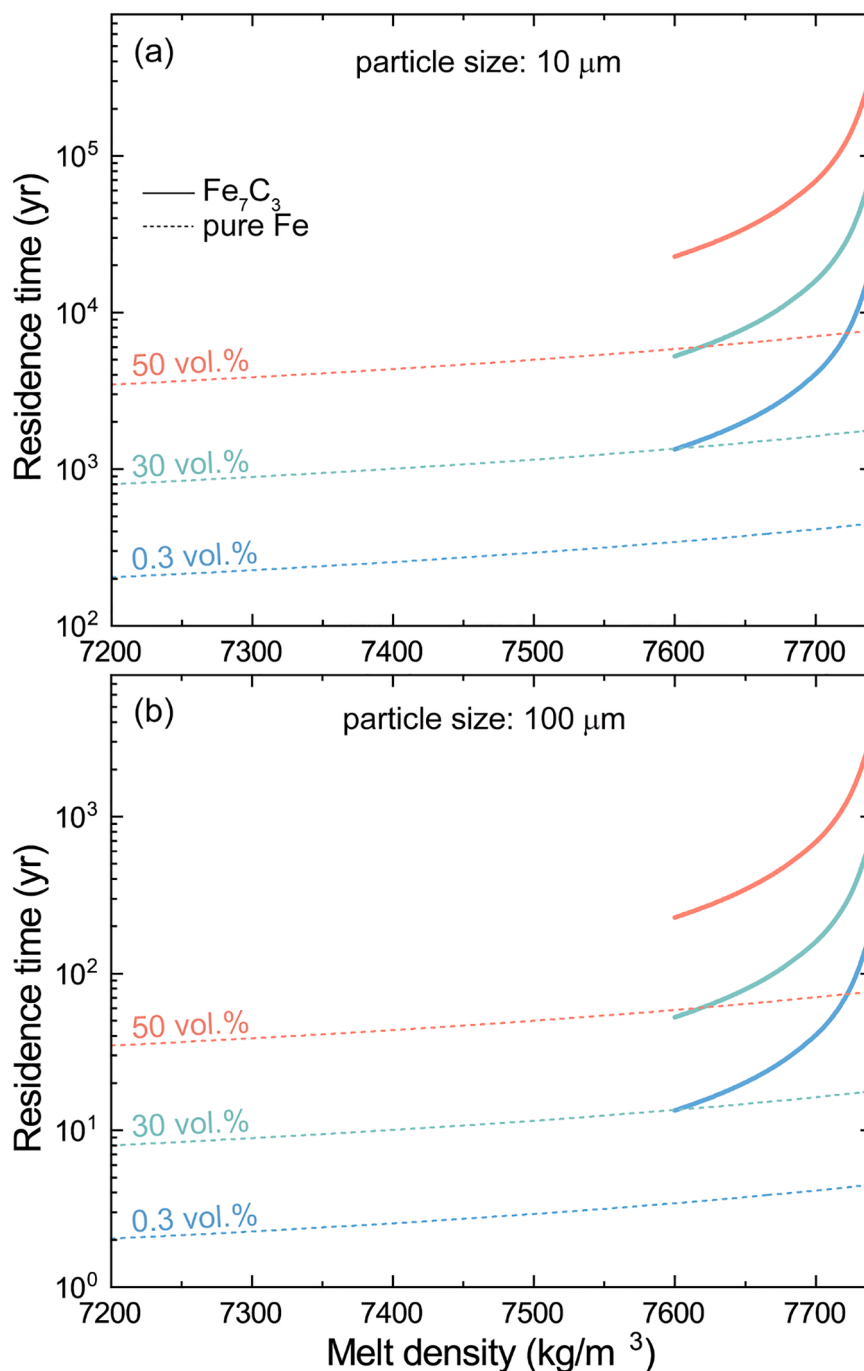


Fig. 5. Residence time of Fe (dashed lines) and Fe_7C_3 (solid lines) crystals as a function of the density of the coexisting liquid, shown for two different particle size (upper and lower panel) and three crystal fractions. The intersections of the density contours at 15 GPa and 1900 K with the liquidus lines along the “Fe+L” and “ Fe_7C_3 +L” fields indicate a minimum liquid in coexistence with Fe and Fe_7C_3 of 7200 and 7600 kg/m^3 , respectively.

the residence time, which increases by approximately one order of magnitude when the crystal fraction rises from 0.3 vol % to 50 vol %, and by roughly two orders of magnitude when the particle size increases by a factor of ten. The effect of density contrast becomes particularly significant when the difference in densities between the crystal and the liquid is small, as is the case for Fe_7C_3 . The reduced density contrast between Fe_7C_3 ($\sim 7.75 \text{ g/cm}^3$ at 15 GPa and 1900 K; Nakajima et al., 2011) and the surrounding Fe-C-S liquid results in a residence time for 10- μm grains as long as 10^5 years. Moreover, considering the potential presence of silicon in Mercury's core (e.g. Chabot et al., 2014) and its high solubility in solid Fe (Edmund et al., 2022), the simultaneous crystallization of Fe_7C_3 and Fe-Si solid solution can be anticipated, especially for high bulk C content (Miozzi et al., 2022). This scenario is supported by the comparable liquidus of Fe- Fe_7C_3 on the C-rich side (Fei and Brosh, 2014) and that of Fe-FeSi (Edmund et al., 2022). Given the similar densities of Fe_7C_3 and Fe-Si solid alloys ($\sim 7.71 \text{ g/cm}^3$ for Fe-9 wt %Si at 15 GPa and 1900 K; Fischer et al., 2014; and $\sim 7.7 \text{ g/cm}^3$ for Fe-5wt %Si at the same condition, Edmund et al., 2019), the suspension of crystallized grains of Fe_7C_3 and Fe-Si solid solution could potentially lead, at least locally, to a mush-like outer core. In such a scenario, the generated dynamo is qualitatively expected to be significantly weaker than that produced in a 'Fe snow' model.

5. Conclusions

The melting relation and phase assemblage of the Fe-C-S ternary system were determined at 5 and 15 GPa up to 1900 K. These findings were applied to model the cooling processes of the Moon's and Mercury's cores. In a ternary Fe-C-S metallic core, Fe and Fe_3C are the most plausible candidates for the Moon's inner core, while Fe and Fe_7C_3 are favored for Mercury's inner core at 1900 K, with the liquid outer core composed of Fe-C-S melts. For both bodies, a layered inner core structure, comprising both Fe and carbide phases, is theoretically possible. For Mercury, our crystal settling model indicates that 'Fe snow' settles more efficiently than ' Fe_7C_3 snow', primarily due to the higher density contrast between the solid and liquid phases, although particle size and melt fraction also influence this process. In a C-enriched core, the lower settling rate of Fe_7C_3 could result at least locally, in a mush-like outer core.

Future work should focus on determining the density of C-rich ternary Fe-C-S liquids and extending analyses to Fe-C-S-Si quaternary compositions. Such studies are particularly timely, given the high-precision measurements of Mercury's topography, gravity, and magnetic field anticipated from the BepiColombo mission (Genova et al., 2021). These advancements deepen our understanding of Mercury's internal structure and offer broader insights into the differentiation and evolution of small telluric bodies under reducing conditions.

CRediT authorship contribution statement

Bin Zhao: Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Jintao Zhu:** Writing – review & editing, Investigation, Formal analysis. **Daniele Antonangeli:** Writing – review & editing, Validation, Investigation, Funding acquisition. **Guillaume Morard:** Writing – review & editing, Validation, Investigation. **Qi Chen:** Writing – review & editing, Visualization, Validation, Methodology, Investigation, Funding acquisition, Formal analysis. **Takashi Yoshino:** Writing – review & editing, Validation, Formal analysis.

Declaration of competing interest

The authors declare that there is no known competing interest that could affect the work reported in this manuscript.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.epsl.2026.120087.

Data availability

All data have been published in an online repository (declared in the main text)

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