

Supporting Information

Magnetic collapse and low conductivity of Fe₃N in the interior of Earth and other terrestrial planets

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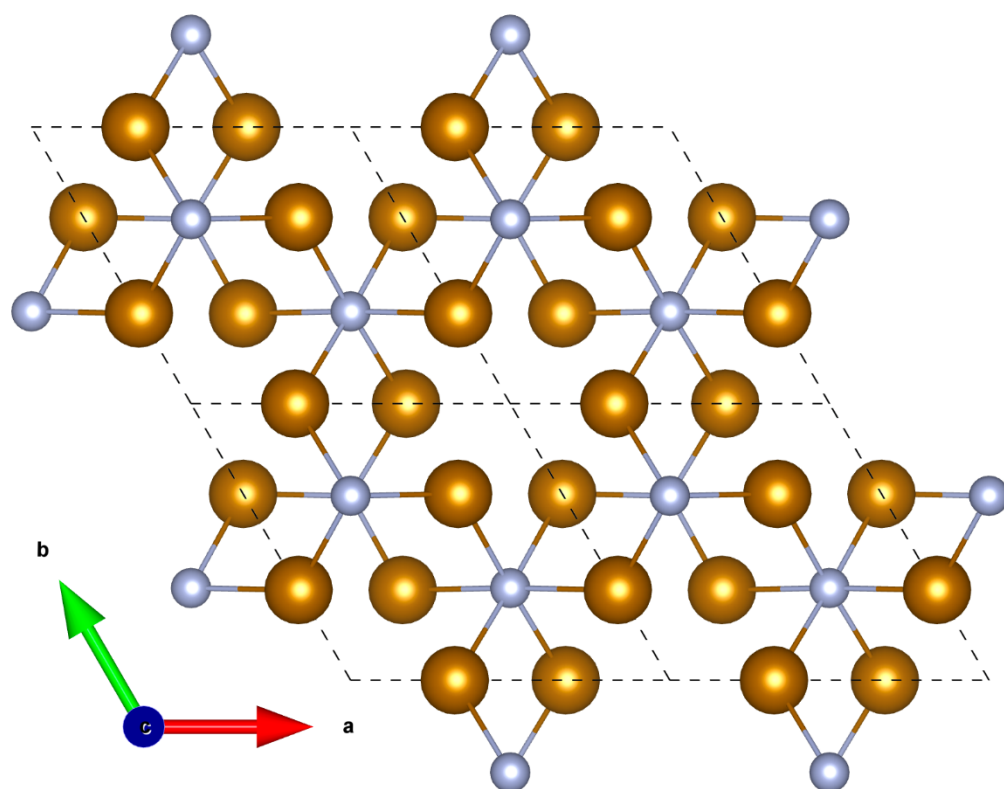
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Figure S1. The crystal structure of Fe₃N at ambient conditions. It has a hexagonal structure with the space group *P*312.

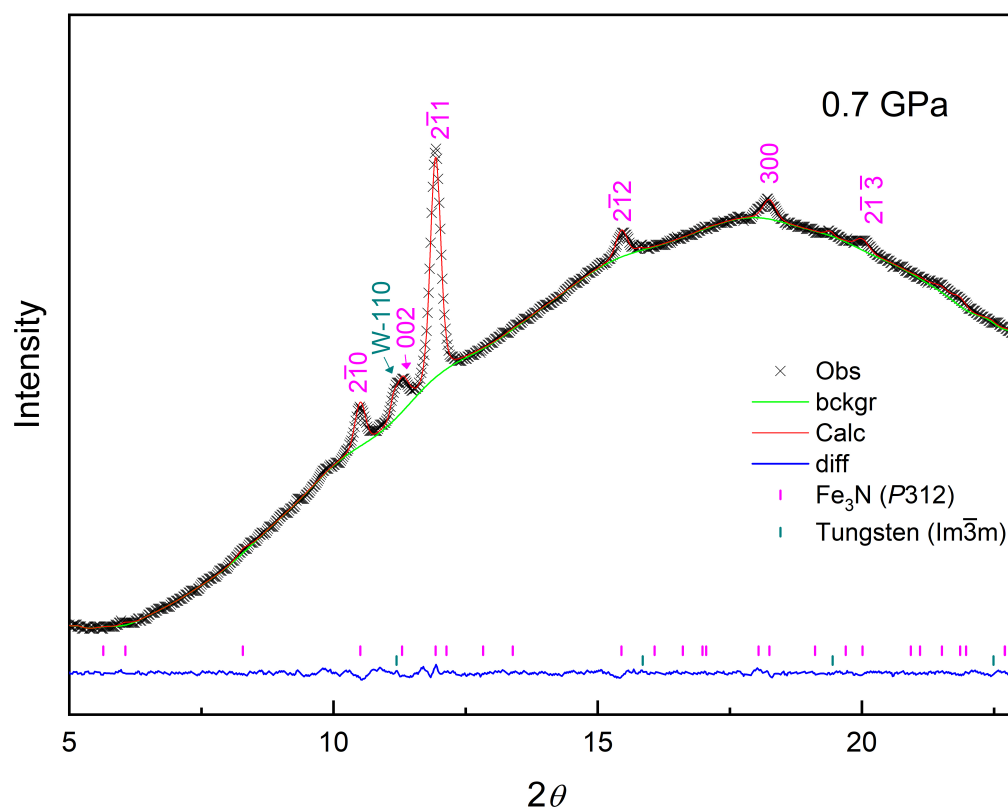


Figure S2. Rietveld refinement analyses of Fe₃N at 0.7 GPa and room temperature ($R_I =$
30 0.0041 and $R_2 = 0.0027$). The wavelength (λ) is 0.4340 Å.

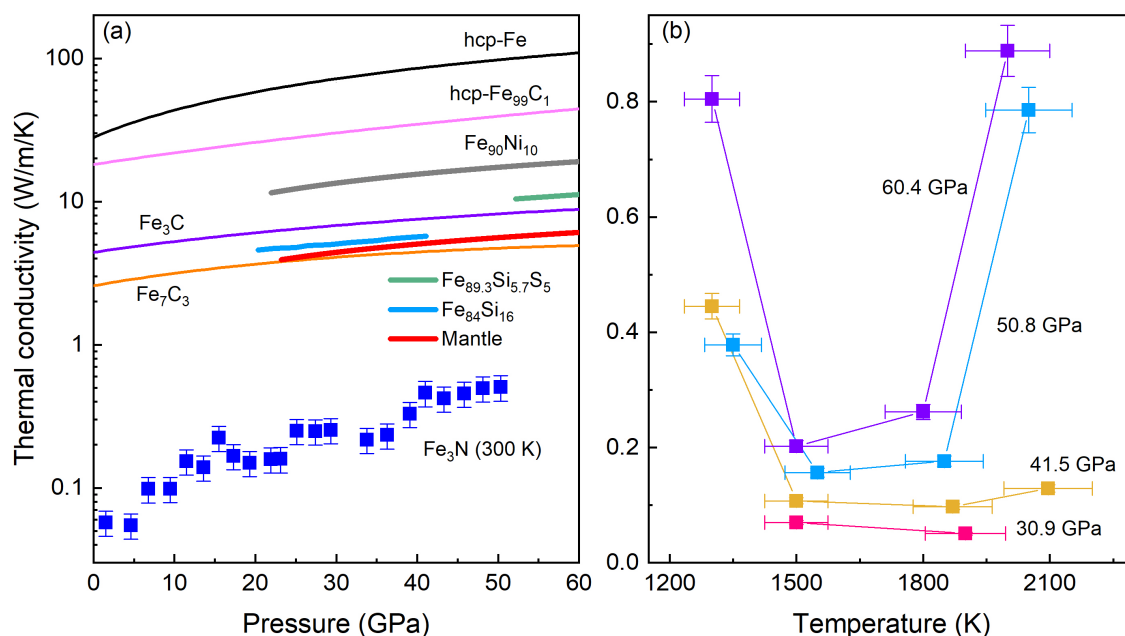
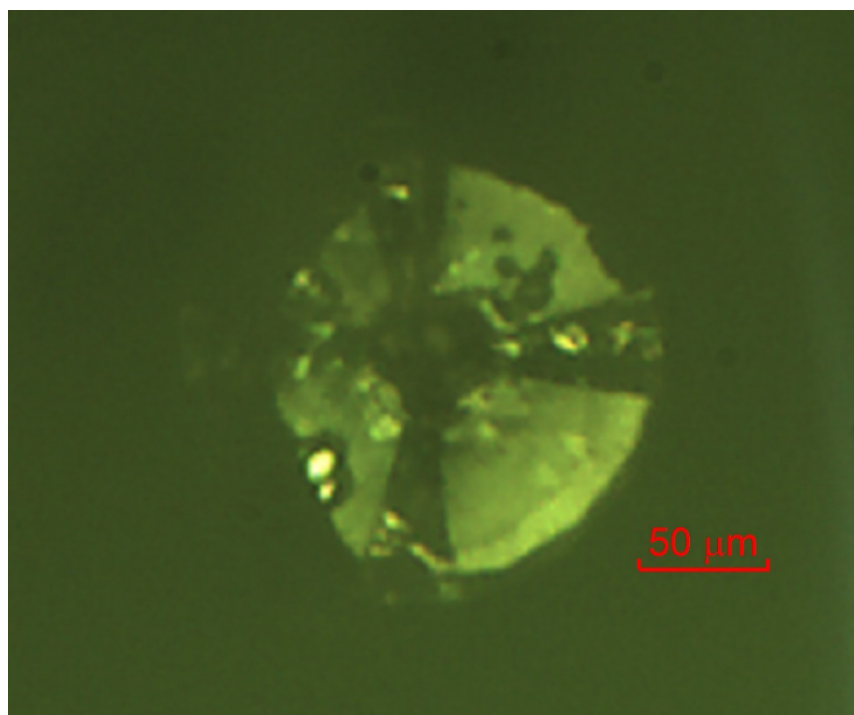


Figure S3. (a) The pressure-dependent TC of Fe₃N compared with other iron alloys at room temperature. Squares: Fe₃N, this study; Black, magenta, purple, and orange curves: hcp-Fe, hcp-Fe₉₉C₁, Fe₃C, and Fe₇C₃, respectively (Zhang et al., 2018); Gray curve: Fe₉₀Ni₁₀ (Gomi & Hirose, 2015); Green and blue curves: Fe_{89.3}Si_{5.7}S₅ and Fe₈₄Si₁₆, respectively (Seagle et al., 2013); Red curve: pyrolytic mantle at 2000 K (Hsieh et al., 2018). (b) The TC of Fe₃N under high pressure and temperature conditions. The TC data were deduced from the EC values by using the Wiedemann-Franz law. The error bar is derived from the EC.



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Figure S4. Optical microscopic image of Fe₃N after laser heating in a diamond-anvil cell. The sample was sandwiched between two NaCl layers as the pressure medium and thermal insulation, together with the intact connection of four probes. Cubic boron nitride (cBN) insert was used as electrical insulation. The laser spot is about 30 μm.

45 **Table SI.** Lattice parameters and atomic coordinates from structural refinement at 0.7 GPa and room temperature.

Space group		Lattice parameters (Å)			Atomic coordinates			
						<i>x</i>	<i>y</i>	<i>z</i>
Fe ₃ N	<i>P</i> 312	<i>a</i>	<i>b</i>	<i>c</i>	Fe	0.00	0.666(1)	0.25
		4.740(1)	4.740(1)	4.409(2)	N1	0.33(1)	0.666(1)	0.50
					N2	0.66(1)	0.333(1)	0.00

Table SII. Pressure-volume data of Fe₃N at 300 K.

P (GPa, ruby)	P (GPa, Au)	a (Å)	c (Å)	V (Å ³)	ρ (g/cm ³)
0.7		4.740(1)	4.409(2)	85.67(80)	7.04(70)
3.5		4.728(5)	4.364(4)	84.47(84)	7.13(71)
7.2		4.688(5)	4.338(4)	82.57(83)	7.30(73)
9.2		4.663(5)	4.328(4)	81.48(82)	7.40(74)
14.2	13.1(1)	4.613(5)	4.306(4)	79.35(79)	7.60(76)
16.3	17.6(2)	4.581(5)	4.275(4)	77.70(78)	7.76(78)
22.5	21.7(2)	4.549(5)	4.234(4)	75.89(76)	7.94(79)
24.4	25.6(3)	4.525(5)	4.207(4)	74.31(74)	8.11(81)
30.7	29.2(3)	4.490(4)	4.220(4)	73.68(74)	8.18(82)
34.2	33.1(3)	4.477(4)	4.204(4)	72.95(73)	8.26(83)
38.3	37.1(4)	4.457(4)	4.171(4)	71.74(72)	8.40(84)
42.1	40.9(4)	4.442(4)	4.171(4)	71.34(71)	8.45(85)
	42.4(4)	4.425(4)	4.167(4)	70.65(71)	8.53(85)
	44.1(4)	4.421(4)	4.157(4)	70.35(70)	8.57(86)
	46.8(5)	4.407(4)	4.155(4)	69.87(69)	8.63(86)
	49.8(5)	4.389(4)	4.164(4)	69.45(69)	8.68(87)
	52.3(5)	4.386(4)	4.160(4)	69.30(69)	8.71(87)

The number in parentheses is the uncertainty corresponding to the last digits of the quantity value.

Table SIII. EC and TC of Fe₃N at 300 K.

P (GPa)	Resistance (Ω)	Thickness (μm)	EC σ (S/m)	TC k (W/m/K)
0.5(2)	14.2(2)	48.3(96)	9.75(95)E+02	2.84(57)E-02
4.6(5)	12.8(2)	44.9(89)	1.16(23)E+03	4.01(81)E-02
6.8(7)	8.3(1)	42.7(84)	1.88(38)E+03	6.96(139)E-02
9.5(9)	13.8(3)	39.8(79)	1.21(24)E+03	4.69(94)E-02
11.5(11)	9.5(1)	38.0(76)	1.85(37)E+03	7.43(15)E-02
13.6(14)	10.3(2)	36.1(72)	1.80(36)E+03	7.41(15)E-02
15.5(16)	7.3(3)	34.3(68)	2.65(53)E+03	1.11(22)E-01
17.3(17)	8.1(2)	32.8(65)	2.50(50)E+03	1.07(21)E-01
21.9(22)	8.9(2)	29.0(58)	2.57(51)E+03	1.14(23)E-01
23.1(23)	8.8(2)	28.1(56)	2.67(53)E+03	1.20(24)E-01
25.1(25)	8.1(2)	26.6(53)	3.08(61)E+03	1.40(28)E-01
27.5(27)	13.3(5)	24.8(49)	1.99(39)E+03	9.17(18)E-02
30.6(31)	13.4(5)	22.8(45)	2.09(42)E+03	9.77(19)E-02
33.8(34)	10.1(3)	20.83(41)	3.16(63)E+03	1.50(31)E-01
36.3(36)	9.3(3)	19.3(38)	3.70(74)E+03	1.78(36)E-01
39.1(39)	9.9(3)	17.8(35)	3.75(75)E+03	1.82(36)E-01
41.1(41)	7.5(3)	16.9(33)	5.27(105)E+03	2.58(52)E-01
43.3(43)	8.5(2)	15.8(31)	4.92(98)E+03	2.43(48)E-01
45.8(46)	8.6(2)	14.8(29)	5.23(105)E+03	2.61(53)E-01
48.1(48)	7.8(1)	13.9(28)	6.09(92)E+03	3.06(61)E-01
50.3(50)	7.1(1)	13.1(26)	7.07(94)E+03	3.58(72)E-01

50 The number in parentheses is the uncertainty corresponding to the last digits of the quantity value.

Table SIV. EC and TC of Fe₃N under high P - T conditions.

Run#	P (GPa)	T (K)	Resistance (Ω)	Thickness (μm)	EC σ (S/m)	TC k (W/m/K)
1	30.9(12)	1500(75)	7.4(8)	23(5)	1.49(3)E+03	6.99(13)E-02
		1900(95)	8.8(6)		1.08(2)E+03	5.06(21)E-02
2	41.5(36)	1300(65)	0.9(1)	27(6)	9.07(18)E+03	4.45(9)E-01
		1500(75)	3.7(4)		2.19(4)E+03	1.07(2)E-01
		1870(94)	4.1(6)		1.98(4)E+03	9.72(19)E-02
		2096(105)	3.1(5)		2.63(5)E+03	1.29(3)E-01
3	50.8(52)	1350(68)	2.2(4)	15(4)	6.73(14)E+03	3.78(8)E-01
		1550(78)	5.3(1)		2.74(6)E+03	1.56(3)E-01
		1850(93)	4.2(3)		3.48(7)E+03	1.76(4)E-01
		2050(103)	0.9(4)		1.55(31)E+04	7.85(15)E-01
4	60.4(58)	1300(65)	1.3(3)	11(6)	1.55(3)E+04	8.05(16)E-01
		1500(75)	5.1(2)		3.88(8)E+03	2.02(4)E-01
		1800(90)	3.9(2)		5.03(10)E+03	2.62(5)E-01
		2000(100)	1.2(1)		1.71(5)E+04	8.88(17)E-01

The number in parentheses is the uncertainty corresponding to the last digits of the quantity value.