Supplementary

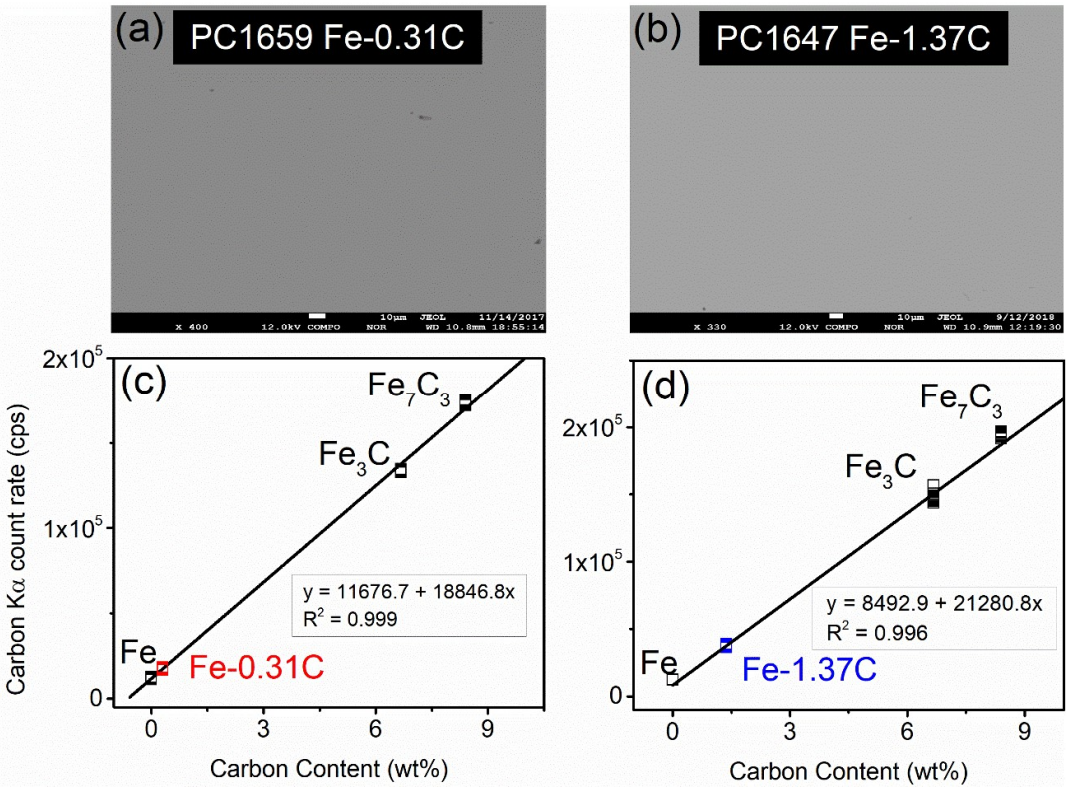

Figure S1. Carbon analysis for recovered Fe-C samples by electron microprobe. (**a**,**b**) Back scattered electron images for recovered samples from Run# PC1659 and PC1647. (**c**,**d**) Carbon count rates as a function of carbon content; count rates (counts per second) for each standard are average of more than 20 measurements made on randomly selected spots on each standard using an electron beam with 12 keV accelerating voltage, 30 nA current, and a diameter of 1 micron; Counts rates for each sample are average of more than 40 randomly selected spots under the same analytical conditions.

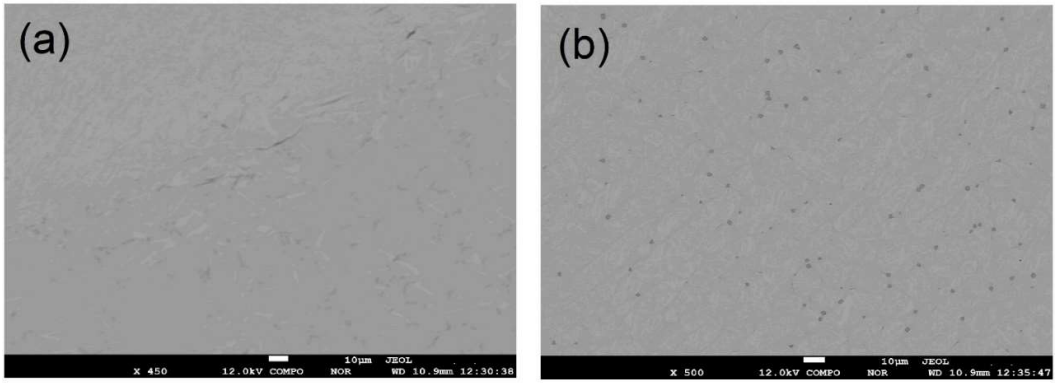

Figure S2. Back scattered electron images for unsuccessful synthesis runs. (**a**) inhomogeneous recovered sample due to the lack of enough heating time; (**b**) quenched texture from a melt product.

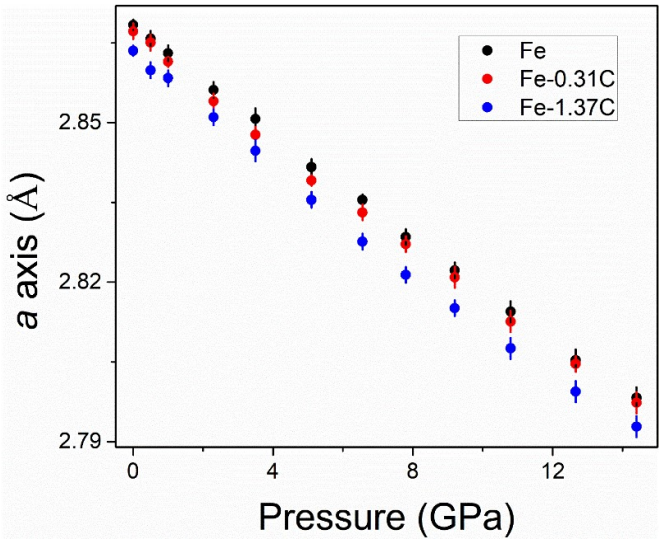

Figure S3. The length of lattice constant *a* as a function of pressure for Fe, Fe-0.31C, and Fe-1.37C.

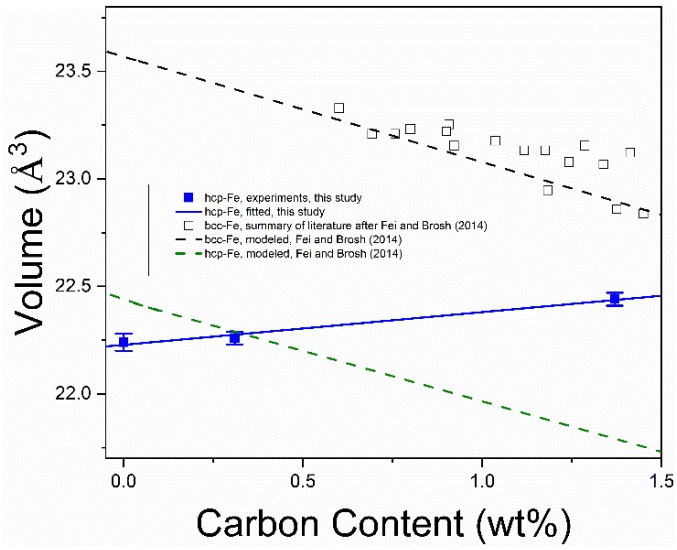

Figure S4. Unit cell volume of bcc- and hcp-Fe as a function of carbon content at ambient condition. Blue symbols are for hcp-Fe in this study; the open symbols are data from literature results that were summarized in Fei and Brosh (2014) [1]; black and green dash lines are linear fitting for bcc- and hcp-Fe data reported by Fei and Brosh (2014) [1].

Table S1. Compression data for pure-Fe, Fe-0.31C and Fe-1.37C in bct structure using Au as the pressure calibrant.

P_{Au} (GPa)	Fe	Fe-0.31C	Fe-1.37C
	a (Å)	*a* (Å)	*a* (Å)
0.5(1)	2.868(1)	2.867(2)	2.864(1)
1.0(1)	2.866(2)	2.865(2)	2.860(2)
2.3(1)	2.863(2)	2.862(1)	2.858(2)
3.5(2)	2.856(2)	2.854(2)	2.851(2)
5.1(2)	2.851(2)	2.848(2)	2.845(2)
6.6(1)	2.842(2)	2.839(1)	2.836(2)
7.8(2)	2.836(1)	2.833(2)	2.828(2)
9.2(3)	2.829(2)	2.827(2)	2.821(2)
10.8(2)	2.822(2)	2.821(2)	2.815(2)
12.7(3)	2.815(2)	2.813(2)	2.808(2)
14.4(2)	2.805(2)	2.805(2)	2.799(2)

Table S2. Compression data for pure-Fe, Fe-0.31C and Fe-1.37C in hcp phases using Ne as the pressure calibrant.

P_{Ne} (GPa)	a (Å)	Δa (Å)	c (Å)	Δc (Å)	V (Å^3)	Density (g/cm^3)
Compression data for Pure-Fe RUN#1						
16.5(2)	2.456	0.003	3.940	0.003	20.581	9.012
18.5(2)	2.450	0.003	3.932	0.005	20.439	9.074
19.9(3)	2.445	0.003	3.922	0.003	20.304	9.135
21.0(2)	2.440	0.004	3.915	0.004	20.185	9.188
22.4(3)	2.437	0.003	3.911	0.004	20.115	9.221
24.3(3)	2.433	0.003	3.902	0.004	20.003	9.272
27.0(2)	2.425	0.004	3.890	0.004	19.810	9.362
30.0(4)	2.419	0.003	3.878	0.004	19.652	9.438
31.7(4)	2.413	0.003	3.870	0.004	19.514	9.505
33.5(3)	2.408	0.004	3.860	0.005	19.383	9.569
35.5(3)	2.403	0.004	3.852	0.005	19.262	9.629
37.1(4)	2.399	0.003	3.847	0.003	19.173	9.673
38.5(3)	2.396	0.004	3.842	0.005	19.101	9.710
39.6(4)	2.394	0.004	3.837	0.005	19.044	9.739
41.2(4)	2.390	0.003	3.832	0.003	18.956	9.784
43.5(4)	2.387	0.003	3.826	0.003	18.879	9.824
Compression data for Pure-Fe RUN#2						
25.9 (2)	2.428	0.003	3.892	0.001	19.871	9.334
37.6(4)	2.398	0.001	3.845	0.003	19.148	9.686
49.8(4)	2.371	0.003	3.806	0.004	18.531	10.009
74.6(5)	2.329	0.004	3.738	0.004	17.559	10.557
86.9(7)	2.313	0.004	3.713	0.004	17.202	10.782
111.9(7)	2.282	0.003	3.656	0.004	16.486	11.250
117.1(7)	2.276	0.004	3.646	0.004	16.354	11.341
121.7(8)	2.27	0.003	3.636	0.004	16.227	11.430
126.1(9)	2.265	0.004	3.630	0.006	16.128	11.500
135.6(9)	2.258	0.005	3.614	0.001	15.956	11.624
Compression data for Fe-0.31C RUN#1						
16.2(2)	2.461	0.004	3.943	0.005	20.681	8.868
18.7(2)	2.453	0.003	3.934	0.004	20.500	8.946
19.8(3)	2.448	0.003	3.929	0.003	20.390	8.994
21.0(2)	2.445	0.003	3.922	0.004	20.304	9.032
22.2(3)	2.441	0.003	3.914	0.004	20.198	9.080
24.7(3)	2.435	0.003	3.904	0.004	20.046	9.149
27.2(2)	2.427	0.003	3.891	0.004	19.846	9.241
30.7(4)	2.419	0.003	3.878	0.004	19.652	9.332
32.4(4)	2.414	0.003	3.871	0.004	19.535	9.388
34.4(3)	2.410	0.003	3.863	0.004	19.430	9.438
36.4(4)	2.405	0.003	3.856	0.004	19.315	9.495
37.9(3)	2.401	0.003	3.848	0.003	19.210	9.546
39.6(4)	2.397	0.003	3.843	0.004	19.122	9.591
40.8(4)	2.394	0.003	3.839	0.004	19.054	9.625
42.3(4)	2.391	0.003	3.839	0.003	19.006	9.649
43.7(4)	2.388	0.003	3.829	0.004	18.909	9.698
Compression data for Fe-0.31C RUN#2						
25.9(2)	2.431	0.003	3.896	0.003	19.941	9.197
37.5(4)	2.403	0.003	3.851	0.004	19.259	9.522
49.7(4)	2.376	0.004	3.811	0.004	18.631	9.843
75.5(5)	2.33	0.004	3.744	0.004	17.601	10.419
86.5(7)	2.315	0.004	3.715	0.003	17.243	10.635
Compression data for Fe-1.37C RUN#1						
16.2(2)	2.466	0.003	3.945	0.003	20.775	8.501

18.8(2)	2.458	0.003	3.934	0.003	20.583	8.580
20.6(3)	2.452	0.003	3.925	0.004	20.436	8.642
21.2(2)	2.450	0.004	3.919	0.003	20.372	8.669
22.4(3)	2.444	0.003	3.916	0.003	20.256	8.718
24.5(3)	2.441	0.003	3.909	0.004	20.162	8.759
27.5(2)	2.429	0.003	3.898	0.004	19.917	8.867
31.1(4)	2.419	0.004	3.886	0.005	19.692	8.968
33.1(4)	2.415	0.004	3.880	0.005	19.597	9.012
35.2(3)	2.409	0.004	3.870	0.005	19.449	9.080
37.2(4)	2.406	0.004	3.862	0.005	19.361	9.122
39.0(3)	2.401	0.004	3.856	0.005	19.250	9.174
40.5(4)	2.397	0.004	3.849	0.005	19.151	9.221
41.8(4)	2.394	0.004	3.844	0.005	19.079	9.257
43.2(4)	2.392	0.004	3.840	0.005	19.027	9.282
44.7(4)	2.386	0.003	3.836	0.003	18.912	9.338
Compression data for Fe-1.37C RUN#2						
26.1(2)	2.4348	0.001	3.906	0.002	20.055	8.806
37.5(4)	2.405	0.003	3.864	0.004	19.356	9.124
49.7(4)	2.377	0.004	3.822	0.004	18.699	9.445
76.1(5)	2.332	0.005	3.751	0.004	17.665	9.997
87.2(7)	2.315	0.004	3.720	0.004	17.267	10.228
97.5(7)	2.301	0.003	3.699	0.004	16.959	10.414
109.0(7)	2.285	0.004	3.673	0.004	16.607	10.634

Table S3. Thermoelastic parameters used for modeling the density of hcp-Fe, Fe-0.31C and Fe-1.37C along an adiabatic geotherm with T_{ICB} = 5000, 6000 and 7000 K.

Vibrational Grüneisen parameter	$\gamma_{vib} = \gamma_0(\rho_0/\rho)^q, \gamma_0 = 1.74, q = 0.78$
Electronic Grüneisen parameter	$\gamma_e = 2$
Vibrational specific heat	$C_{V,vib} = 9nR(\frac{\theta_D}{T})^{-3}\int_0^{\frac{\theta_D}{T}}\frac{x^4e^x}{(e^x-1)^2}dx$, θ_D = 422 K, R = 8.314 $J\ mol^{-1}\ K^{-1}$
Electronic specific heat	$C_{Ve} = \beta_0(\rho_0/\rho)^k T, \beta_0 = 0.07\ Jkg^{-1}K^{-2}, k = 1.4$

Reference

1. Fei, Y.; Brosh, E. Experimental study and thermodynamic calculations of phase relations in the Fe–C system at high pressure. *Earth Planet. Sci. Lett.* **2014**, *408*, 155–162.