Supplementary Material

Chemical reaction between ferropericlase (Mg,Fe)O and water under high pressure-temperature conditions of the deep lower mantle

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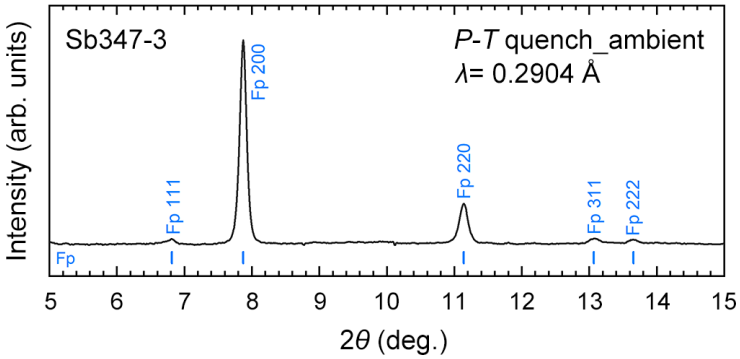

Figure S1. A representative XRD pattern of the run products recovered to ambient conditions. The sample was synthesized in Fp20 at 106 GPa and 2150 K (Run# Sb347-3). The XRD pattern was collected at the laser-heated center. The unit-cell volume of the ferropericlase (Fp) phase was obtained as 75.58(6) $Å^3$ at ambient conditions. The background of the XRD pattern was removed.

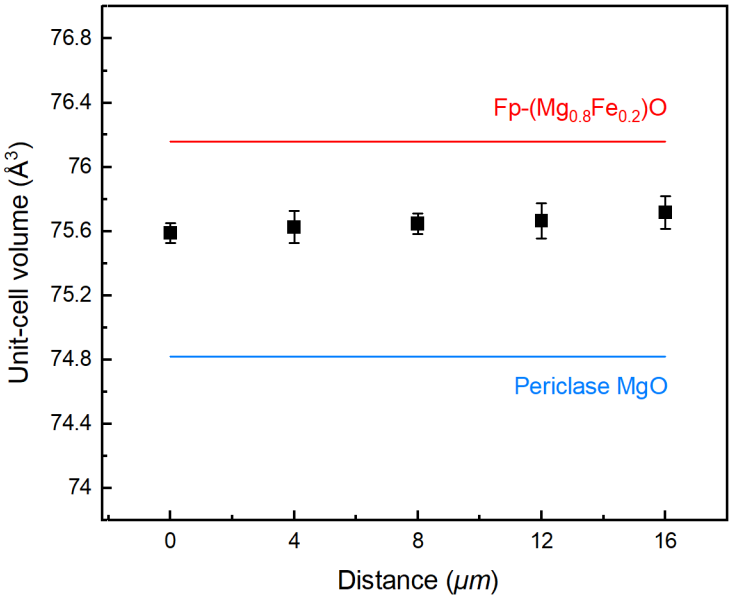

Figure S2. Unit-cell volumes of the Fp-phase after recovered to ambient conditions versus the relative distance to the laser-heated center (Run# Sb347-3). The unit-cell volumes of Fp20 and periclase MgO are plotted for reference [*Fei*, 1999; *Fei et al.*, 2007].

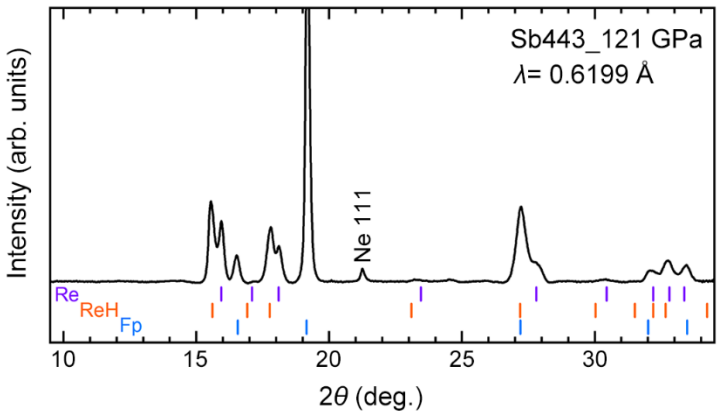

Figure S3. A representative XRD pattern collected near the edge of the sample chamber (Run# Sb443). Incorporation of hydrogen expands the unit-cell volume of Re by 5.57 % [*Anzellini et al.*, 2014]. The unit-cell volumes for the Re and ReH_x are V_{Re}= 24.22(1) Å^3 and V_{ReH}= 25.57(1) Å^3, respectively. The background of the XRD pattern was removed.

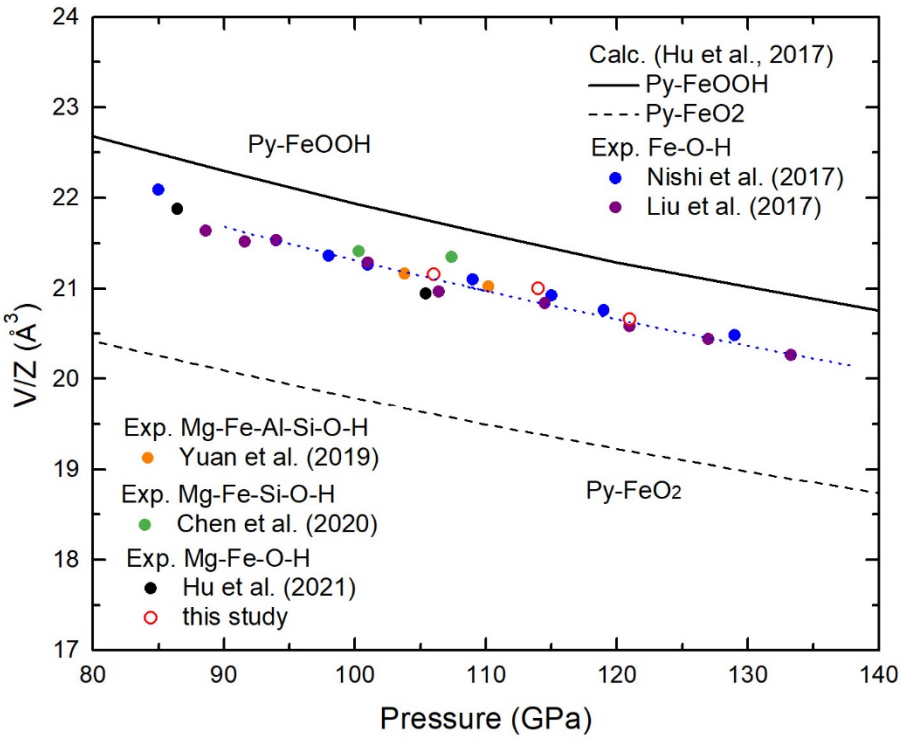

Figure S4. The unit-cell volumes per formula of the Py-phase are plotted as a function of pressure. Solid and dashed lines are calculated equation of state (EOS) for Py-FeOOH and Py-FeO_2 phase, respectively. Experimental data from the references and this study were plotted as solid and open circles, respectively. A least-squares fit of the compression data from this study, Liu et al. (2017) and Yuan et al. (2019) to a Birch-Murnahan EOS yielded a bulk modulus K_{94GPa} = 579(16) GPa and its pressure derivative K'= 4 with V/Z=21.53 Å^3 at 94 GPa (blue dotted line). These data were obtained using consistent pressure scales.

Table S1. The reflections of selected grains for the coexisting Py-phase and Fp-phase at 106 GPa and after *T* quench (Run #Sb347-3). The X-ray wavelength was 0.2904 Å.

Py	#	H	K	L	ω_meas (°)	η_meas (°)	2θ_meas (°)	d (Å)
Grain1	1	-1	-1	-1	8.9	208.4	6.570	2.534
	2	-1	0	2	8.2	103.2	8.485	1.963
	3	1	0	-2	16.8	283.0	8.482	1.963
	4	-2	-1	1	10.4	146.3	9.293	1.792
	5	2	1	-1	26.9	326.1	9.287	1.794
	6	-2	0	2	20.3	116.7	10.734	1.552
	7	0	2	2	28.3	56.9	10.718	1.555
	8	2	0	-2	32.1	296.5	10.728	1.553
	9	2	2	0	7.1	354.0	10.726	1.554
	10	-3	-1	1	25.5	147.6	12.601	1.323
	11	1	-1	-3	26.7	265.4	12.586	1.325
	12	-2	-2	-2	15.9	207.9	13.165	1.267
	13	-3	-1	2	12.1	135.7	14.222	1.173
	14	-1	-2	-3	21.8	229.4	14.222	1.173
	15	-1	2	3	24.4	75.9	14.202	1.175
	16	2	3	1	30.3	15.9	14.194	1.175
Grain2	1	-1	-1	-1	10.8	290.9	6.569	2.534
	2	-1	-1	1	35.6	224.0	6.559	2.538
	3	1	1	-1	26.2	44.0	6.567	2.535
	4	-1	-2	0	39.5	263.0	8.479	1.964
	5	0	-1	-2	31.2	328.9	8.477	1.965
	6	0	1	2	14.7	149.0	8.477	1.965
	7	1	2	0	30.8	83.2	8.481	1.964
	8	-2	-1	1	11.0	229.1	9.300	1.791
	9	-1	-2	-1	31.8	285.8	9.291	1.793
	10	-1	-1	-2	6.1	309.4	9.289	1.793
	11	1	1	-2	37.7	26.7	9.288	1.793
	12	1	2	-1	38.9	60.5	9.288	1.793
	13	0	2	2	32.7	134.0	10.744	1.551
	14	2	2	0	11.8	77.2	10.739	1.552
	15	2	2	-1	16.8	58.6	11.383	1.464
	16	2	2	1	6.2	96.0	11.399	1.462
	17	-1	1	3	28.4	166.0	12.594	1.324
	18	1	3	1	30.4	102.4	12.601	1.323
	19	-2	-2	-2	14.3	291.1	13.162	1.267
	20	-2	-2	2	40.4	223.6	13.149	1.268
	21	-2	0	3	10.1	191.6	13.692	1.218

Grain3	1	-1	1	1	24.8	113.4	6.567	2.535
	2	1	-1	-1	31.8	293.2	6.566	2.535
	3	-2	0	1	8.8	152.1	8.478	1.964
	4	2	0	-1	26.8	332.0	8.483	1.963
	5	-2	1	1	31.8	131.3	9.299	1.791
	6	-1	-2	-1	30.8	231.4	9.289	1.793
	7	-1	2	1	35.7	97.7	9.296	1.792
	8	1	-1	-2	12.8	289.2	9.294	1.792
	9	1	2	1	18.8	51.3	9.292	1.793
	10	0	-2	-2	20.8	260.2	10.736	1.552
	11	2	2	0	34.4	24.0	10.728	1.553
	12	-2	-2	-1	23.8	214.9	11.381	1.464
	13	-3	1	1	35.3	140.2	12.604	1.323
	14	1	3	1	28.7	55.1	12.588	1.324
	15	3	1	-1	25.6	351.2	12.595	1.324
	16	-2	2	2	21.2	113.5	13.161	1.267
	17	2	-2	-2	35.3	293.4	13.159	1.267
	18	0	3	2	19.3	76.4	13.696	1.218

Fp	**#**	**H**	**K**	**L**	**ω_meas (°)**	**η_meas (°)**	**2θ_meas (°)**	**d (Å)**
Grain1	1	-1	-1	-1	10.3	119.4	7.661	2.173
	2	-1	-1	1	9.3	48.7	7.655	2.175
	3	1	1	-1	19.3	228.6	7.654	2.175
	4	1	1	1	18.8	299.2	7.653	2.176
	5	-2	-2	0	8.3	84.0	12.521	1.332
	6	1	1	-3	36.8	197.9	14.691	1.136
	7	1	1	3	29.0	329.5	14.687	1.136
	8	-2	-2	-2	5.8	119.6	15.346	1.087
	9	2	2	-2	24.6	228.3	15.342	1.088
	10	2	2	2	23.3	299.5	15.348	1.087
	11	-3	-1	-3	26.8	128.8	19.369	0.863
	12	3	3	-1	24.8	250.5	19.351	0.864
	13	3	3	1	24.3	277.4	19.353	0.864
Grain2	1	-1	-1	-1	5.8	126.0	7.649	2.177
	2	-1	-1	1	8.3	55.2	7.657	2.175
	3	1	1	-1	17.5	235.2	7.655	2.175
	4	1	1	1	15.3	305.8	7.647	2.177
	5	-2	-2	0	5.5	90.6	12.515	1.332
	6	-3	-1	-1	30.3	109.1	14.687	1.136
	7	-3	-1	1	31.3	73.7	14.677	1.137

	8	1	1	-3	32.0	204.9	14.692	1.136
	9	1	1	3	26.3	336.3	14.683	1.136
	10	2	2	2	20.3	306.1	15.333	1.088
	11	-3	-1	-3	23.8	135.6	19.355	0.864
	12	-3	-1	3	26.3	47.1	19.327	0.865
	13	3	3	-1	22.0	257.1	19.344	0.864
	14	3	3	1	21.3	284.0	19.331	0.865
Grain3	1	0	0	-2	7.5	183.9	8.841	1.884
	2	-2	0	-2	16.9	138.2	12.515	1.332
	3	-2	0	2	6.9	47.7	12.517	1.332
	4	2	0	-2	23.8	227.7	12.524	1.331
	5	2	0	2	35.4	317.9	12.506	1.333
	6	-3	1	1	29.4	73.5	14.668	1.137
	7	-1	1	3	34.4	23.0	14.662	1.138
	8	3	1	1	11.3	291.8	14.694	1.135
	9	-4	0	0	11.8	92.8	17.738	0.942
	10	4	0	0	29.3	272.8	17.734	0.942
	11	-3	1	3	20.3	47.0	19.321	0.865
	12	-4	0	-2	11.8	119.7	19.850	0.842
	13	-4	0	2	7.0	65.9	19.853	0.842
	14	-2	0	-4	7.7	157.7	19.860	0.842
	15	2	0	-4	31.4	208.2	19.872	0.842
	16	4	0	-2	28.8	245.9	19.861	0.842
	17	4	0	2	34.8	299.7	19.844	0.843
Grain4	1	-1	-1	1	19.8	64.8	7.639	2.180
	2	1	1	-1	28.3	244.6	7.646	2.178
	3	-2	-2	0	27.5	99.0	12.496	1.334
	4	0	2	2	8.3	332.1	12.496	1.334
	5	2	2	0	40.3	278.8	12.503	1.333
	6	-1	-3	-1	2.1	122.2	14.676	1.137
	7	1	3	1	19.3	302.0	14.671	1.137
	8	-2	-2	-2	35.3	133.1	15.353	1.087
	9	-2	-2	2	15.7	64.5	15.309	1.090
	10	-1	-3	-3	1.8	148.4	19.335	0.865
	11	1	3	3	37.8	328.3	19.326	0.865
	12	2	4	0	25.8	283.2	19.835	0.843
	13	-2	-4	-2	7.8	127.4	21.762	0.769
	14	-2	-2	4	1.3	45.2	21.736	0.770
	15	2	2	-4	31.5	225.3	21.772	0.769
	16	2	4	-2	21.8	259.2	21.771	0.769