Electronic Supplementary Information

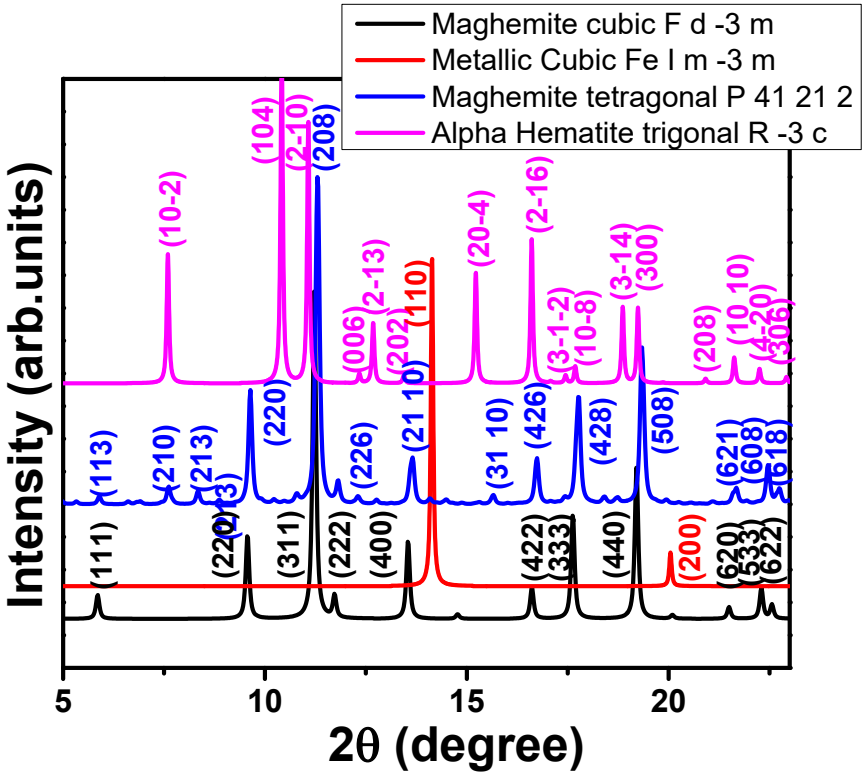
Hydrostatic pressure induced reversible phase transformation in iron oxide nanoparticles.

Arkaprava Das[1]*, Anumeet Kaur[2], and Parwinder Kaur[3]

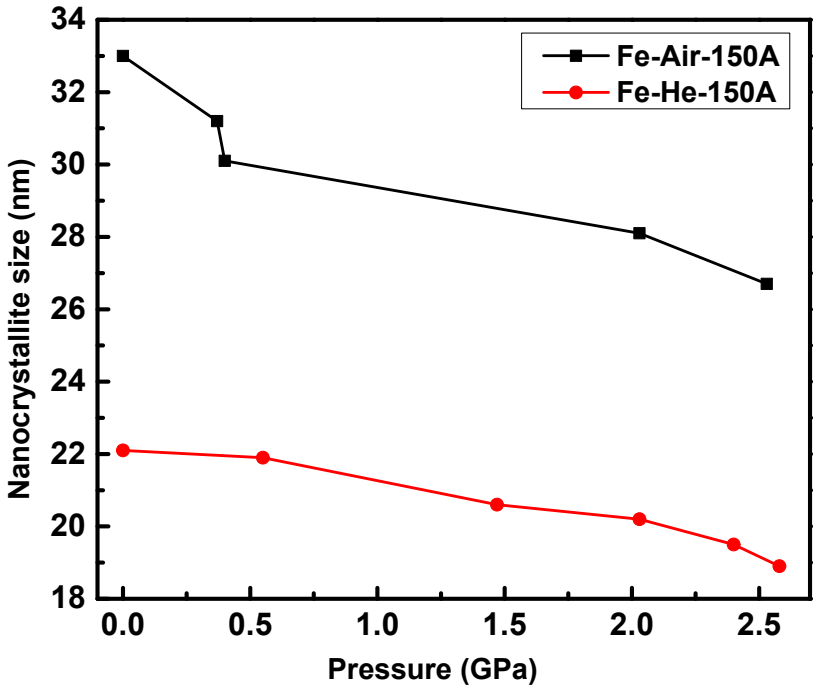
[1]Chimie des Interaction Plasma surface, Université of Mons, Mons, Belgium

[2]Department of Applied Sciences and Humanities, Global Group of Institutes, Amritsar, Punjab, 143501, India

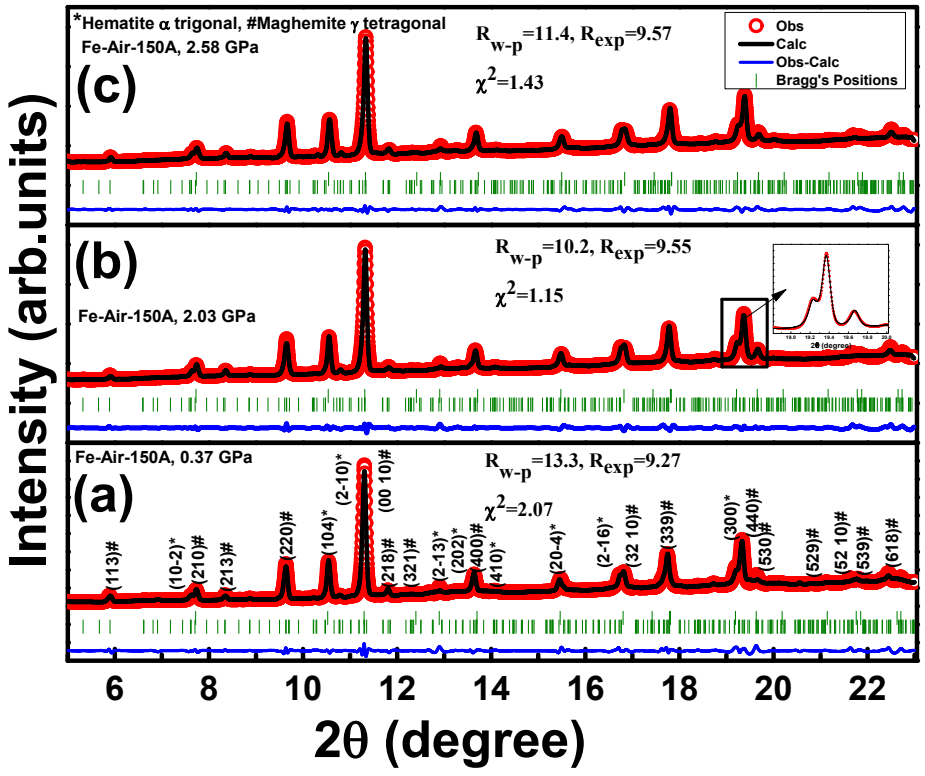
[3]Department of Applied Sciences, Bhai Gurdas Group of Institutes, Sangrur, Punjab 148001, India



ESF1: Standard XRD patterns for cubic, tetragonal maghemite iron oxide and metallic Fe phase



ESF2: Reducing nanocrystallite size with increasing pressure for Fe-Air-150A and Fe-He-150A sample.



ESF3: Reitveld Refinement for Fe-Air-150A sample at 0.37 (a), 2.03 (b) and 2.58 GPa (c) pressure

EST1: Nanocrystallite size at different pressure for both Fe-Air-150A and Fe-He-150A samples

Sample	Pressure (GPa)	Peak	Peak position (2^{θ})	FWHM	Crystallite Size (nm)
Fe-Air-150A	0.00	(313)	11.29	0.071	33.0
Fe-Air-150A	0.37	(313)	11.30	0.082	31.2
Fe-Air-150A	0.40	(313)	11.30	0.085	30.1
Fe-Air-150A	2.03	(313)	11.32	0.091	28.1
Fe-Air-150A	2.53	(313)	11.34	0.096	26.7
Fe-He-150A	0.00	(110)	14.04	0.116	22.1
Fe-He-150A	0.55	(110)	14.05	0.117	21.9
Fe-He-150A	1.47	(110)	14.08	0.124	20.6
Fe-He-150A	2.03	(110)	14.09	0.127	20.2
Fe-He-150A	2.40	(110)	14.10	0.132	19.5
Fe-He-150A	2.58	(110)	14.11	0.136	18.9

EST2: Refinement results for Fe-Air-150A sample at 0 GPa pressure

Results of the Reitveld refinement for Fe-Air-150A sample at 0 GPa pressure						
Trigonal α phase with space group $R\bar{3}c$, **Cell parameters:- a = b = 5.033 (6) Å, c = 13.741 (26) Å, Volume = 348.049 (0.008) (Å)^3**						
Atom	**Position**	***x***	***y***	***z***	**B_{iso}(Å^2)**	**Occupancy**
Fe0	12*c*	0.000	0.000	0.145	2.261	0.365
O1	18*e*	0.000	0.273	0.750	0.001	0.987
Tetragonal maghemite phase with space group *P* 41 21 2 **Cell parameters:- a = b = 8.332 (8) Å, c = 25.089 (30) Å ,Volume = 1741.951 (0.031) (Å)^3**						
Atom	**Position**	***x***	***y***	***z***	**B_{iso}(Å^2)**	**Occupancy**
Fe1	8*b*	0.771	0.946	0.063	0.216	1.000
Fe2	8*b*	0.775	0.982	0.353	0.009	0.974
Fe3	8*b*	0.714	1.044	0.849	0.035	0.999

Fe4	4*a*	0.372	0.372	0.000	1.474	**0.495**
Fe5	8*b*	0.634	0.666	0.346	1.190	0.927
Fe6	8*b*	0.232	0.876	0.948	0.002	1.000
Fe7	8*b*	0.442	0.842	0.323	0.901	0.961
Fe8	8*b*	0.299	0.929	0.672	0.038	1.000
Fe9	4*a*	0.143	0.143	0.000	0.036	**0.421**
O1	8*b*	0.614	0.666	-0.008	0.001	0.712
O2	8*b*	0.575	0.963	0.370	0.002	0.851
O3	8*b*	0.675	0.859	0.625	0.001	0.713
O4	8*b*	0.059	0.327	0.057	2.194	1.000
O5	8*b*	0.302	0.410	0.308	0.001	1.000
O6	8*b*	0.088	0.322	0.669	0.094	0.820
O7	8*b*	0.146	0.869	0.012	0.001	1.000
O8	8*b*	0.117	0.907	0.328	0.001	0.981
O9	8*b*	0.052	0.911	0.712	2.720	1.000
O10	8*b*	0.387	0.627	-0.001	0.001	1.000
O11	8*b*	0.414	0.647	0.339	0.001	0.956
O12	8*b*	0.364	0.616	0.669	0.001	1.000
%Molar	**84.22 % (Tetragonal)**		**15.78 % (Trigonal)**		**$R_{w\text{-}p}$ = 10, R_{exp} = 6.65**	
	$R_{B(Tetragonal)}$ = 2.63		**$R_{B(Trigonal)}$ = 0.70**		**χ^2 = 2.32**	

EST3: Refinement results for Fe-He-150A sample at 0 Gpa pressure

Results of the Reitveld refinement for Fe-He-150A sample at 0 GPa pressure					
Metallic Cubic Fe phase with space group *Im* $\bar{3}$*m*, **Cell parameters:- a = b = c = 2.860 (01) Å, Volume = 23.624 (0.002) (Å)^3**					
Atom	***x***	***y***	***z***	**B_{iso}(Å^2)**	**Occupancy**
Fe	0.00000	0.00000	0.0000	0.010	0.920
Cubic maghemite phase with space group *Fd-3m*					

Cell parameters:- a = b = c = 8.332 (8) Å, Volume = 588.621 (0.002) (Å)^3						
Atom	**Position**	***x***	***y***	***z***	**B_{iso}(Å^2)**	**Occupancy**
Fe1	8*a*	0.125	0.125	0.125	0.001	0.461
Fe2	16*d*	0.500	0.500	0.500	0.009	0.864
O	32*e*	0.651	0.651	0.651	0.000	1.000
%Molar	**61.8 % (cubic metallic Fe)** $R_{B(cubic\ Fe)}$ **= 1.10**		**38.2 % (Cubic maghemite)** $R_{B(cubic\ Maghemite)}$ **= 2.36**		$R_{w\text{-}p}$ **= 9.56,** R_{exp} **= 8.14** χ^2 **= 1.38**	

EST4: Refinement results for Fe-He-150A sample at 0.55 GPa pressure

Results of the Reitveld refinement for Fe-He-150A sample at 0.55 GPa pressure						
Metallic Cubic Fe phase with space group *Im* $\bar{3}$*m*, **Cell parameters:- a = b = c = 2.865 (0) Å, Volume = 23.521 (0.008) (Å)^3**						
Atom		***x***	***y***	***z***	**B_{iso}(Å^2)**	**Occupancy**
Fe0		0.000	0.000	0.000	0.001	0.910
Tetragonal maghemite phase with space group *P*41212 **Cell parameters:- a = b = 8.334 (0) Å, c = 25.097 (0) Å ,Volume = 1743.434 (0.031) (Å)^3**						
Atom	**Position**	***x***	***y***	***z***	**B_{iso}(Å^2)**	**Occupancy**
Fe1	8*b*	1.291	0.897	0.036	0.003	0.943
Fe2	8*b*	1.077	1.034	0.385	0.050	1.000
Fe3	8*b*	0.728	4.007	0.708	0.050	1.000
Fe4	4*a*	0.776	0.776	0.000	0.005	**0.484**
Fe5	8*b*	0.615	0.615	0.319	0.004	0.778
Fe6	8*b*	0.389	0.863	0.997	0.005	1.000
Fe7	8*b*	0.374	0.887	0.331	0.050	1.000
Fe8	8*b*	0.306	0.848	0.667	0.050	1.000
Fe9	4*a*	0.129	0.129	0.000	0.036	**0.548**
O1	8*b*	0.994	0.866	0.013	0.050	1.000

O2	8*b*	0.662	0.797	0.338	0.005	1.000
O3	8*b*	1.058	0.873	0.663	0.005	1.000
O4	8*b*	0.192	0.346	0.000	0.005	1.000
O5	8*b*	0.017	0.193	0.340	0.001	1.000
O6	8*b*	0.088	0.322	0.669	0.094	0.820
O7	8*b*	0.123	0.353	0.671	0.005	0.762
O8	8*b*	0.177	0.816	0.331	0.050	0.816
O9	8*b*	0.133	0.853	0.670	0.050	1.000
O10	8*b*	0.383	0.626	0.000	0.001	1.000
O11	8*b*	0.406	0.626	0.338	0.001	0.912
O12	8*b*	0.387	0.617	0.676	0.050	0.878
%Molar	**19.88 % (Cubic Fe)** $R_{B(cubic\ Fe)}$ **= 7.00**		**80.12 % (Tetragonal maghemite)** $R_{B(Tetragonal)}$ **= 0.42**		$R_{w\text{-}p}$ **= 8.37,** R_{exp} **= 7.80** χ^2 **= 1.15**	

EST5: Refinement results for Fe-He-150A sample at 2.40 GPa pressure

Results of the Reitveld refinement for Fe-He-150A sample at 2.40 GPa pressure					
Metallic Cubic Fe phase with space group *Im* $\bar{3}$*m*, **Cell parameters:- a = b = c = 2.854 (001) Å, Volume = 23.270 (0.002) (Å)^3**					
Atom	***x***	***y***	***z***	B_{iso}**(Å^2)**	**Occupancy**
Fe	0.000	0.000	0.00	0.010	0.920
Cubic maghemite phase with space group *Fd* $\bar{3}$*m* **Cell parameters:- a = b = c = 8.332 (8) Å, Volume = 579.205 (0.031) (Å)^3**					
Atom	**Position**	***x***	***y***	***z***	B_{iso}**(Å^2)**	**Occupancy**
Fe1	8*a*	0.125	0.125	0.125	0.001	0.517
Fe2	16*d*	0.500	0.500	0.500	0.009	0.717
O	32*e*	0.250	0.250	0.250	0.000	1.000
%Molar	**17.33 % (cubic metallic Fe)** $R_{B(cubic\ Fe)}$ **= 1.17**		**82.67 % (Cubic maghemite)** $R_{B(cubic\ maghemite)}$ **= 20**		$R_{w\text{-}p}$ **= 10.2,** R_{exp} **= 8.90** χ^2 **= 1.31**	