

Correlating the Size and Cation Inversion Factor in Context of Magnetic and Optical behavior of CoFe₂O₄ nanoparticles

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Supplementary Information

Table S1: Variation in X-ray Energy for Measuring Fe *K*-edge and Co *K*-edge XANES-Imaging Spectra

Element	Variation from Main Edge	Actual Variation (eV)	Step (eV)
Fe	-20 to 80	7092 to 7192	1
Co	-20 to 80	7689 to 7789	1

Table S2: Input files for A-site and B-site occupancies of metal ions in CoFe₂O₄ nanoparticles

A-site						
## This Atoms file was generated by Demeter 0.9.18						
## Demeter written by and copyright (c) Bruce Ravel, 2006-2013						
Space = fd3m						
a	=	8.3858299	b	= 8.3858299	c	= 8.3858299
alpha	=	90.00000	beta	= 90.00000	gamma	= 90.00000
r _{max}	=	8.00000	core = Fe1			
shift	=	0.00000	0.00000	0.00000		
atoms						
# el.	x	y	z	tag		
Co	0.12500	0.12500	0.12500	CoA		
Fe	0.50000	0.50000	0.50000	FeA		
O	0.26000	0.26000	0.26000	O		
B-site						
## This Atoms file was generated by Demeter 0.9.18						
## Demeter written by and copyright (c) Bruce Ravel, 2006-2013						
Space = fd3m						
a	=	8.3858299	b	= 8.3858299	c	= 8.3858299
alpha	=	90.00000	beta	= 90.00000	gamma	= 90.00000
r _{max}	=	8.00000	core = Co1			
shift	=	0.00000	0.00000	0.00000		
atoms						
# el.	x	y	z	tag		
Fe	0.12500	0.12500	0.12500	FeB		
Co	0.50000	0.50000	0.50000	CoB		
O	0.26000	0.26000	0.26000	O		

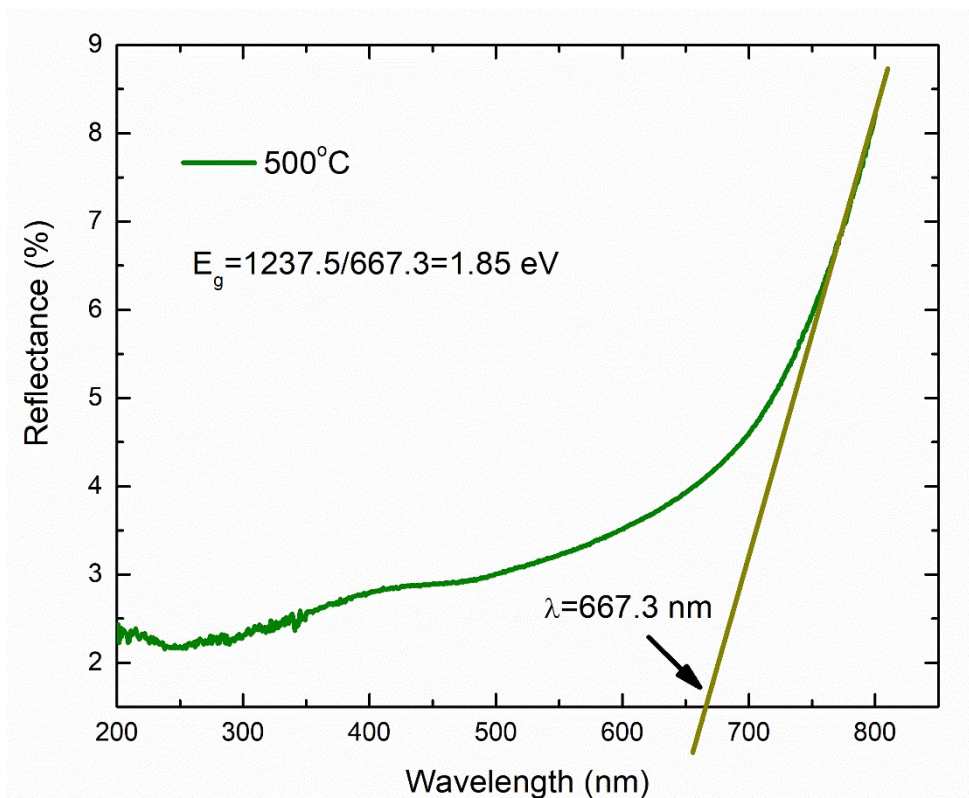


Fig. S1: Estimation of optical band-gap from diffuse reflectance spectrum for representative nanoparticle

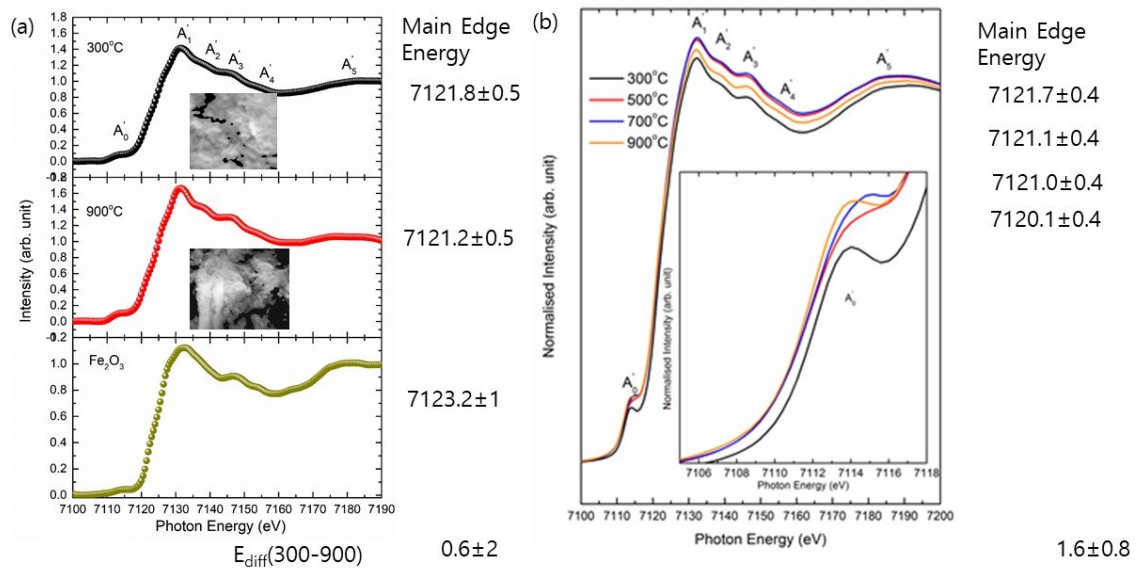


Fig. S2: Fe K-edge (a) XANES spectra extracted from transmission X-ray microscopic imaging and (b) bulk XANES spectra for CoFe₂O₄ nanoparticles.

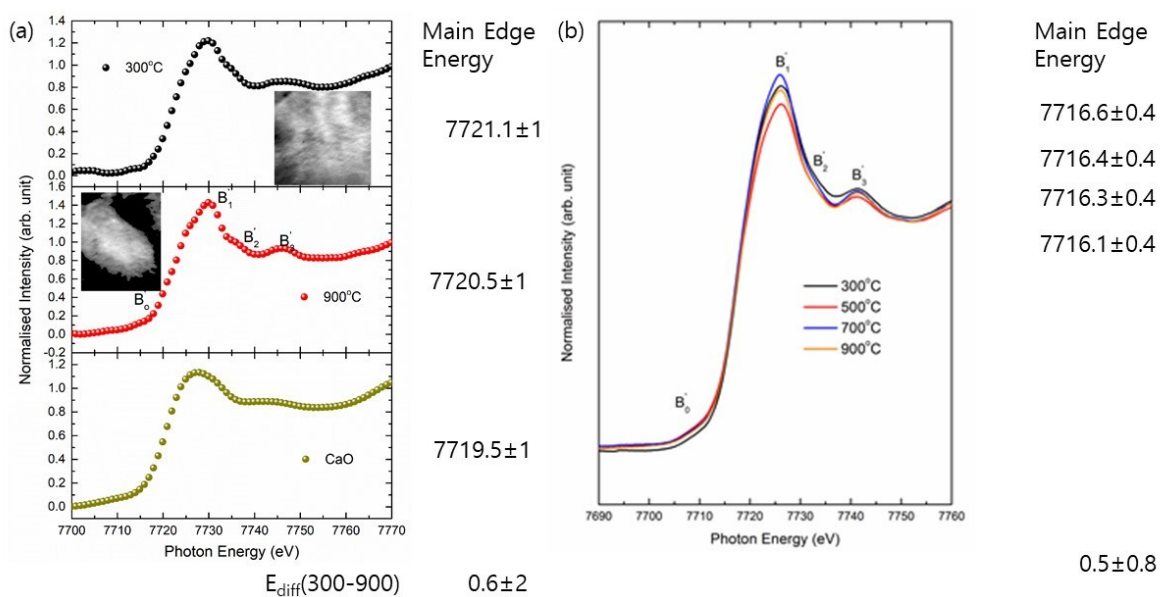


Fig. S3: Co K-edge (a) XANES spectra extracted from transmission X-ray microscopic imaging and (b) bulk XANES spectra for CoFe₂O₄ nanoparticles. (The main energy difference for same sample by two methods is due to calibration related issues.)

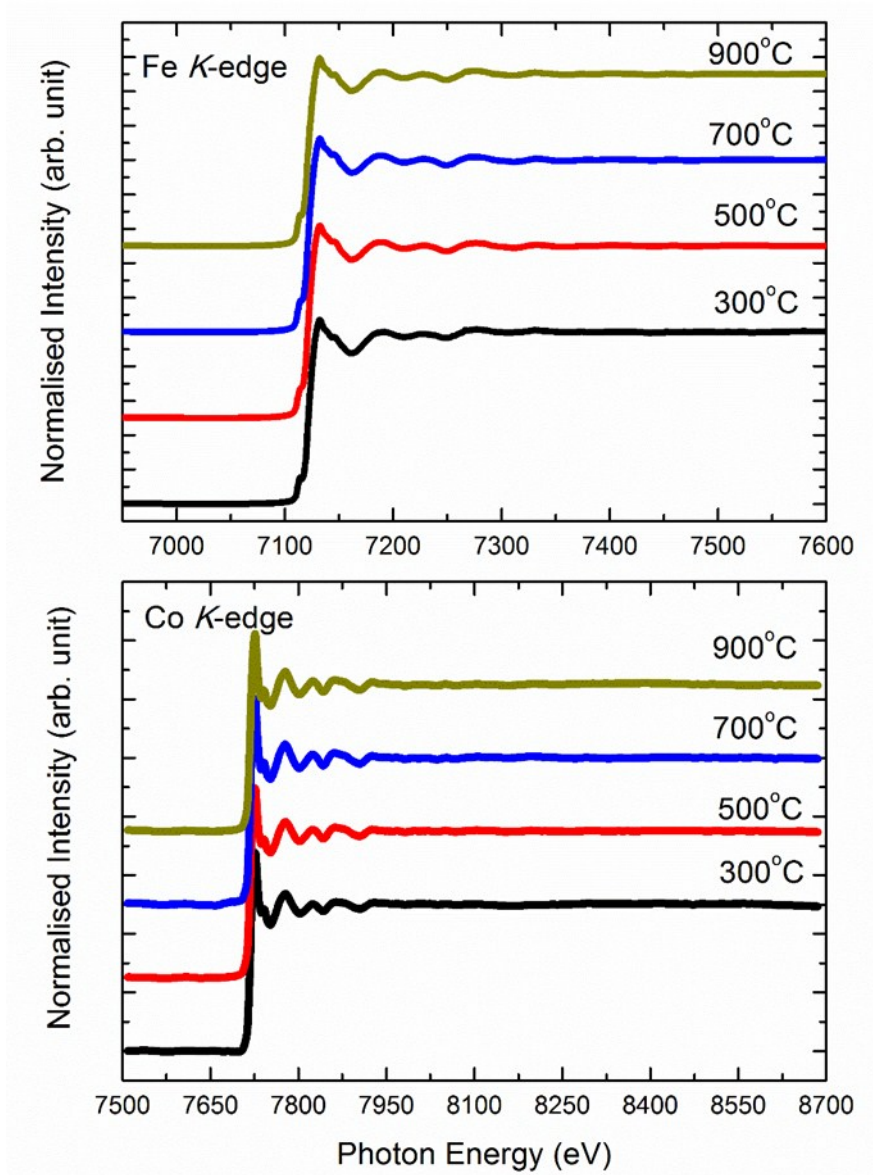


Fig. S4: Fe & Co K-edge EXAFS spectra for CoFe_2O_4 nanoparticles synthesized at 300, 500, 700 and 900°C

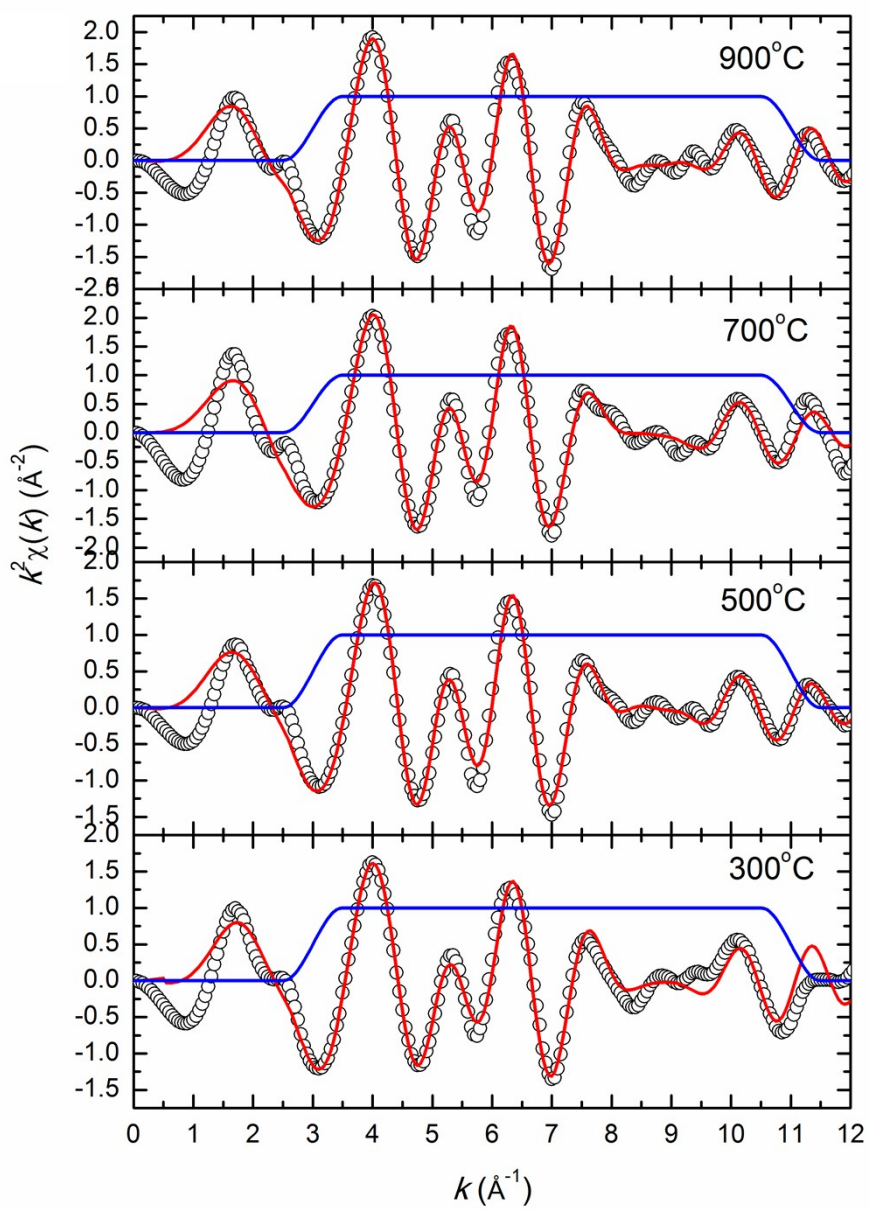


Figure S5: Simulated k -weight Co K -edge EXAFS spectra for CoFe_2O_4 nanoparticles synthesized at 300, 500, 700 and 900°C.

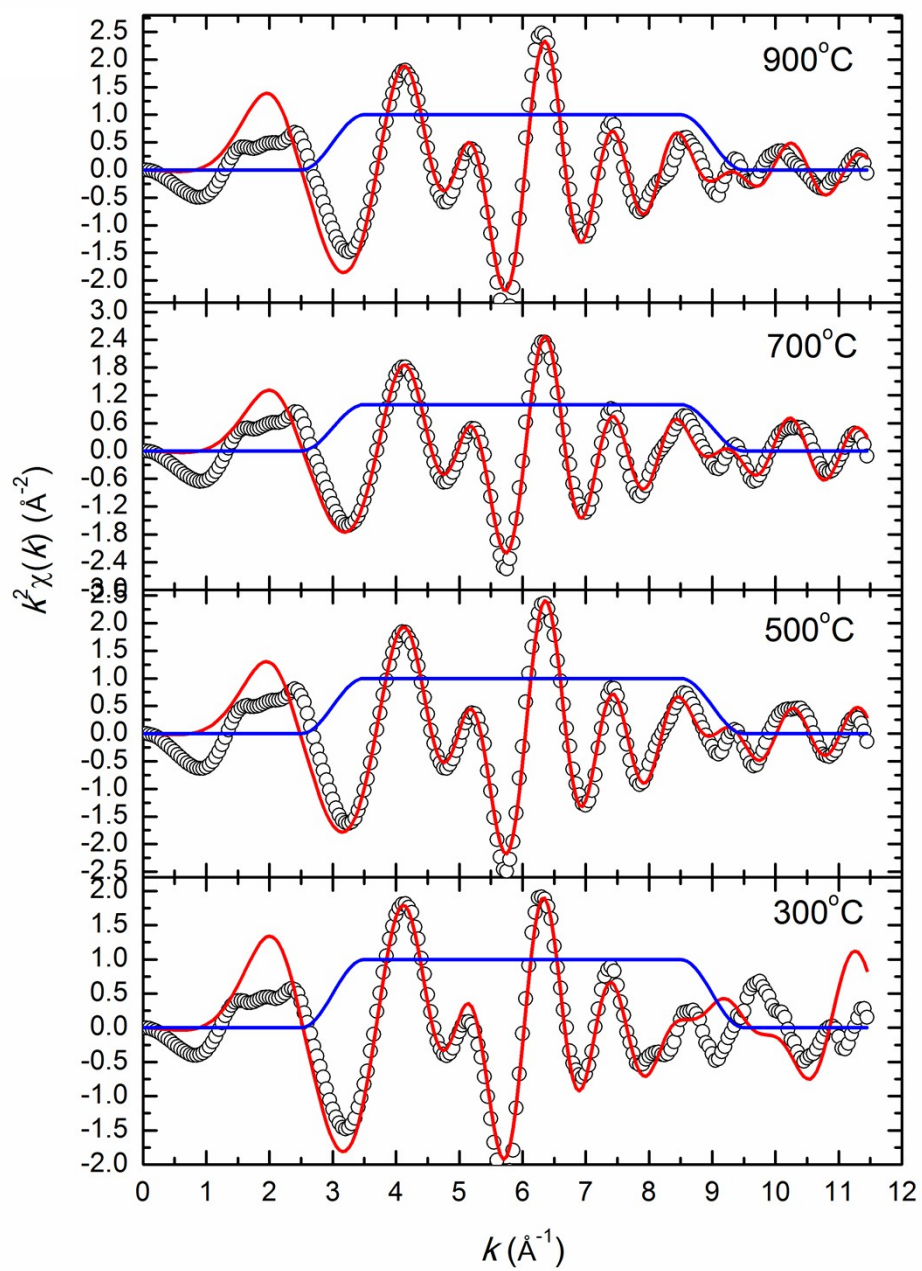


Figure S6: Simulated k -weight EXAFS spectra at Fe K -edge for CoFe_2O_4 nanoparticles synthesized at 300, 500, 700 and 900°C