

Supplementary information

Kinetics of spontaneous phase transitions from wüstite to magnetite in superparamagnetic core-shell nanocubes of iron oxides

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Structural characterization

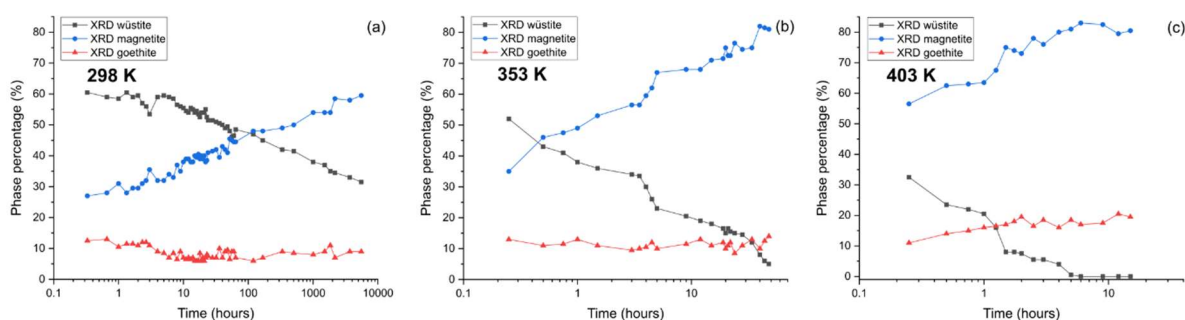


Figure S1. The percentage of wüstite (black), magnetite (blue), and goethite (red) calculated by Rietveld refinement from time-resolved XRD data for (a) 298 K, (b) 353 K, and (c) 403 K. The lines are added to lead the eye.

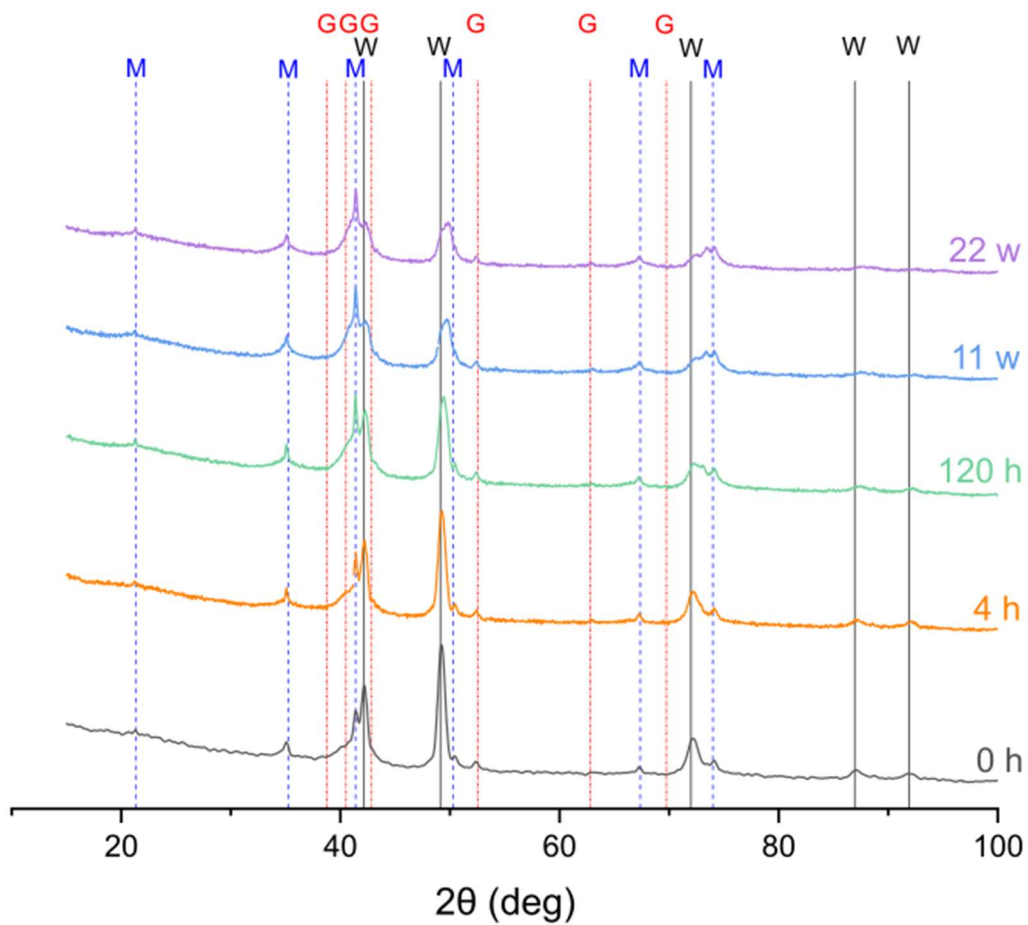


Figure S2. XRD diffractograms of samples after synthesis in several time (0 hours, 4 hours, 120 hours, 11 weeks, and 22 weeks) at 298 K. The characteristic diffractions of wüstite (FeO) are depicted by vertical solid black lines, magnetite (Fe₃O₄) diffractions are depicted by vertical dotted blue lines, and goethite (FeOOH) diffractions are depicted by vertical dash-dotted red lines.

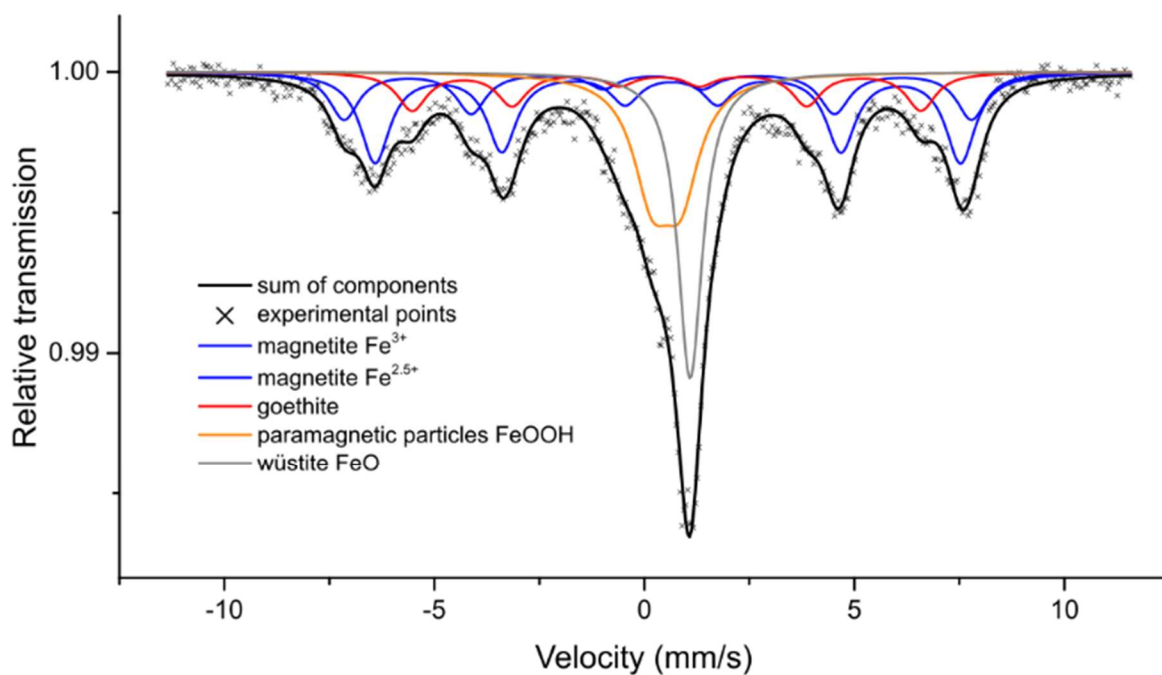


Figure S3. The Mössbauer spectra of the 23 nm core-shell sample measured at 293 K we published previously in collaboration. [19]

Table S1. The relative contents of fitted phases by MS and their hyperfine parameters.

Phase fitted	Content (<i>Fe</i> atomic fraction)	Sextet			Doublet		Singlet
		Isomer shift (mm/s)	Quadrupole Shift (mm/s)	Hyperfine induction (T)	Isomer shift (mm/s)	Quadrupole Shift (mm/s)	Isomer shift (mm/s)
Magnetite Fe ³⁺	0.16	0.27	0.27	46.5			
Magnetite Fe ^{2.5+}	0.30	0.61	0.09	43.3			
Wüstite	0.20						1.10
Goethite	0.13	0.46	0.17	37.7			
Paramag. FeOOH	0.21				0.54	0.68	

Theoretical description of transition kinetics

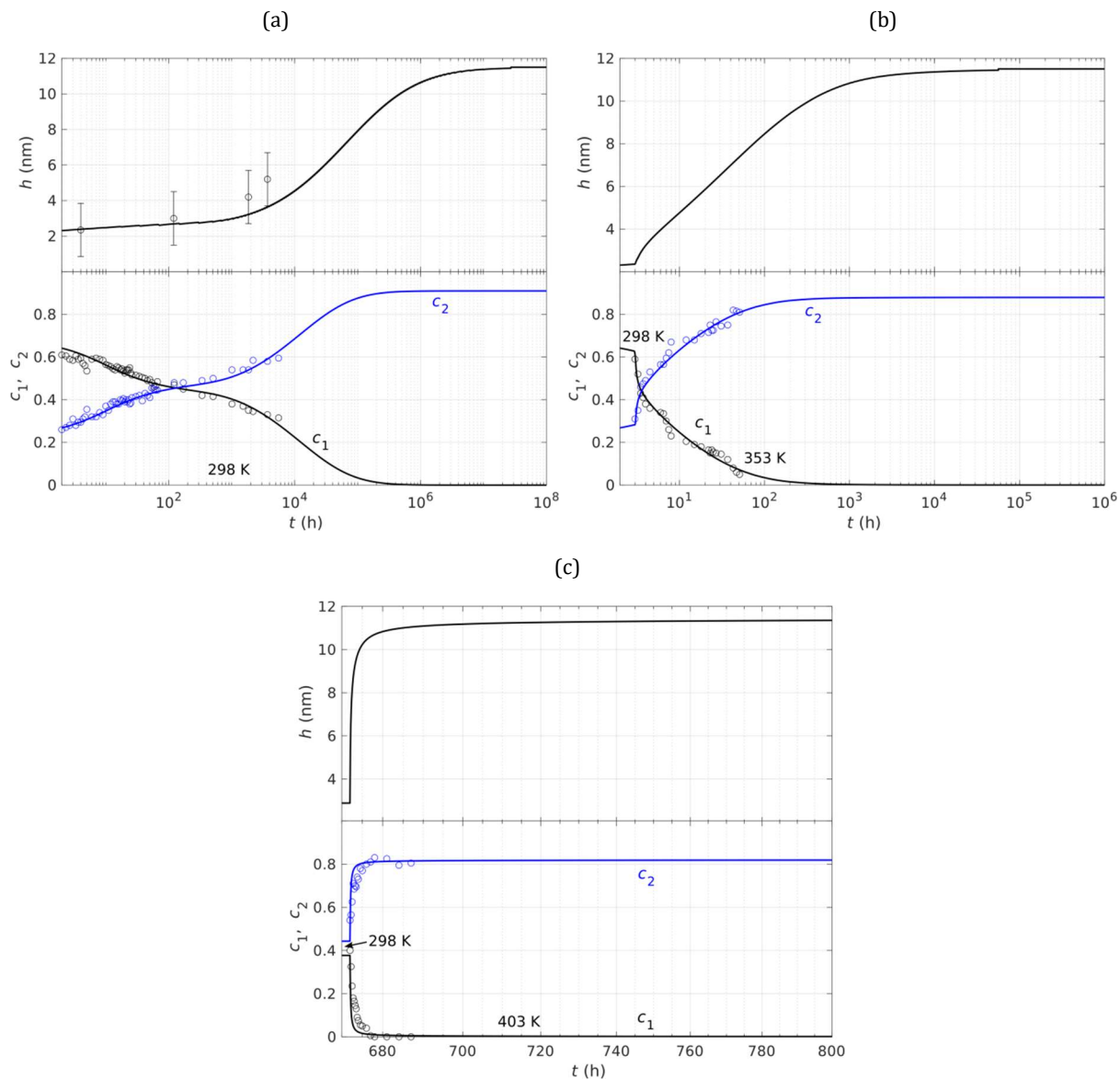


Figure S4. Long-term predictions of the position of the phase boundary (h) and the concentrations of wüstite (c_1) and magnetite (c_2) for NPs held at the temperature of (a) 298 K, (b) 353 K, and (c) 403 K.