Supporting Information for

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Mackinawite formation from elemental iron and sulfur

Figure S1: SEM image of the used iron powder. EDX analyses shows the presence of iron and very small fractions of carbon, oxygen and sulfur.

Figure S2: SEM image of an iron plate after the reaction with sulfur at room temperature in deoxygenated water.

Figure S3: EDX analysis of a washed mackinawite sample free from chloride.

Figure S4: Plot of the not oxidized sulfur content of reference mackinawite samples versus the reaction time at 130°C from mackinawite dissolution experiments.

Figure S5: PXRD pattern of a typical deactivated mackinawite sample obtained from the reaction between iron and sulfur in a 0.01 M sodium chloride solution at room temperature after 12 hours reaction time without any residual iron or sulfur.

Table TS1: Fitting parameters of the Rietveld fit of a PXRD of mackinawite prepared from elemental iron and sulfur.

link to video

https://upload.uni-jena.de/data/601276cfa9cf47.37056468/64fach.mp4

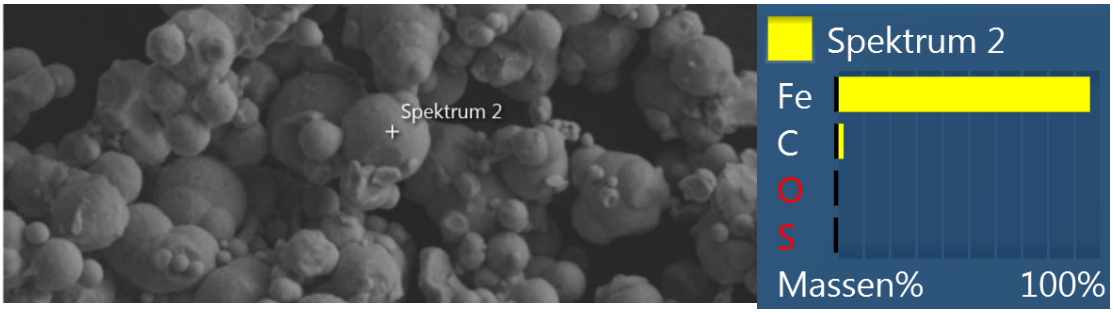

Figure S1: (left) SEM image of the used iron powder. (right) EDX analyses showing the presence of iron and very small fractions of carbon, oxygen and sulfur.

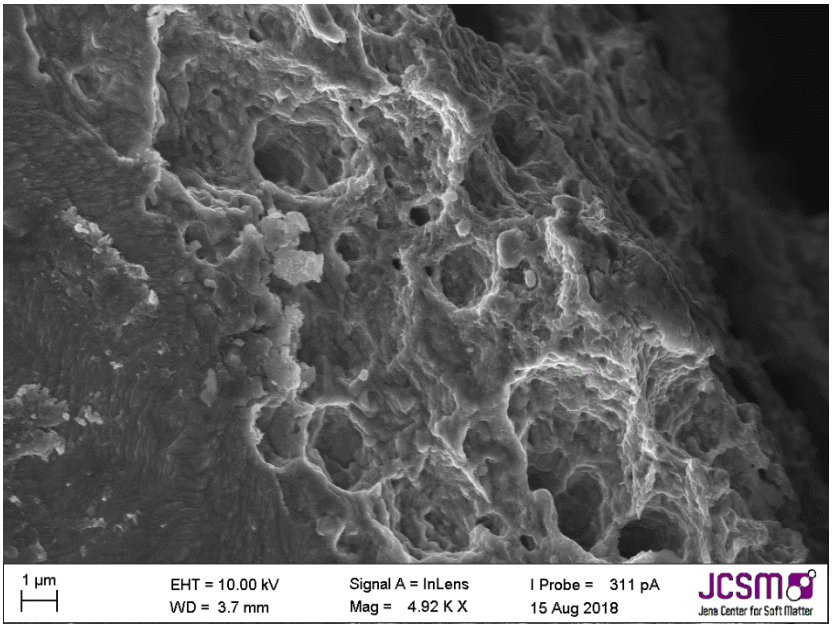

Figure S2: SEM image of an iron plate after the reaction with sulfur at room temperature in deoxygenated water.

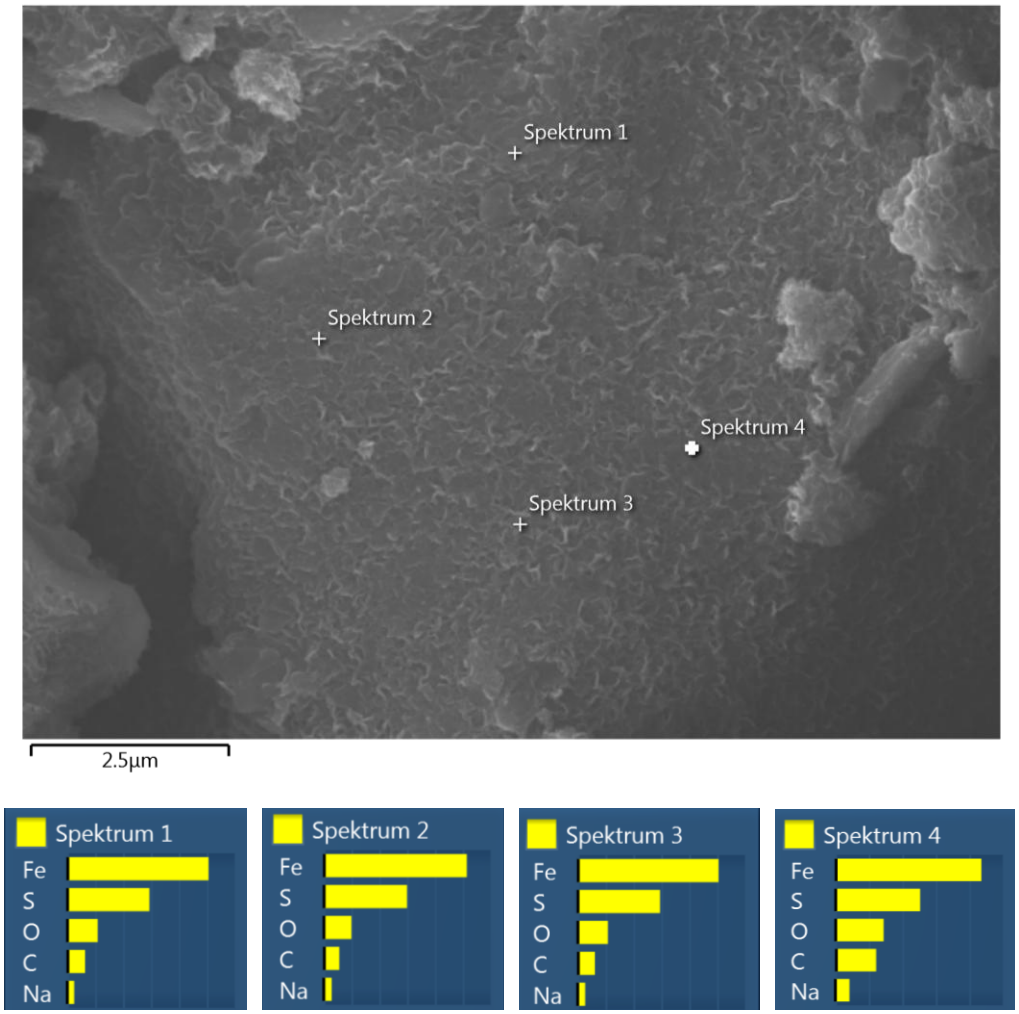

Figure S3: EDX analysis of a washed mackinawite sample free from chloride.

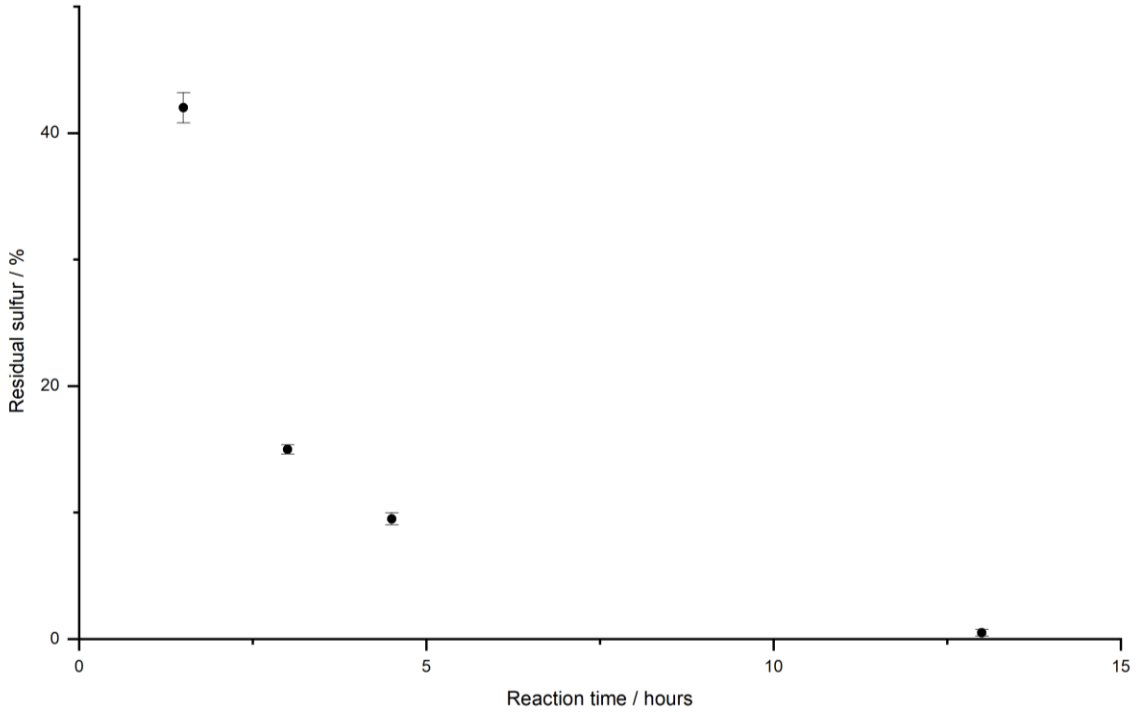

Figure S4: Plot of the not oxidized sulfur content of reference mackinawite samples versus the reaction time at 130°C from mackinawite dissolution experiments.

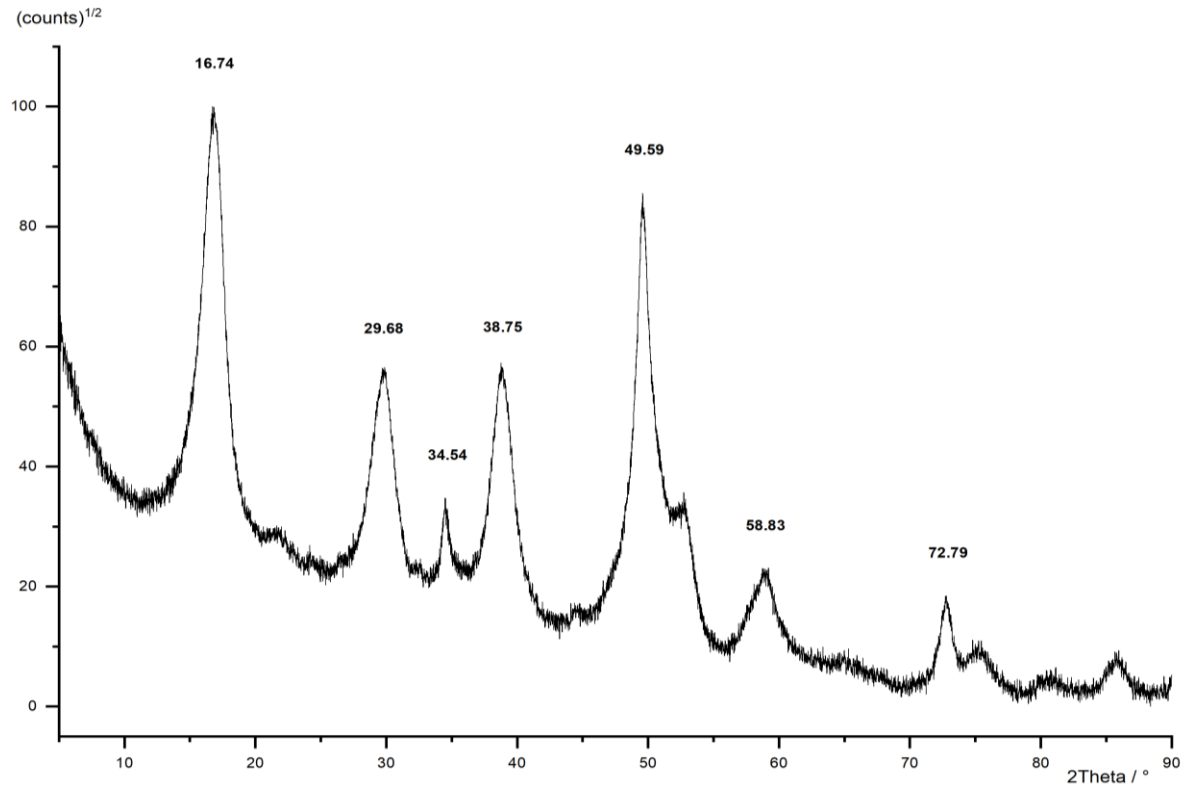

Figure S5: PXRD pattern of a typical deactivated mackinawite sample obtained from the reaction between iron and sulfur in a 0.01 M sodium chloride solution at room temperature after 12 hours reaction time without any residual iron or sulfur.

Table TS1: Fitting parameter of the Rietveld fit of a PXRD of mackinawite prepared from elemental iron and sulfur.

Parameter	Value / explanation
R_{wp}	0.02815
χ^2	1.51
Number of independent parameters	9
a	3.6574 ± 0.0007 Å
c	5.2717 ± 0.011 Å
Temperature factor Fe^{2+} and S^{2-}	0.297 ± 0.075
Size parameter	Additional gaussian convolution as a function of 1/cos(θ)
Strain parameter	Additional gaussian convolution as a function of tan(θ)
Preferred orientation along 001	Reduction of intensities along 001 due to the flat particle shape
Scale parameters (3 Phases)	Relative scale of mackinawite, iron and sulfur