Cross-Sections of Nanocellulose from Wood Analyzed by Quantized Polydispersity of Elementary Microfibrils

Supplementary material

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Contents:

- TEM images of the 18 CNF samples in the study
- Assessment of isotropy in WAXD experiments
- Results from WAXD simulations

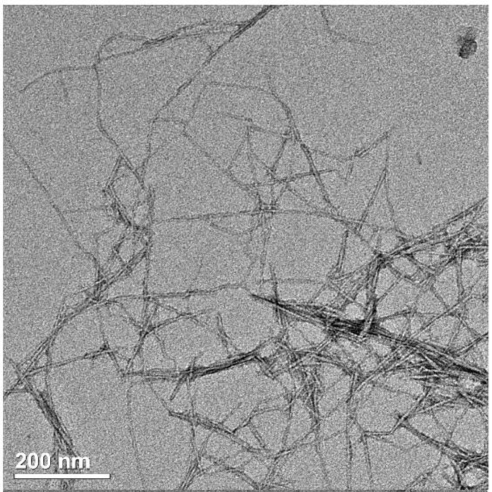
Additionally, a supplementary movie is provided to illustrate the principle of the WAXD simulations.

TEM images of CNF samples

TEMPO-oxidized CNF (low charge)

Sample # TEM

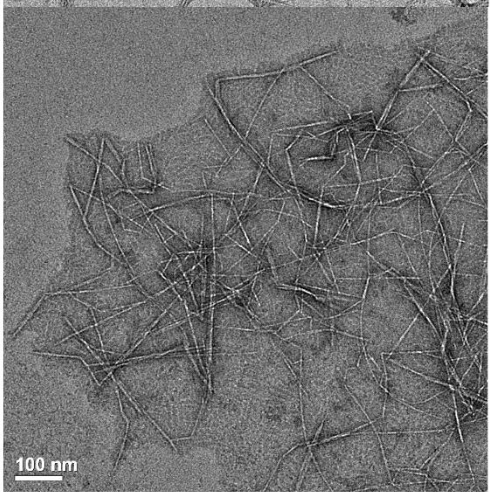
1



Average width based on >60 nanofibrils: 6.9 nm

Standard deviation: 1.4 nm

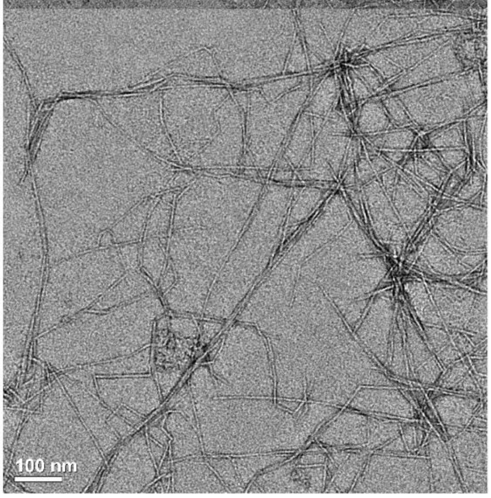
2



Average width based on >60 nanofibrils: 6.3 nm

Standard deviation: 1.3 nm

3



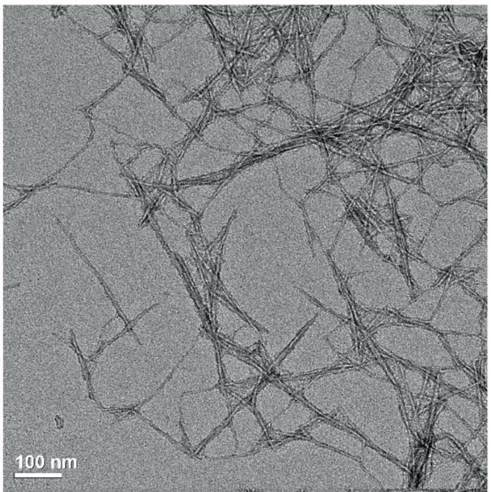
Average width based on >60 nanofibrils: 7.4 nm

Standard deviation: 2.5 nm

TEMPO-oxidized CNF (high charge)

Sample # | TEM

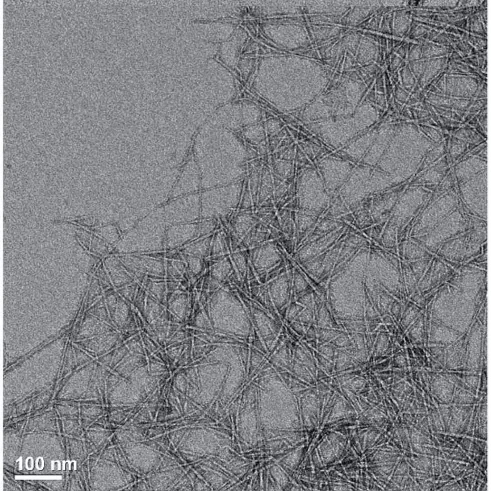
4



Average width based on >60 nanofibrils: 6.9 nm

Standard deviation: 2.3 nm

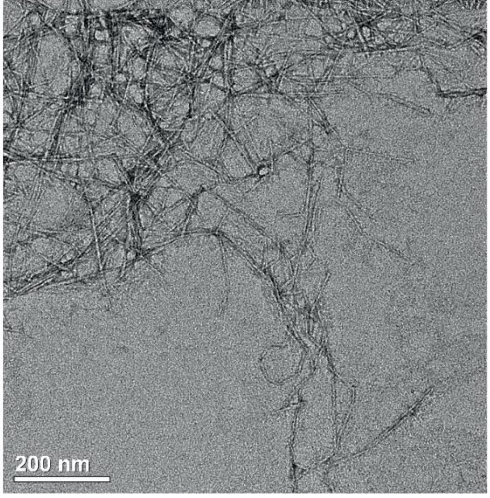
5



Average width based on >60 nanofibrils: 6.0 nm

Standard deviation: 2.4 nm

6



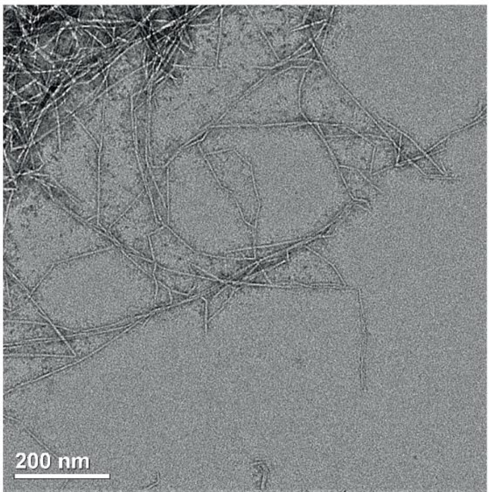
Average width based on >60 nanofibrils: 7.1 nm

Standard deviation: 1.5 nm

Carboxymethylated CNF (lowest charge)

Sample #	TEM	

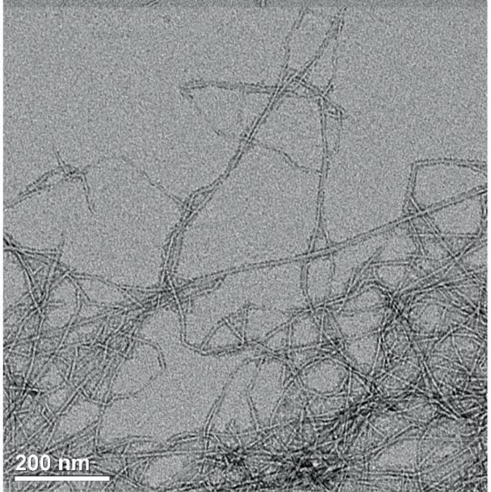
7



Average width based on >60 nanofibrils: 6.2 nm

Standard deviation: 1.1 nm

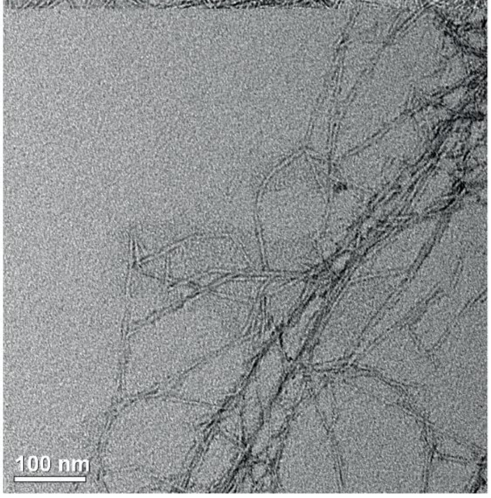
8



Average width based on >60 nanofibrils: 5.9 nm

Standard deviation: 1.1 nm

9



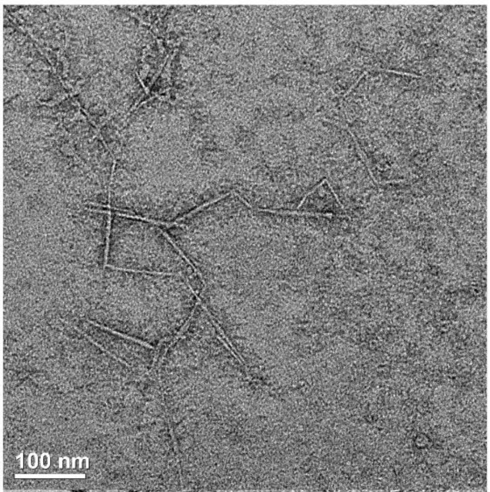
Average width based on >60 nanofibrils: 6.1 nm

Standard deviation: 1.2 nm

Carboxymethylated CNF (low charge)

Sample # | TEM

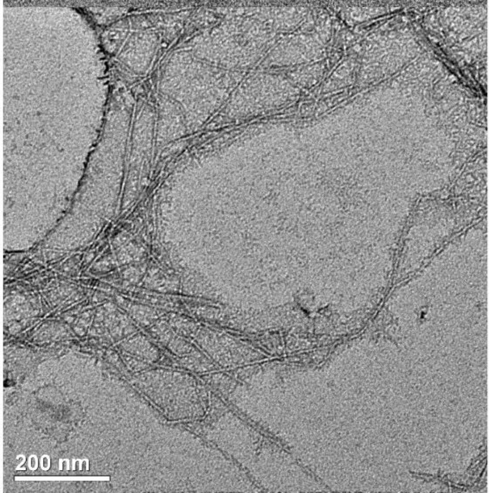
10



Average width based on >60 nanofibrils: 6.3 nm

Standard deviation: 1.3 nm

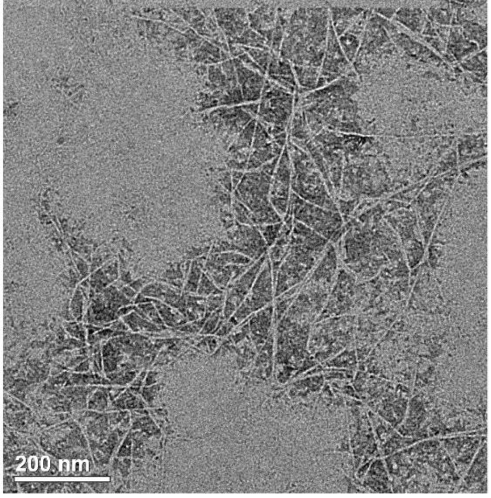
11



Average width based on >60 nanofibrils: 5.8 nm

Standard deviation: 1.2 nm

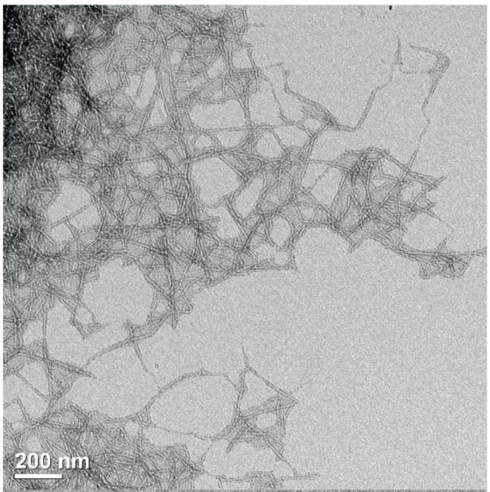
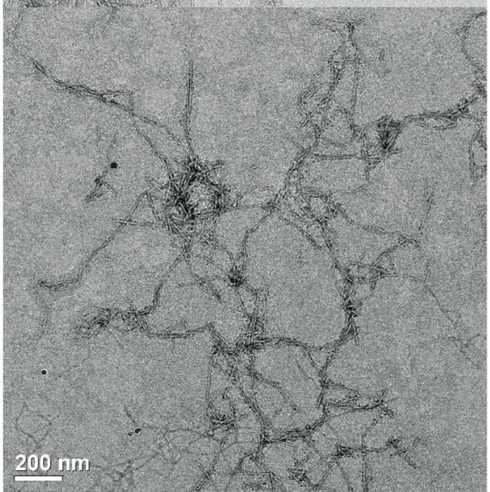
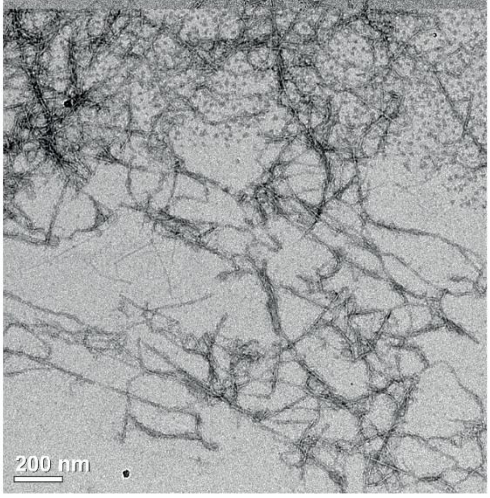
12



Average width based on >60 nanofibrils: 5.9 nm

Standard deviation: 1.2 nm

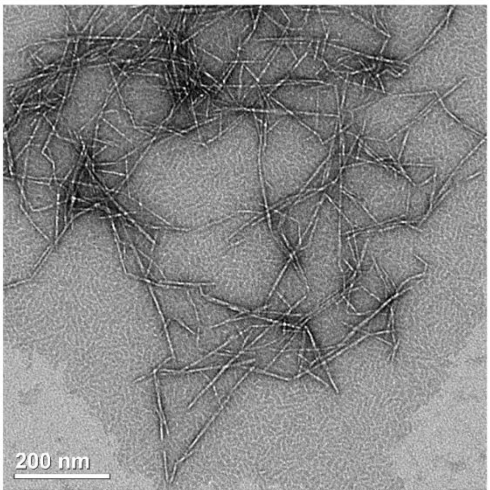
Carboxymethylated CNF (high charge)

Sample #	TEM	
13		Average width based on >60 nanofibrils: 8.2 nm Standard deviation: 2.0 nm
14		Average width based on >60 nanofibrils: 5.0 nm Standard deviation: 1.0 nm
15		Average width based on >60 nanofibrils: 6.9 nm Standard deviation: 1.3 nm

Carboxymethylated CNF (highest charge)

Sample # TEM

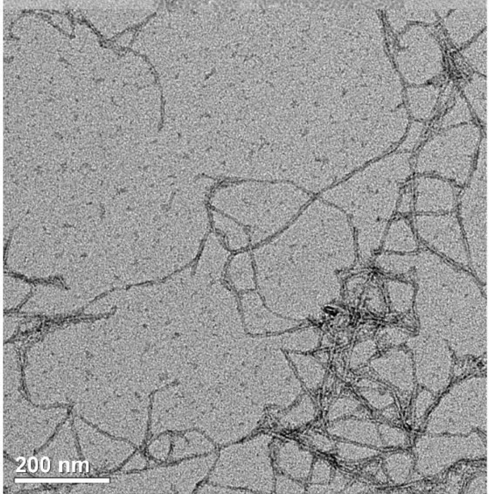
16



Average width based on >60 nanofibrils: 7.7 nm

Standard deviation: 1.8 nm

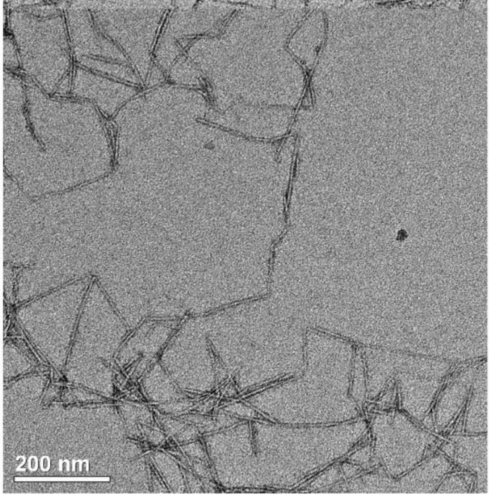
17



Average width based on >60 nanofibrils: 6.8 nm

Standard deviation: 2.0 nm

18



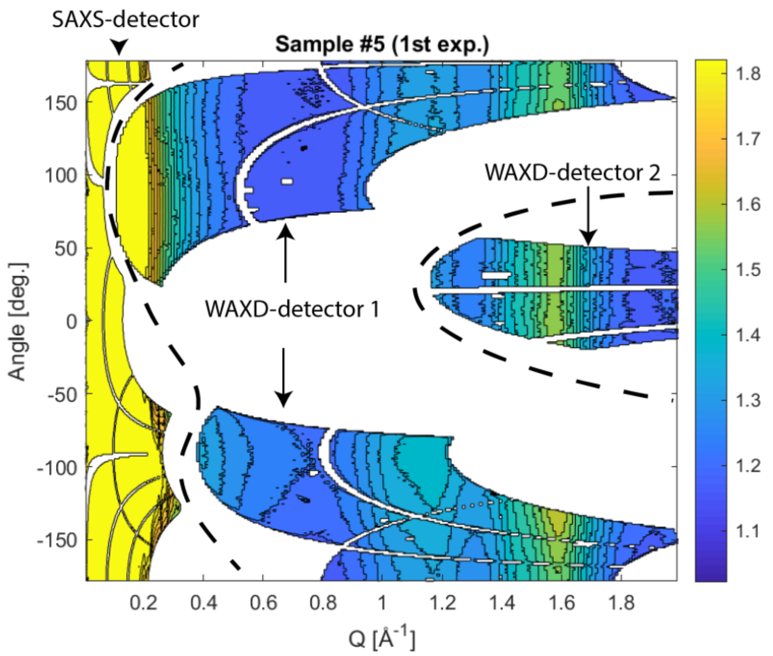
Average width based on >60 nanofibrils: 6.1 nm

Standard deviation: 1.2 nm

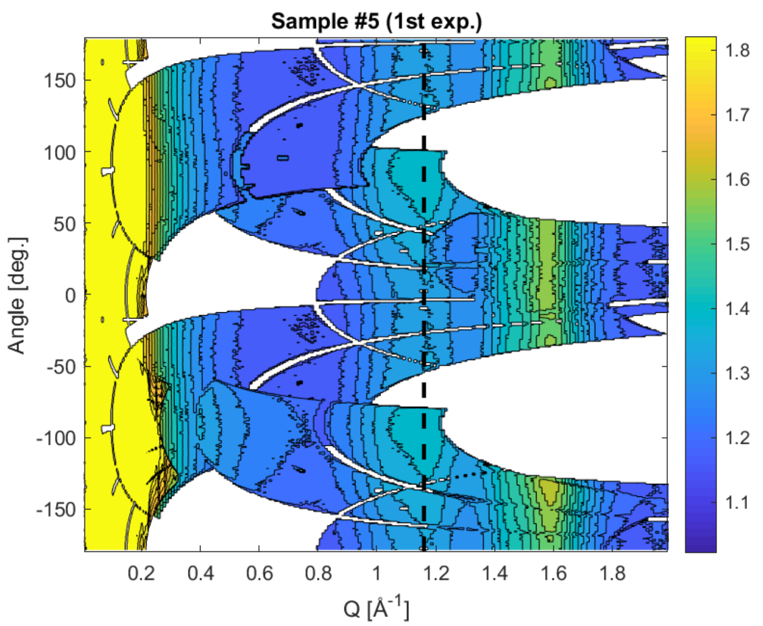
WAXD experiments: ensuring isotropy of samples

Procedure:

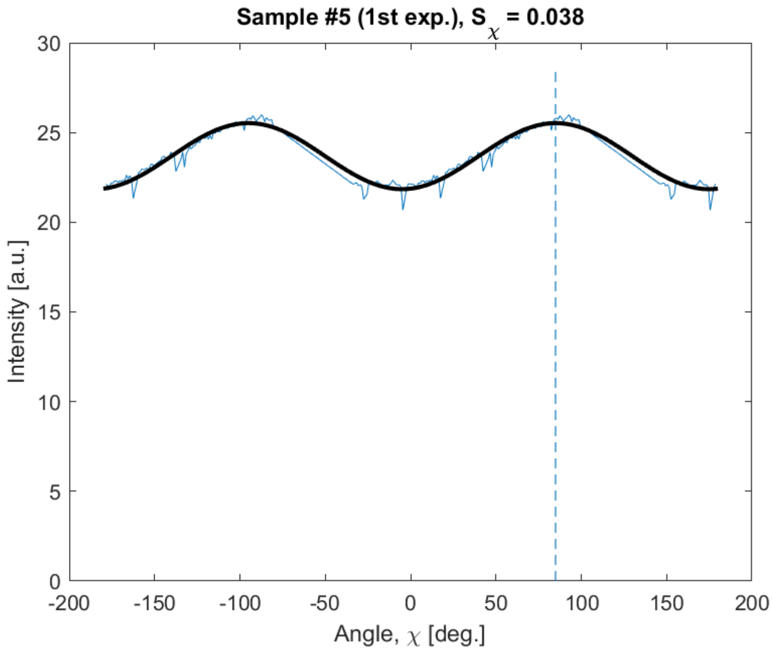
Simultaneous SAXS and WAXD signals were recorded on 3 different detectors (average of 5 different measurement locations, each with 1 s exposure):



The in-accessible (zero) pixels at an angle χ are corrected with data from the corresponding mirror-pixel (if accessible) at $\chi \pm 180°$, due to symmetry:



Note that this mirror-correction does not lead to a perfect matching owing to differences in the intensity due to slight detector tilt. The orientation distribution is evaluated at the location of the (110)-peak at $q = 1.16$ Å^{-1} (thick dashed black line; note that the data at this q-value is only taken from one detector, *i.e.* WAXD-detector 1):



The raw intensity $I(\chi)$ is fitted to a function of form:

$$I_{fit}(\chi) = A\cos\big(2(\chi - \chi_{tilt})\big) + B,$$

where χ_{tilt} indicates the tilt angle (dashed blue line in figure). The order parameter S_χ is calculated through:

$$S_\chi = \int_{-180^\circ}^{180^\circ} I_{fit}(\chi)(2\cos^2(\chi - \chi_{tilt}) - 1)d\chi,$$

Where $I_{fit}(\chi)$ initially is normalized according to:

$$1 = \int_{-180^\circ}^{180^\circ} I_{fit}(\chi)d\chi.$$

Results:

The order parameter of all samples in the study are presented in the table below. Note that every sample was measured in two separate experiments (at different locations).

Sample #	S_χ (1st exp.)	S_χ (2nd exp.)
1	0.023	0.014
2	0.029	0.022
3	0.008	0.016
4	0.016	0.042
5	0.038	0.020
6	0.007	0.009
7	0.002	0.039
8	0.027	0.024
9	0.014	0.016
10	0.006	0.011
11	0.018	0.051
12	0.016	0.029
13	0.025	0.025
14	0.008	0.046
15	0.015	0.015
16	0.032	0.037
17	0.012	0.018
18	0.004	0.008

Since all the samples have an order parameter that fulfill $S_\chi \ll 0.1$, we can safely assume the samples to be isotropic.

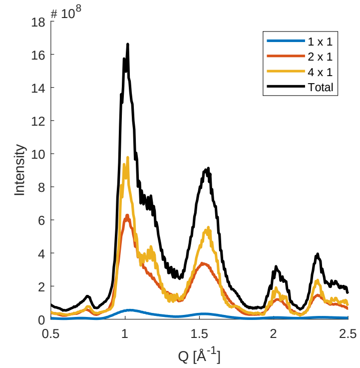
WAXD simulations: Results

Form factor of a CNF chain with semi-axes

1 Å x 1 Å

Model: H1+

Aggregation direction: (1-10)

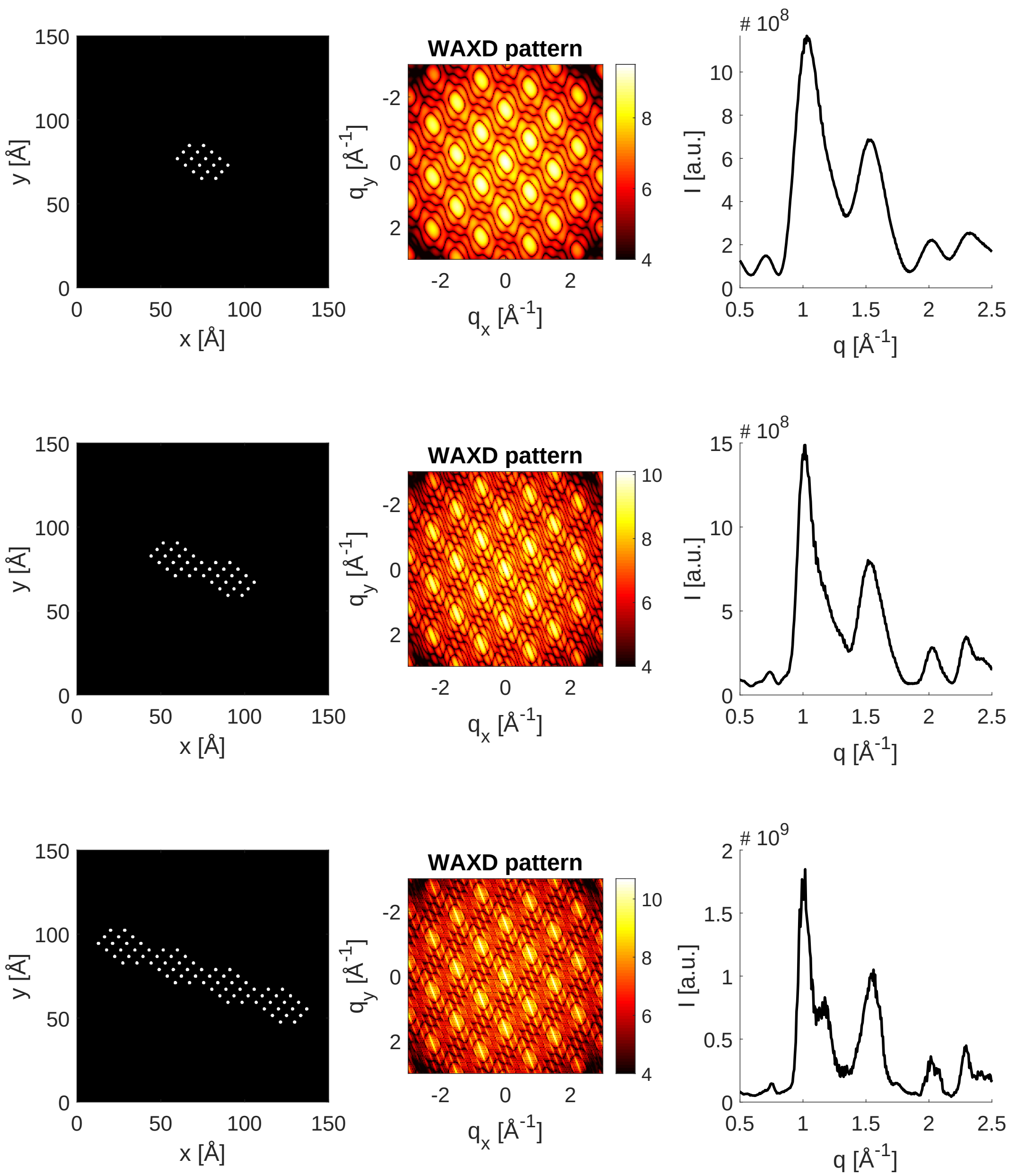


Sample #1

Vol% 1x1: 4.7

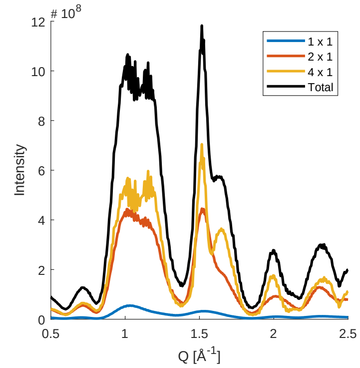
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: H1+

Aggregation direction: (110)

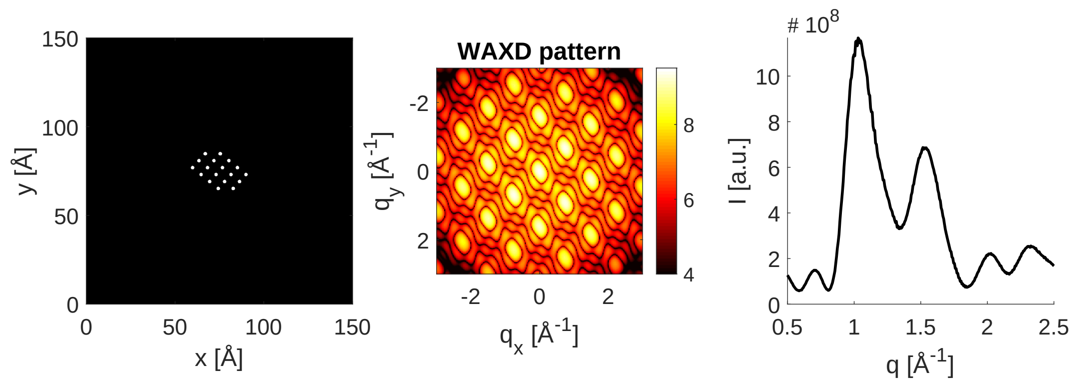


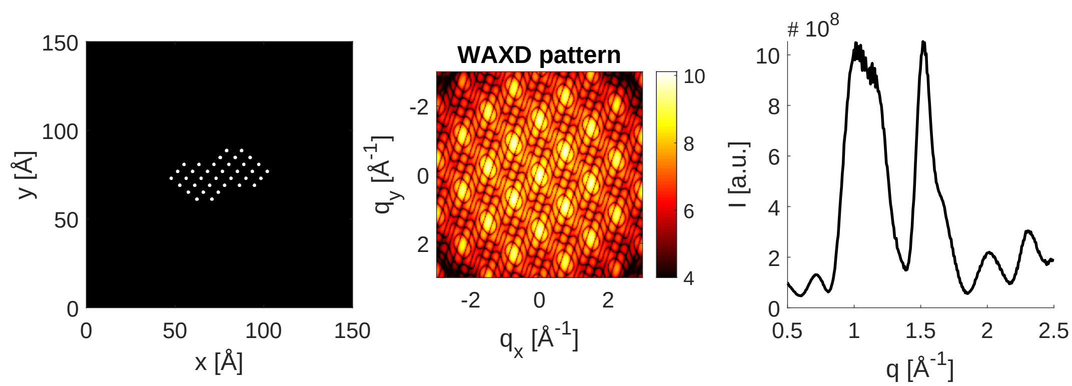
Sample #1

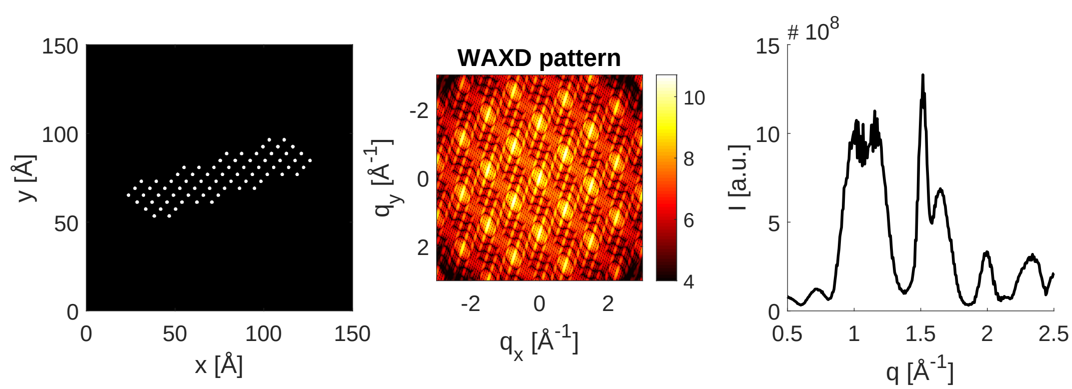
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

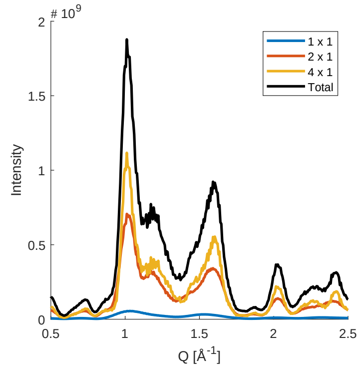






Model: H1+

Aggregation direction: (200)



Sample #1

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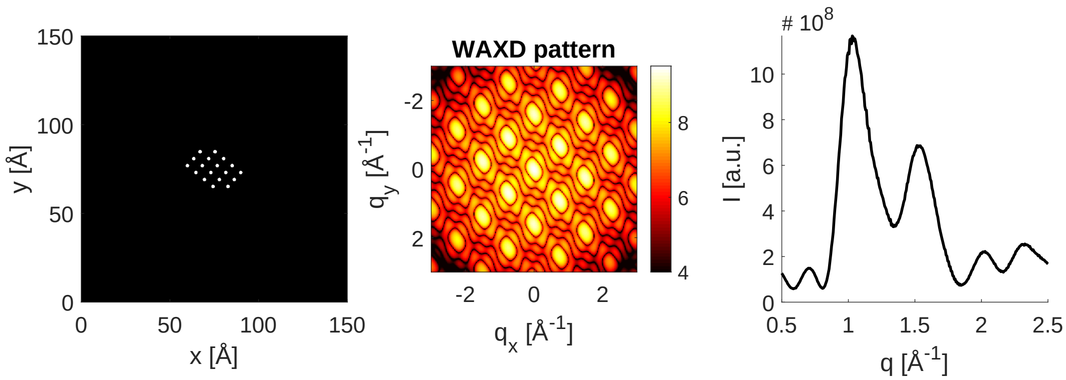
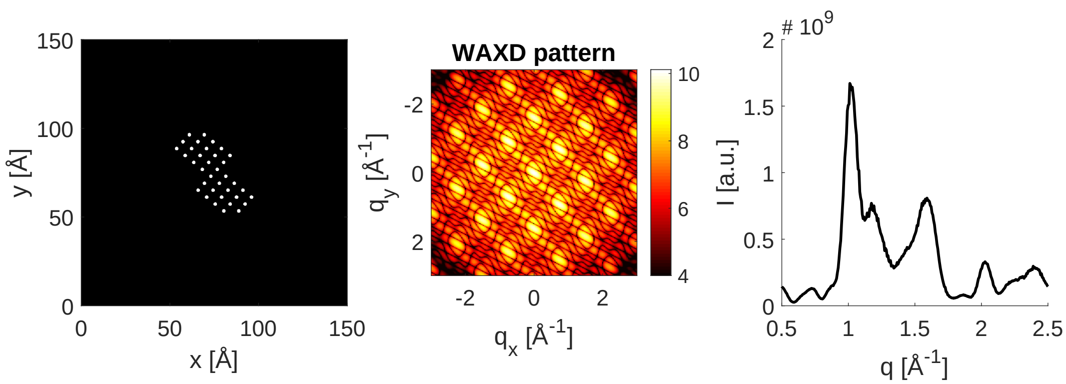
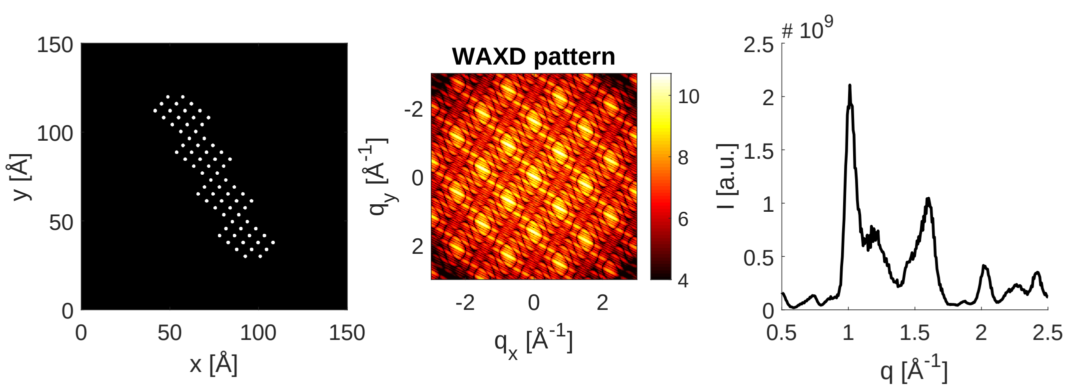
Vol% 4x1: 53.0

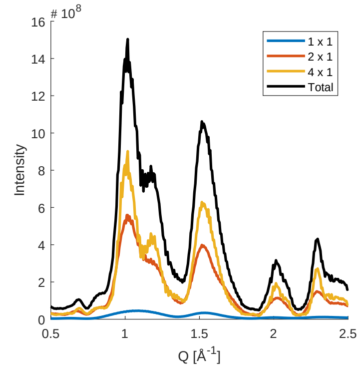






Model: H1-

Aggregation direction: (1-10)

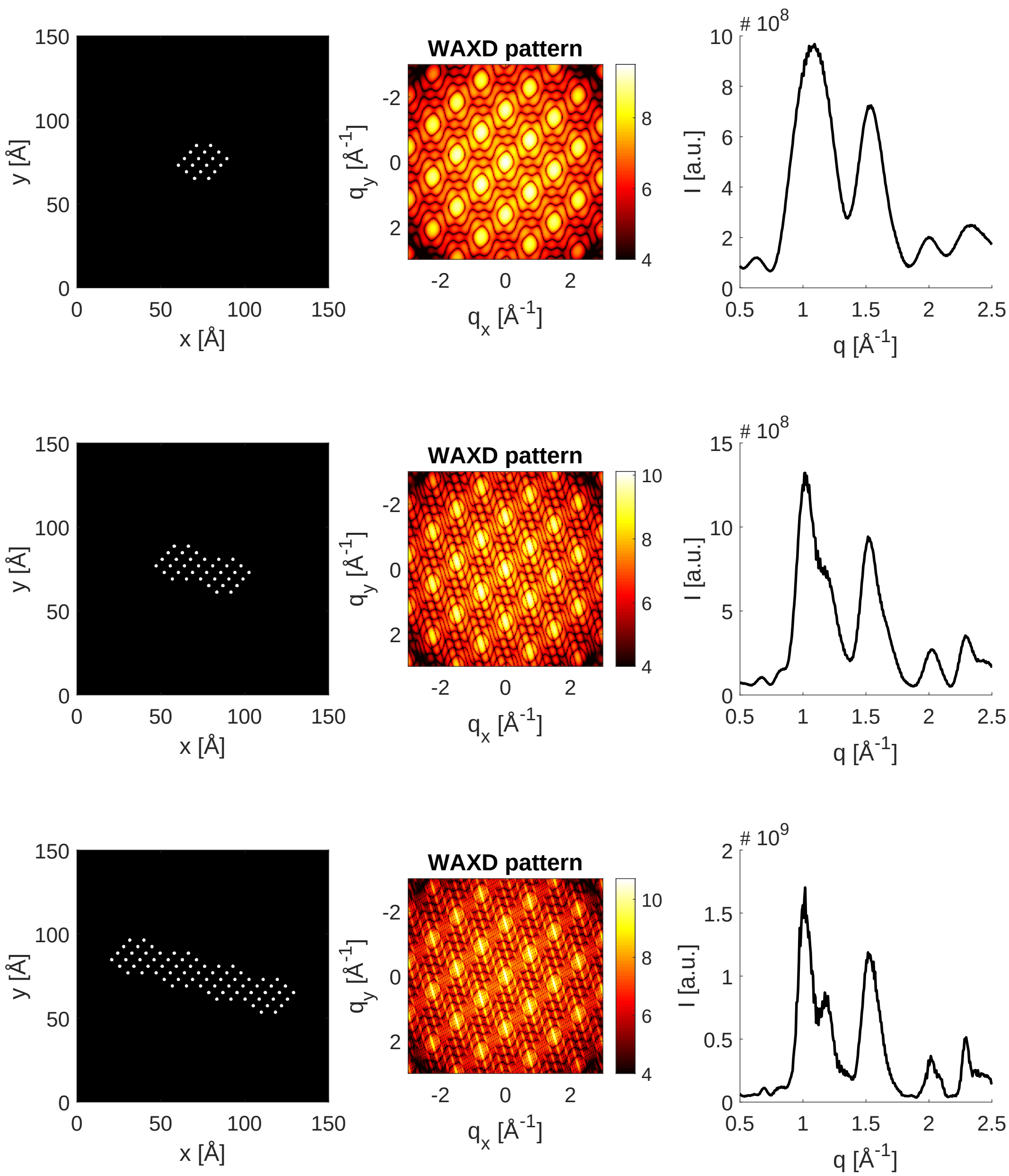


Sample #1

Vol% 1x1: 4.7

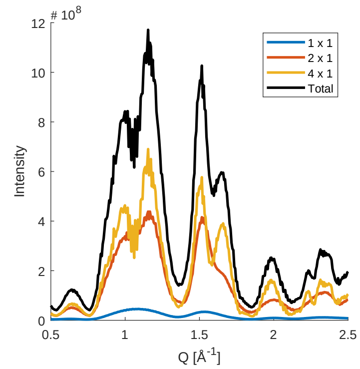
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: H1-

Aggregation direction: (110)



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Vol% 1x1: 4.7

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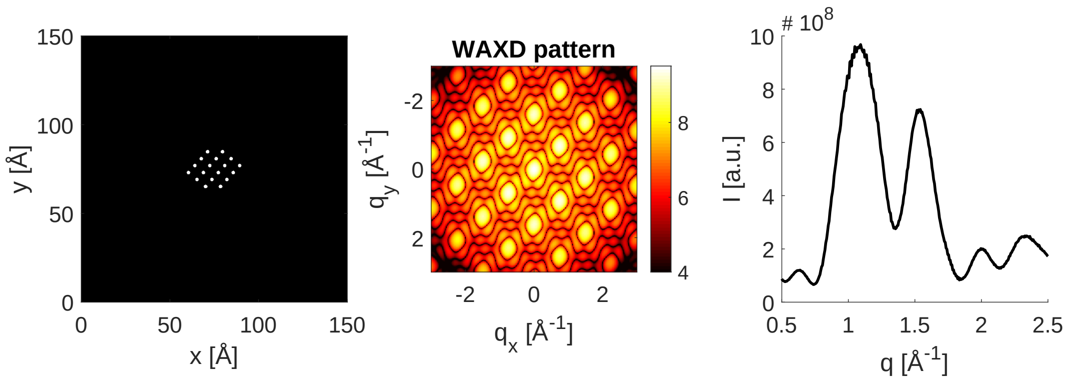
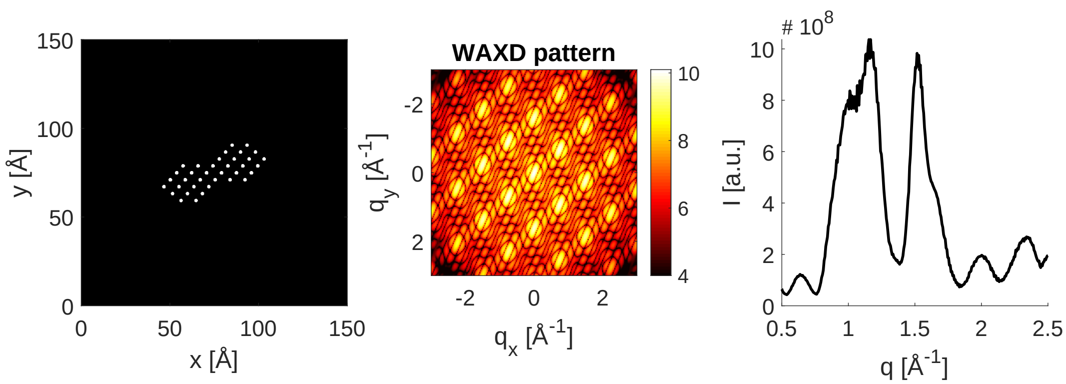
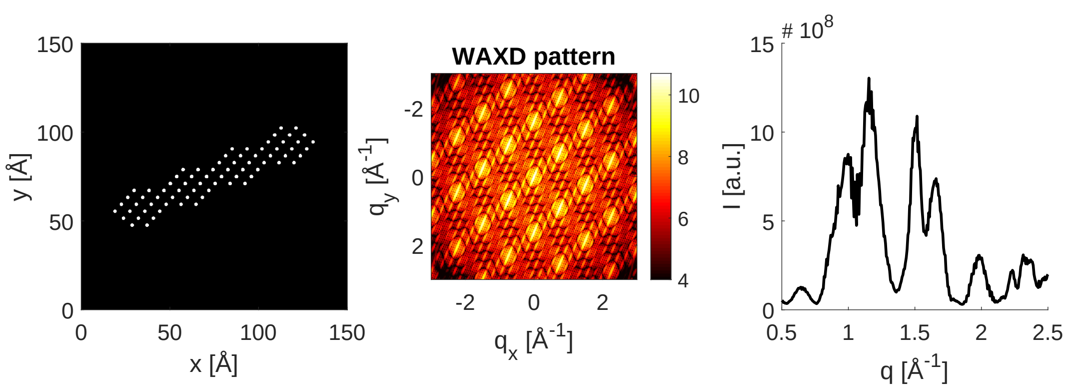
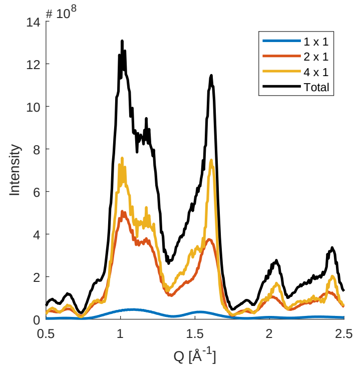






Model: H1-

Aggregation direction: (200)



Sample #1

Vol% 1x1: 4.7

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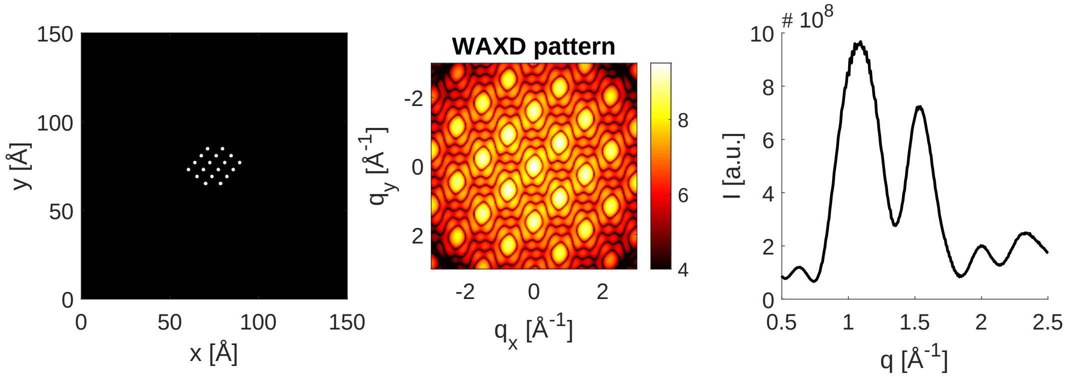
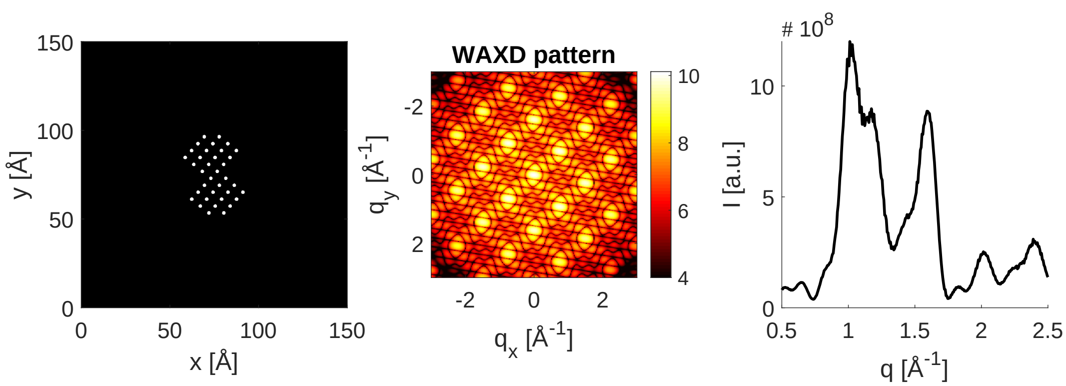
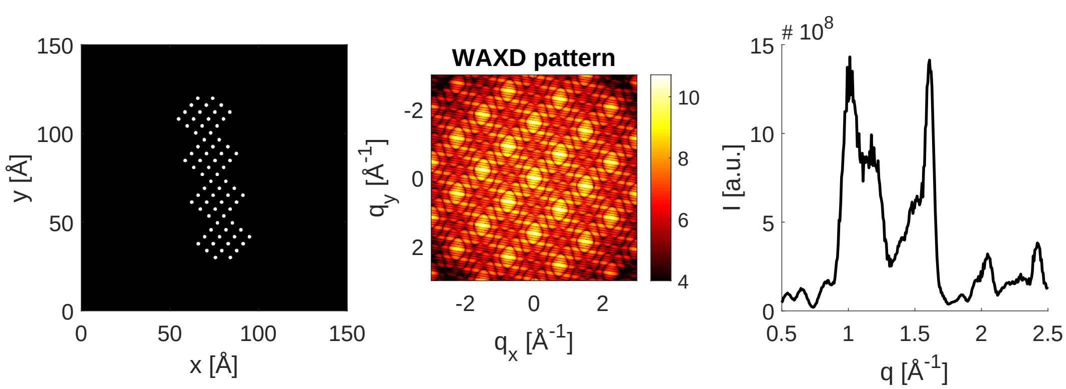
Vol% 4x1: 53.0

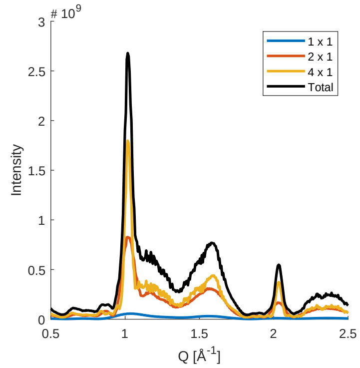






Model: H2+

Aggregation direction: (1-10)

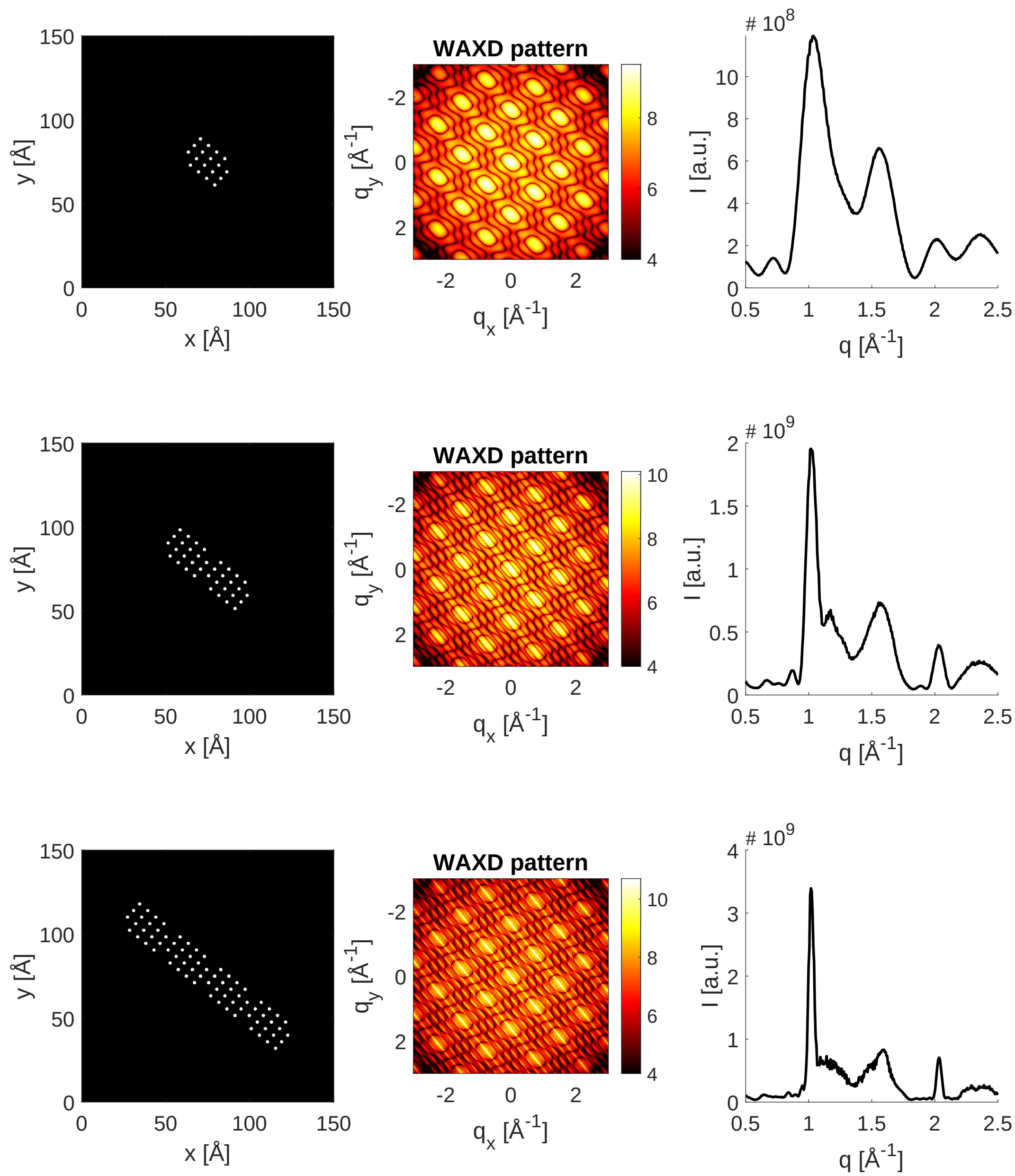


Sample #1

Vol% 1x1: 4.7

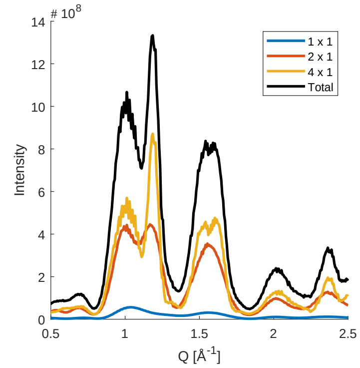
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: H2+

Aggregation direction: (110)

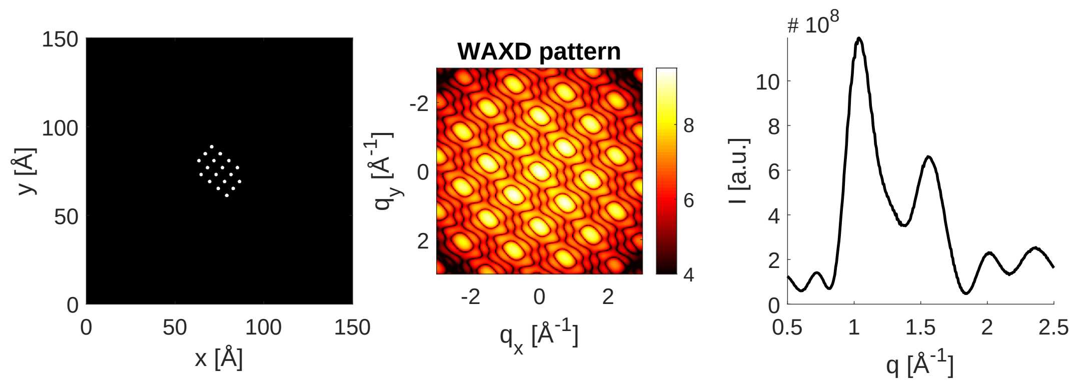


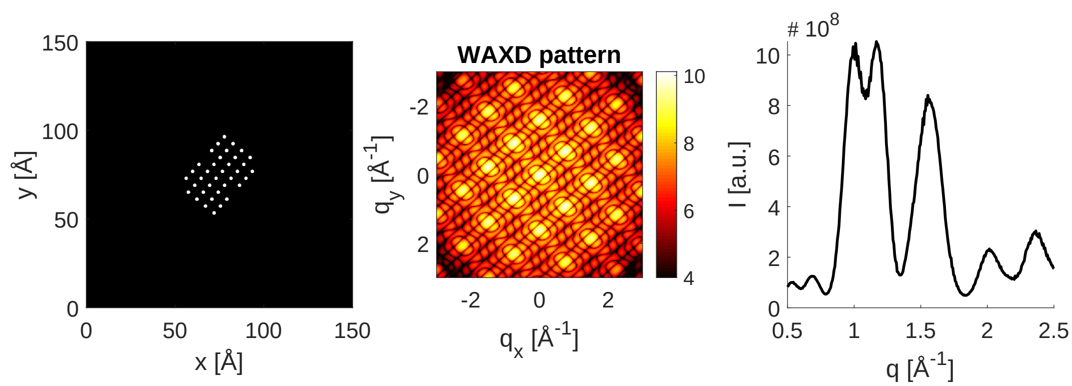
Sample #1

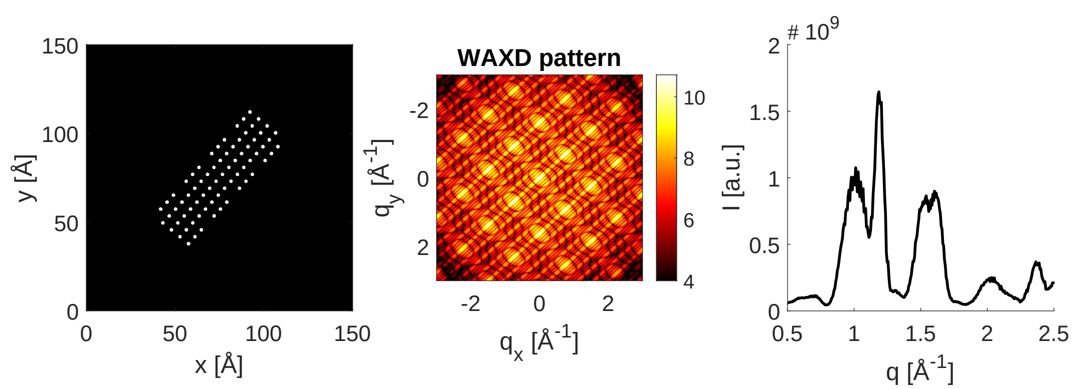
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

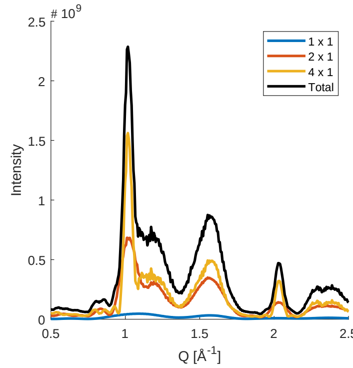






Model: H2-

Aggregation direction: (1-10)



Sample #1

Vol% 1x1: 4.7

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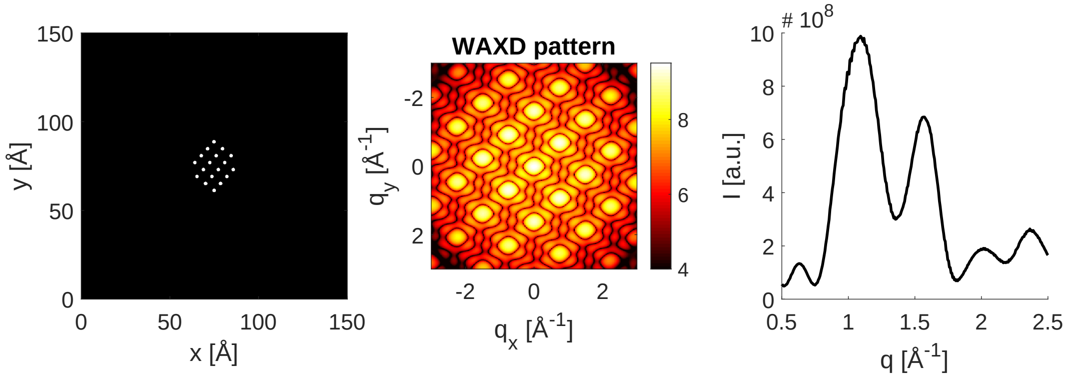
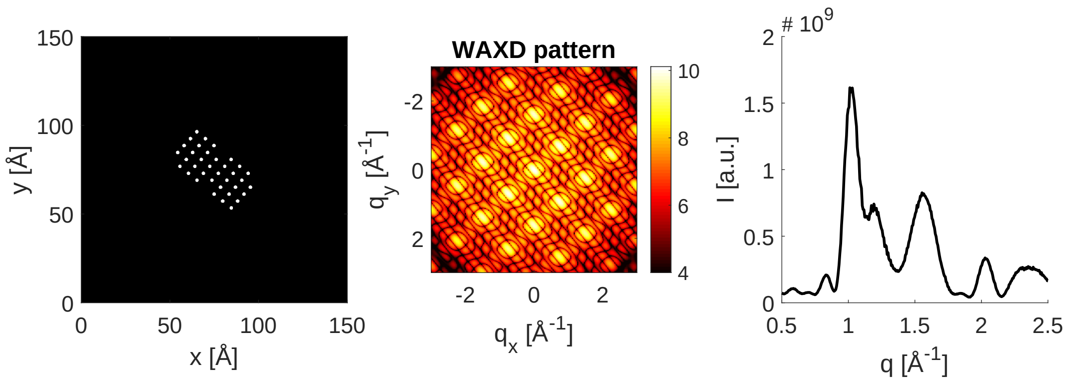
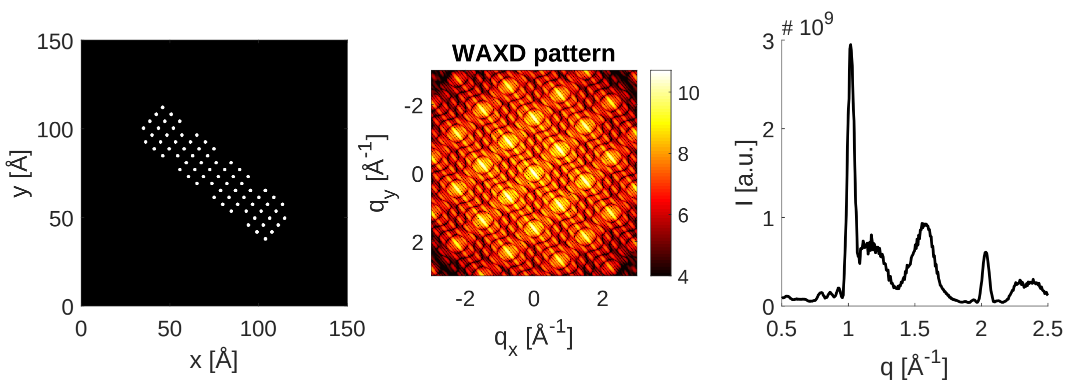
Vol% 4x1: 53.0

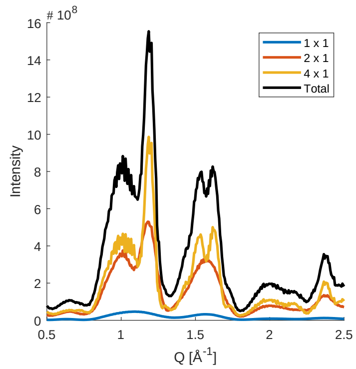






Model: H2-

Aggregation direction: (110)



Sample #1

Vol% 1x1: 4.7

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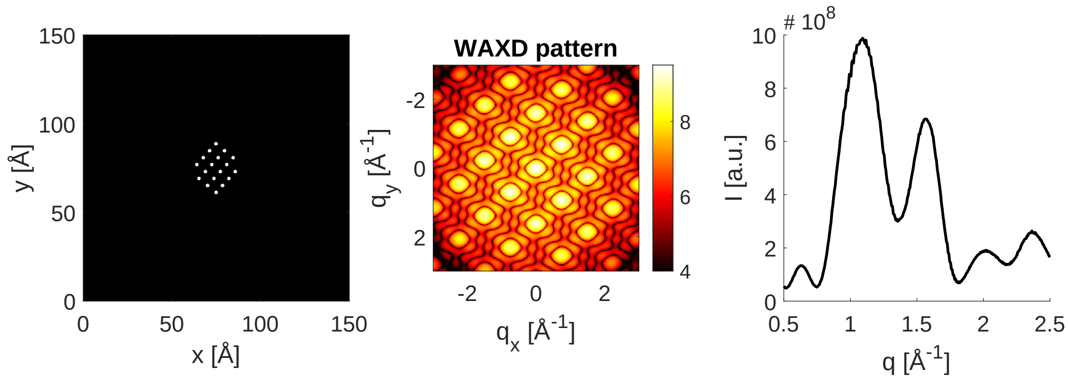
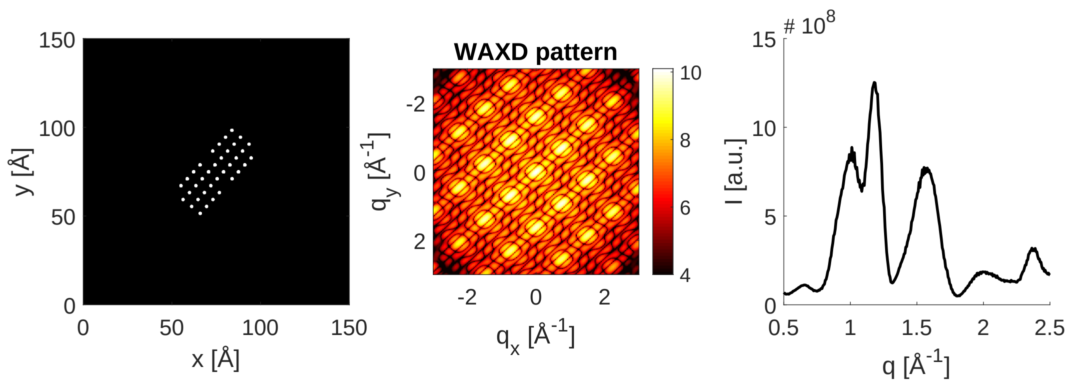
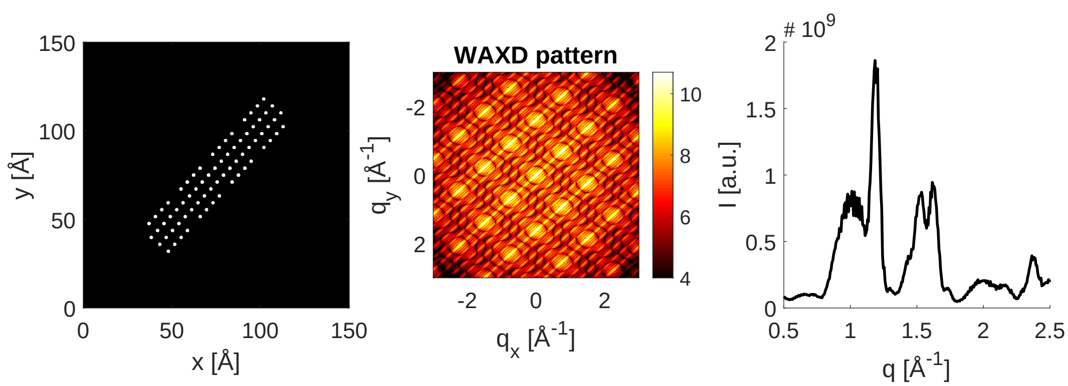
Vol% 4x1: 53.0

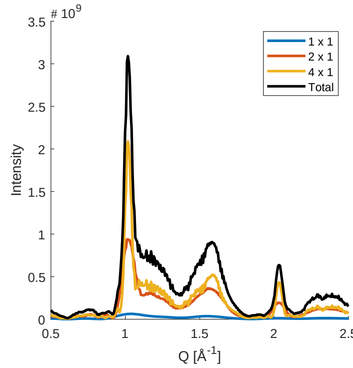






Model: R1+

Aggregation direction: (1-10)

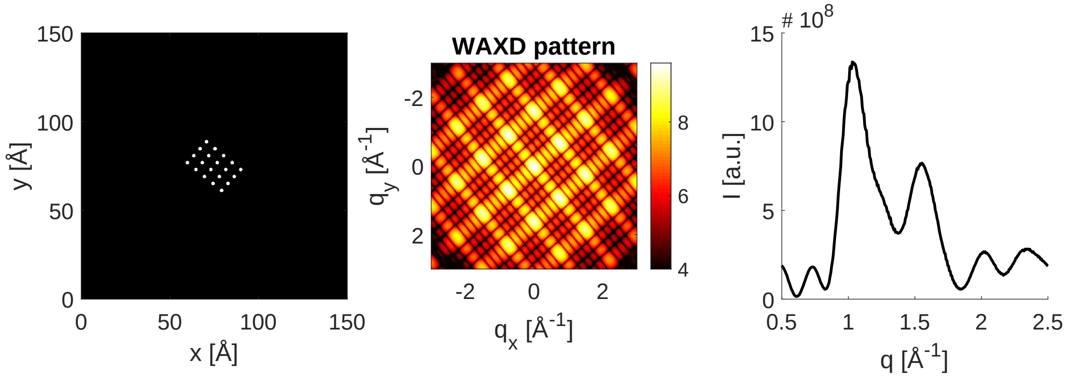


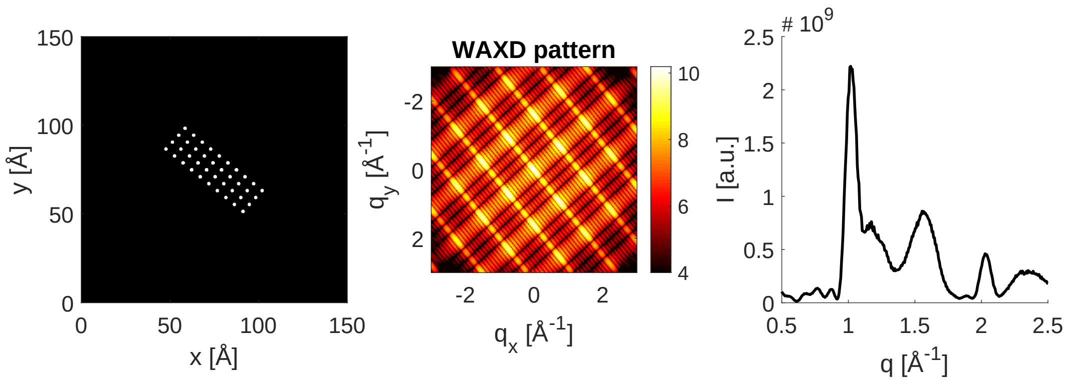
Sample #1

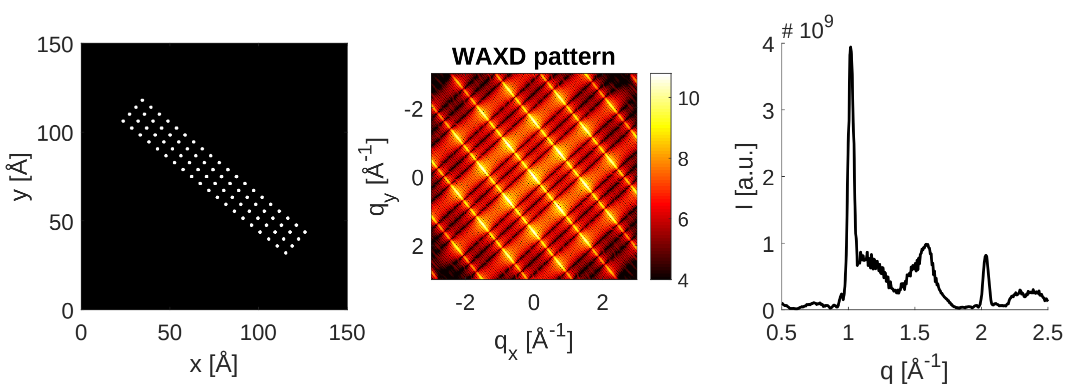
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

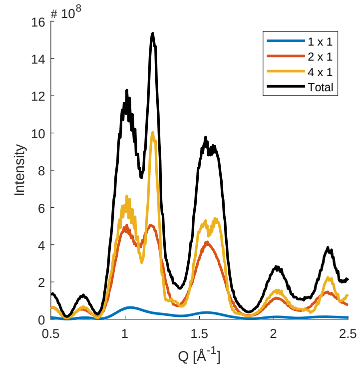






Model: R1+

Aggregation direction: (110)

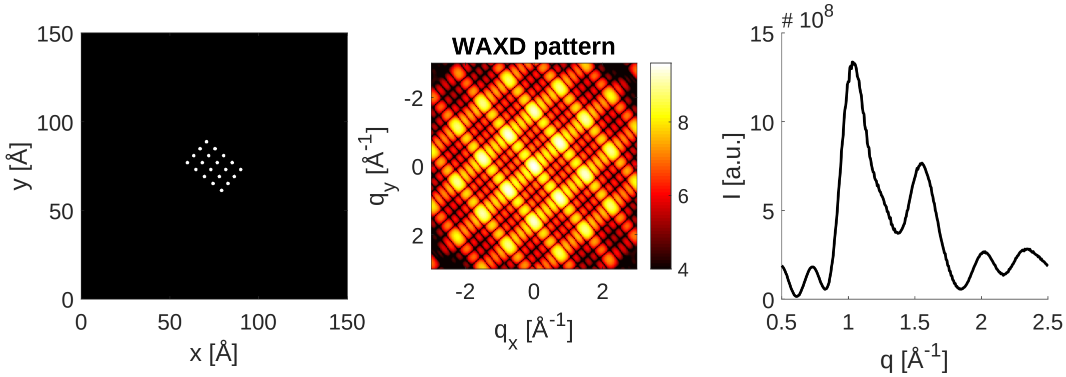


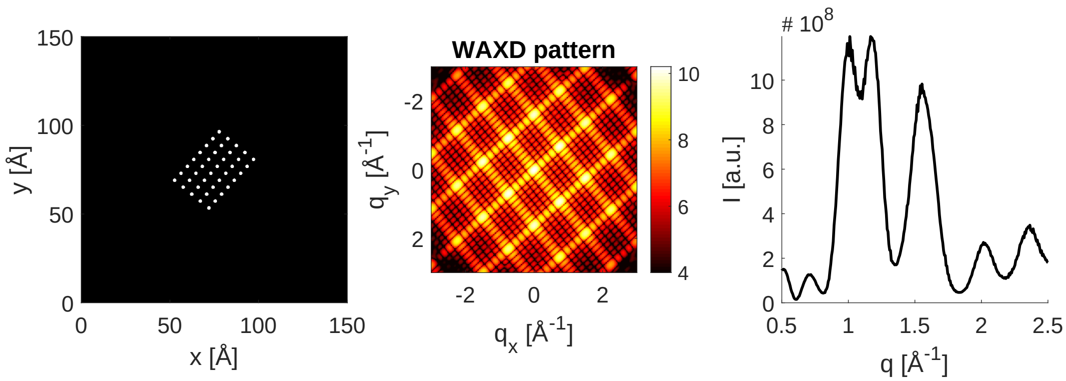
Sample #1

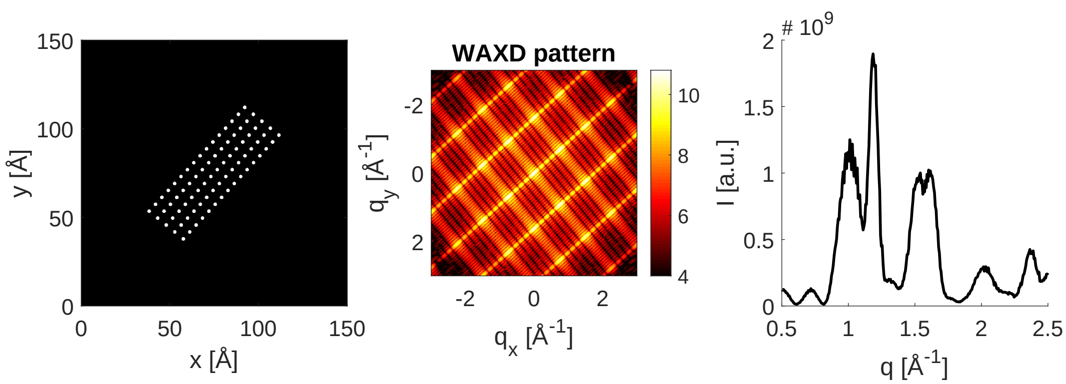
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

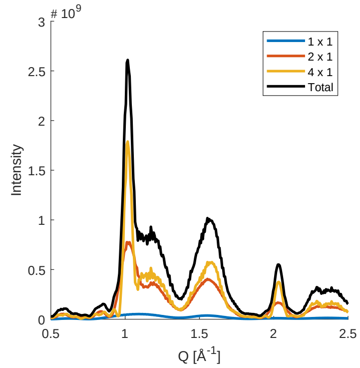






Model: R1-

Aggregation direction: (1-10)

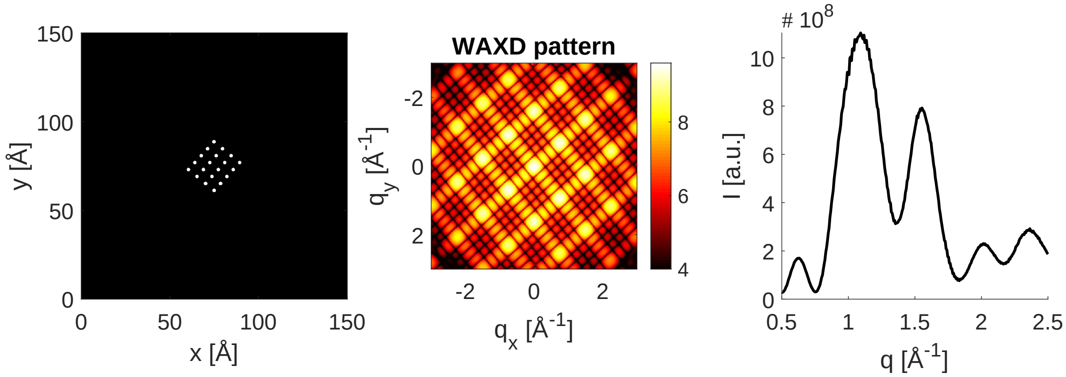


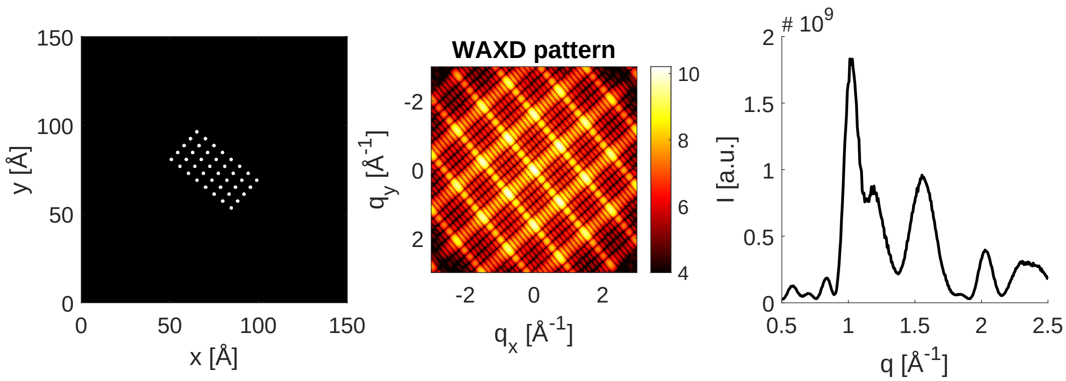
Sample #1

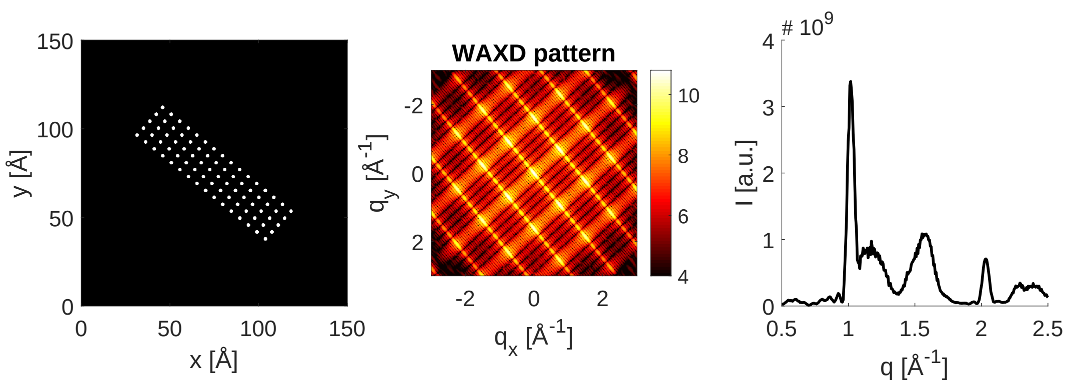
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

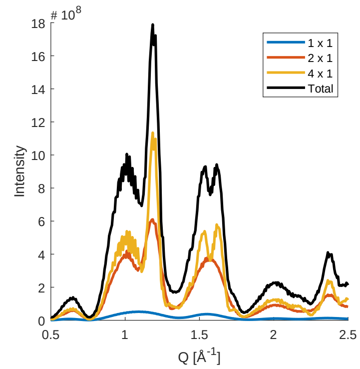






Model: R1-

Aggregation direction: (110)

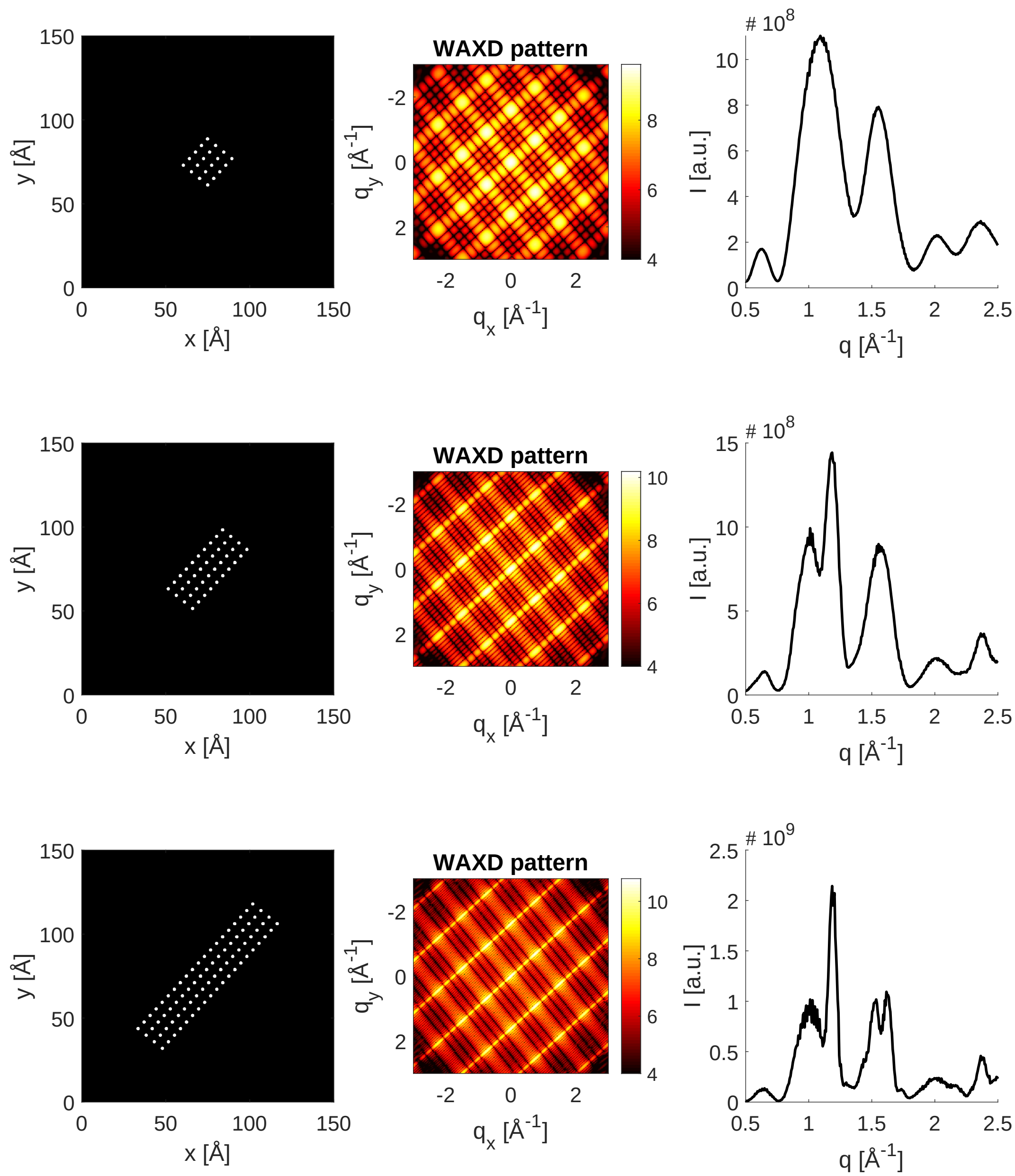


Sample #1

Vol% 1x1: 4.7

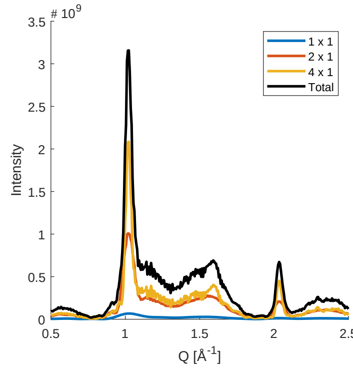
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: R2+

Aggregation direction: (1-10)

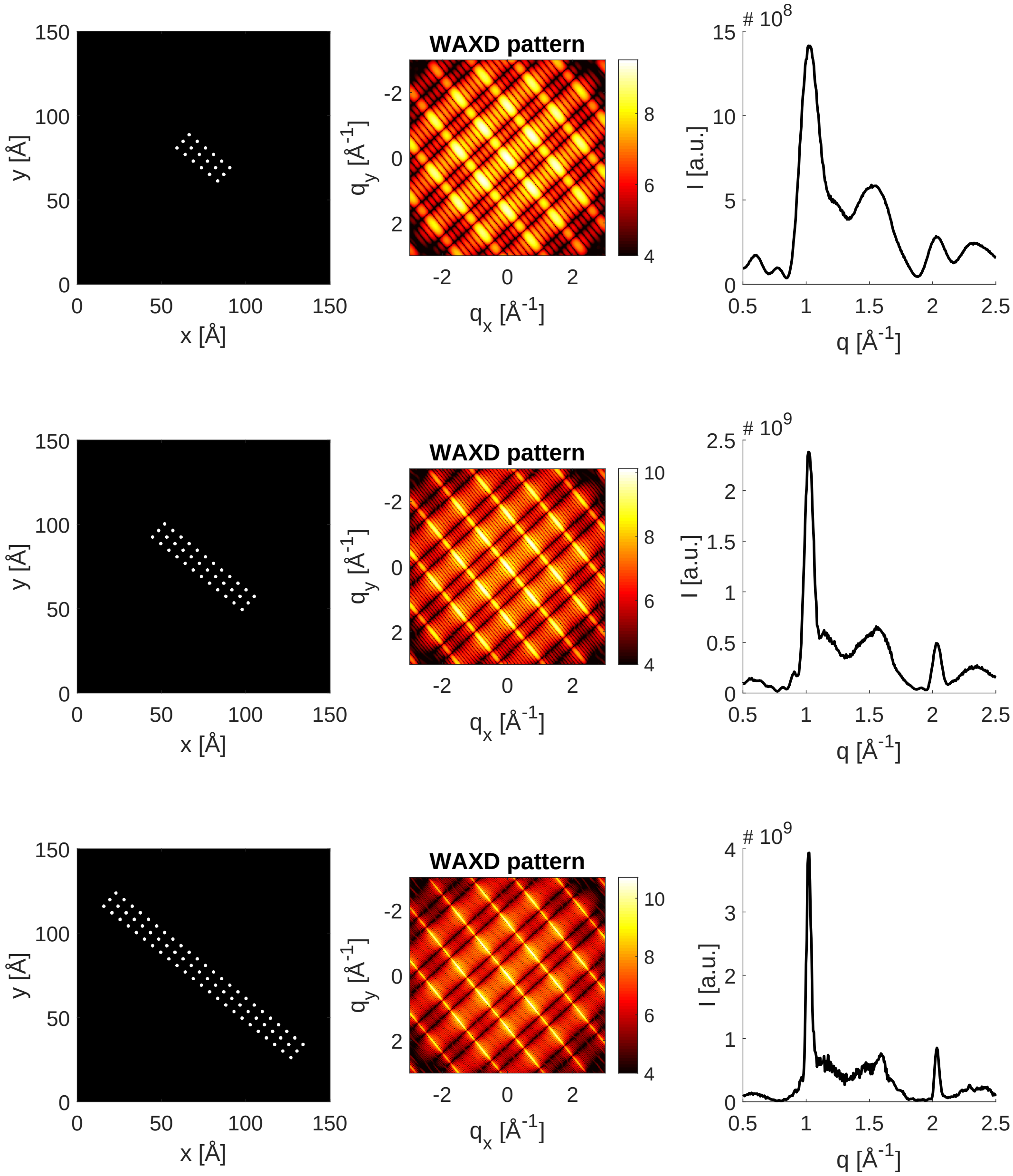


Sample #1

Vol% 1x1: 4.7

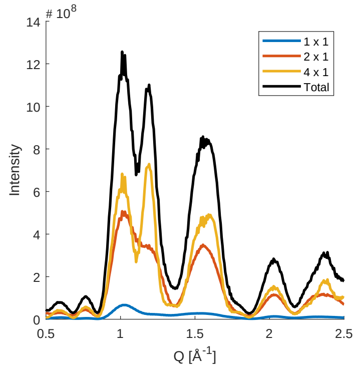
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: R2+

Aggregation direction: (110)

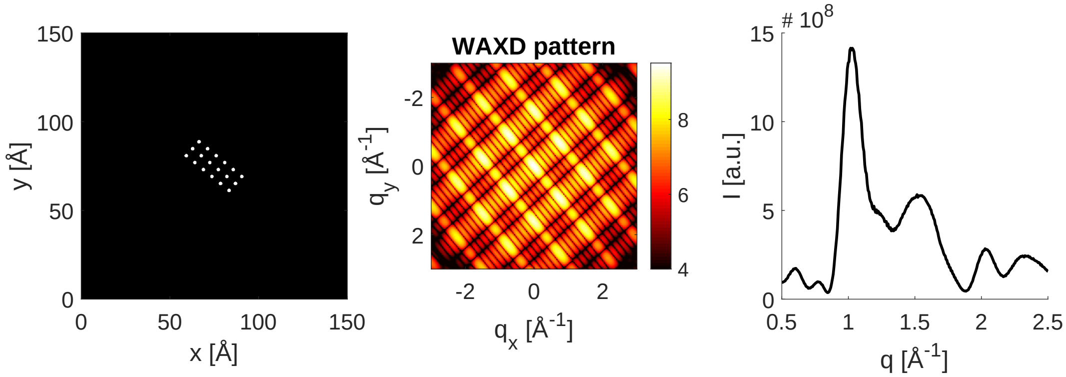


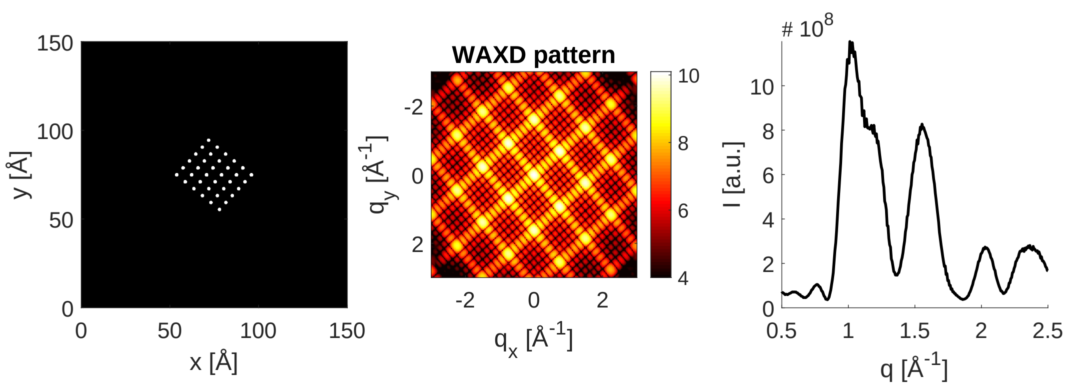
Sample #1

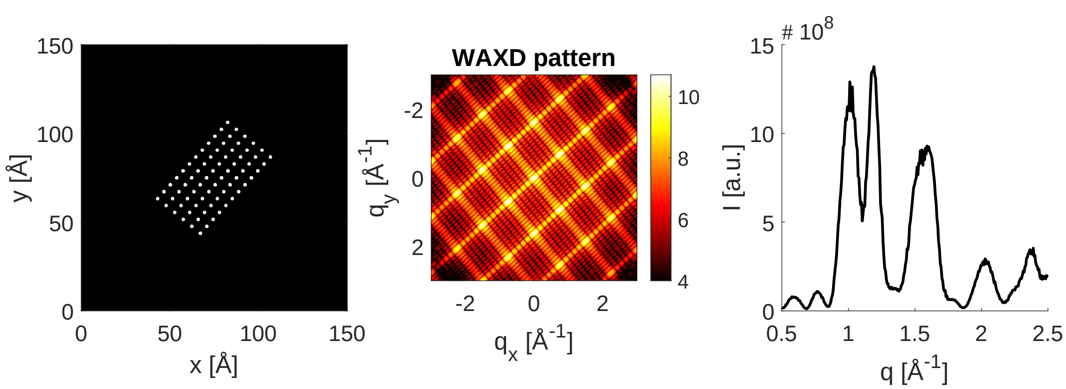
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

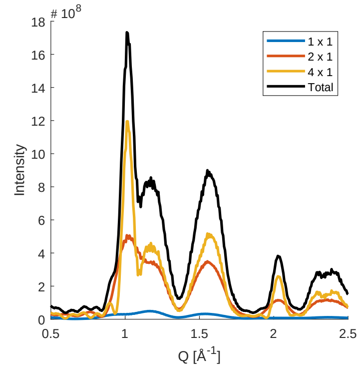






Model: R2-

Aggregation direction: (1-10)

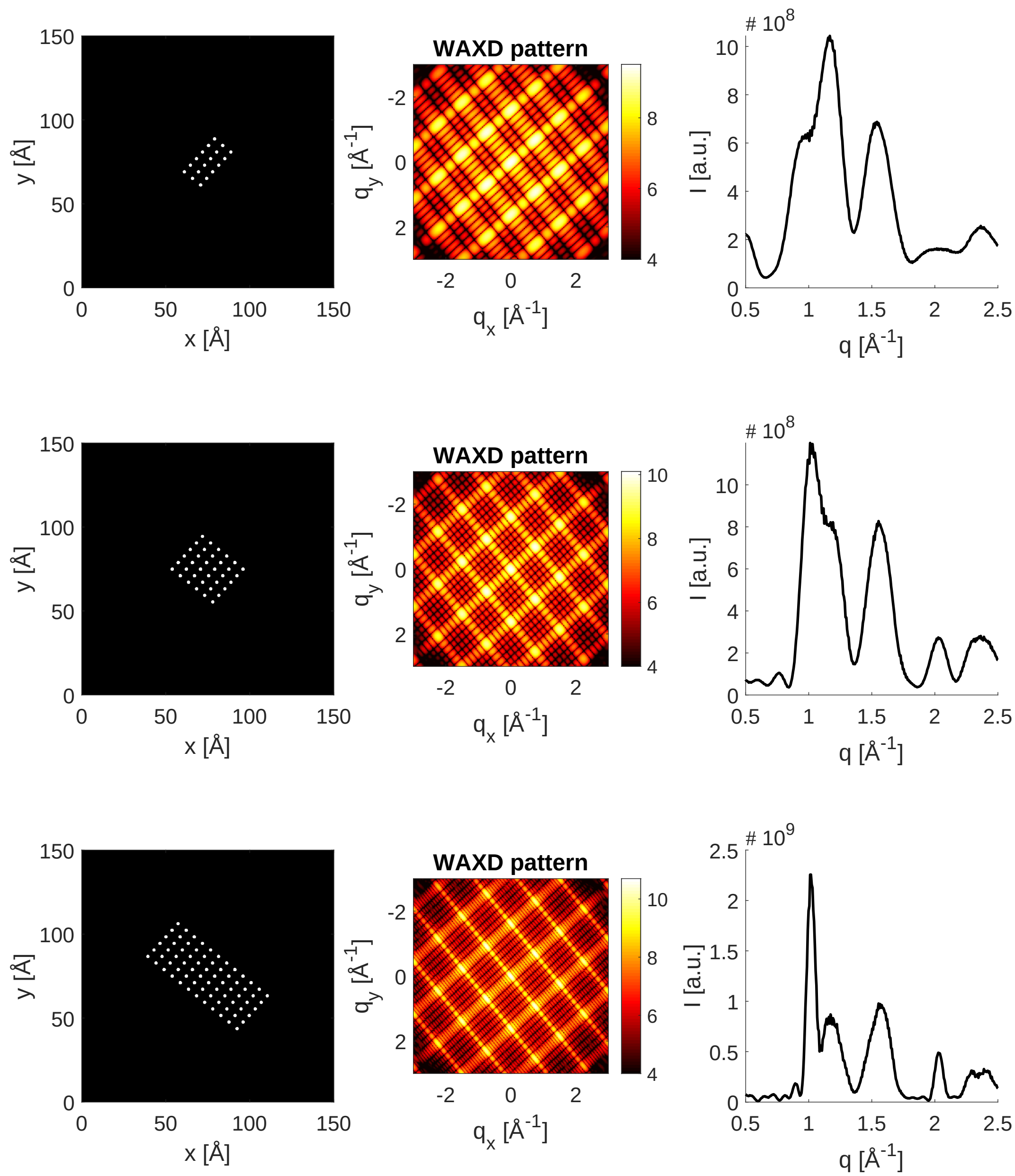


Sample #1

Vol% 1x1: 4.7

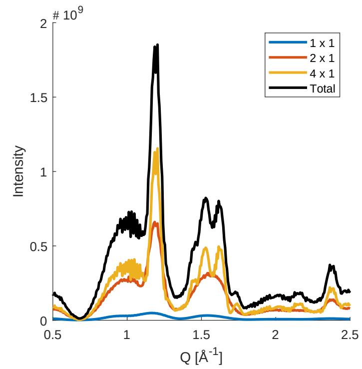
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: R2-

Aggregation direction: (110)

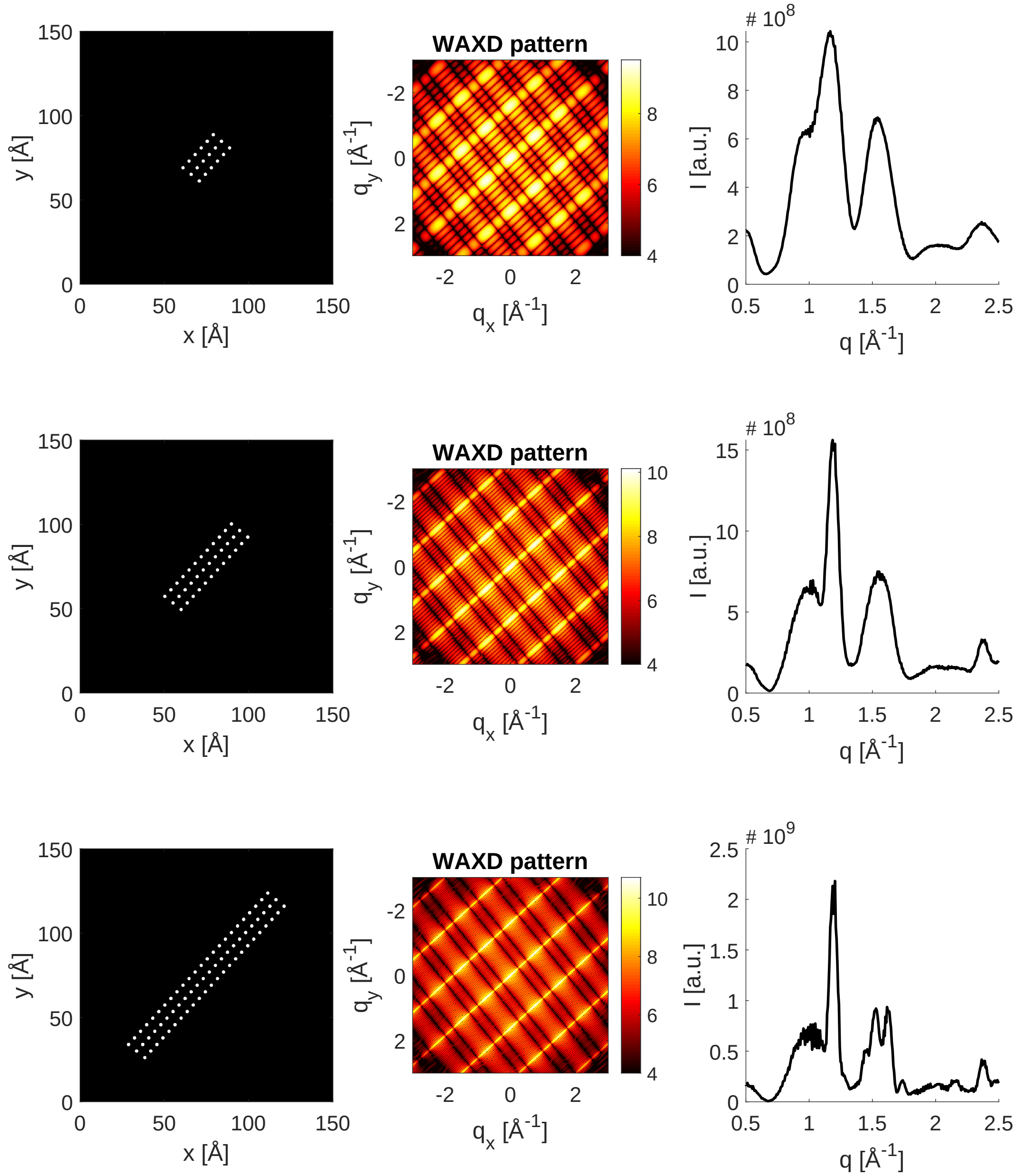


Sample #1

Vol% 1x1: 4.7

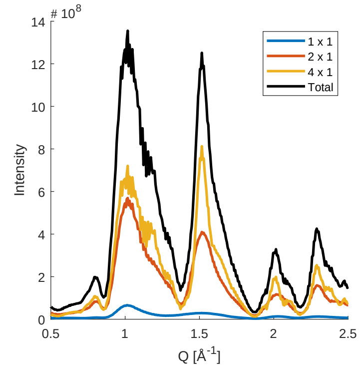
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: Rh1+

Aggregation direction: (110)

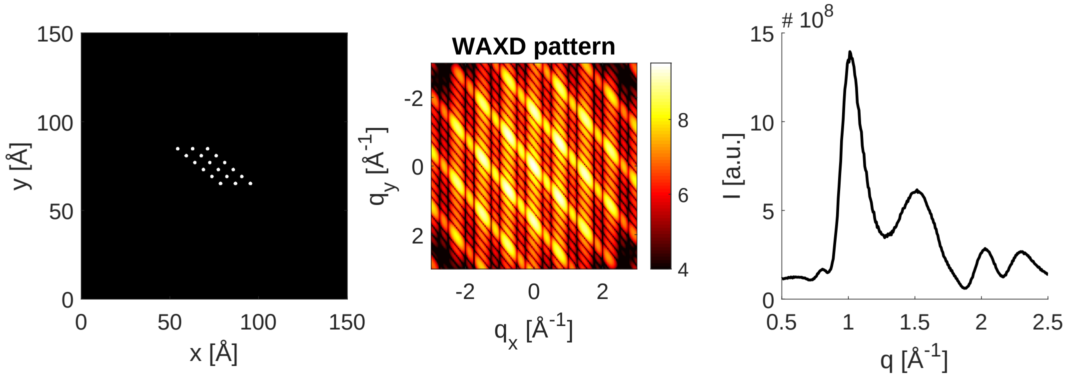


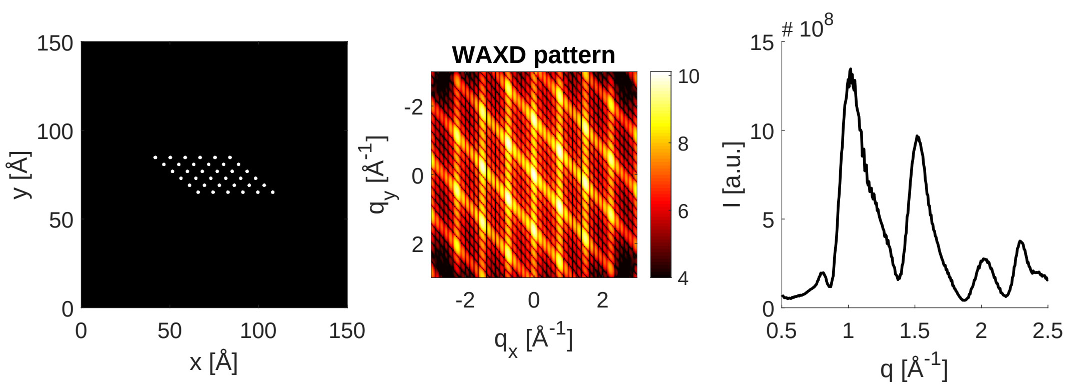
Sample #1

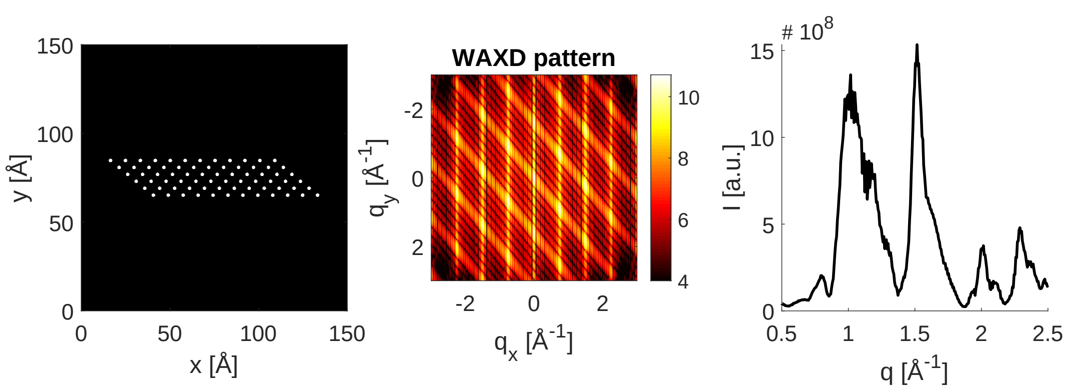
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

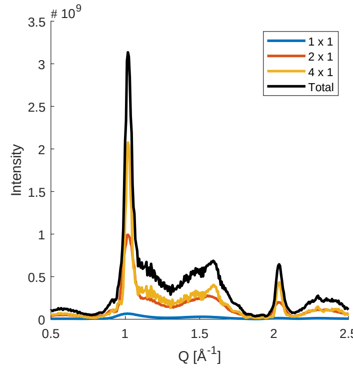






Model: Rh1+

Aggregation direction: (200)

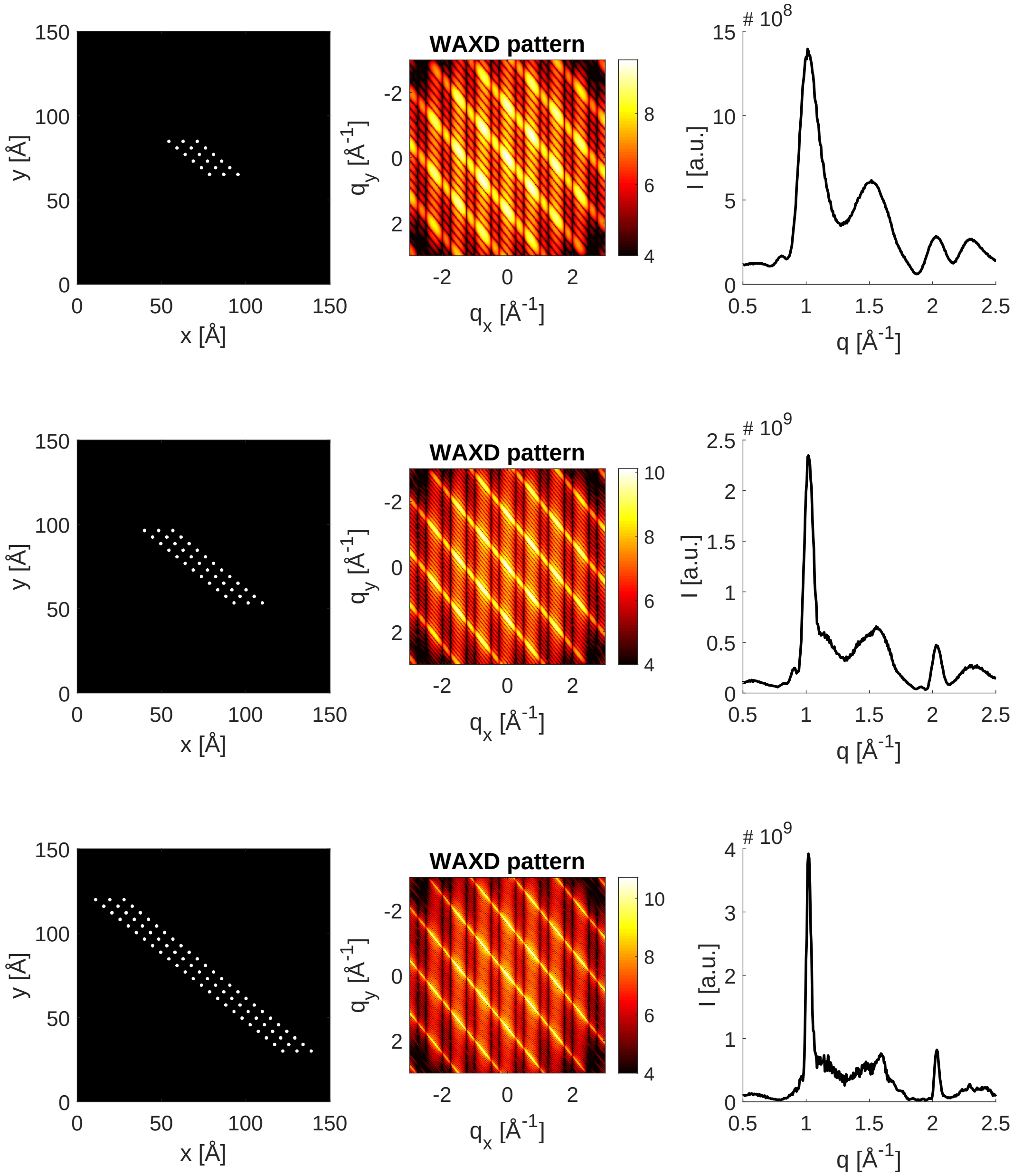


Sample #1

Vol% 1x1: 4.7

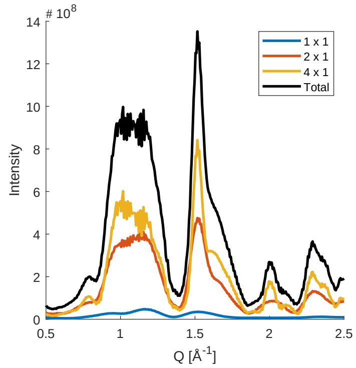
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: Rh1-

Aggregation direction: (1-10)

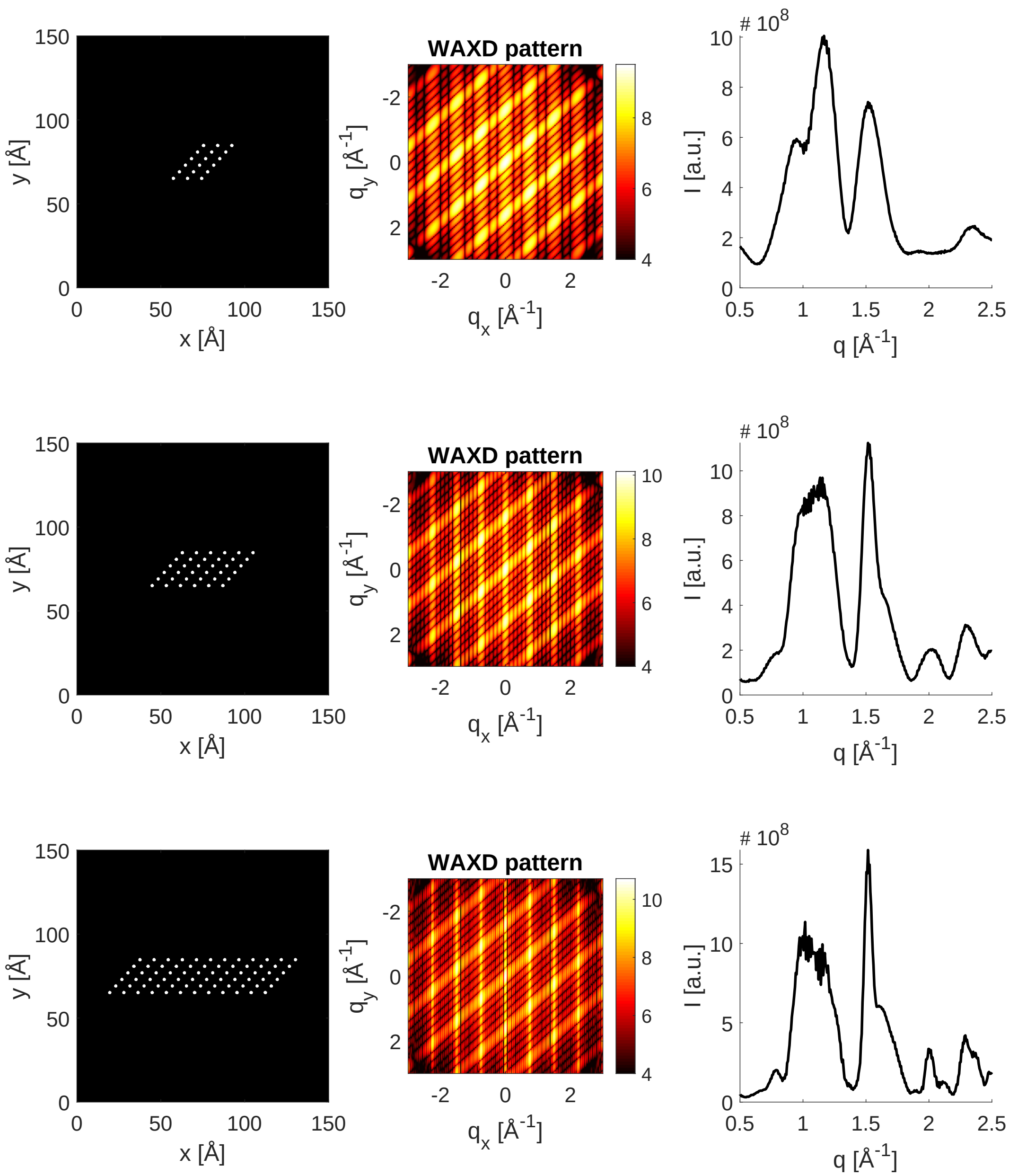


Sample #1

Vol% 1x1: 4.7

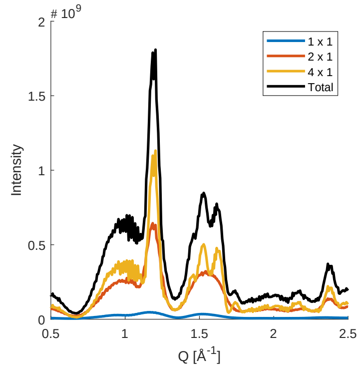
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: Rh1-

Aggregation direction: (200)

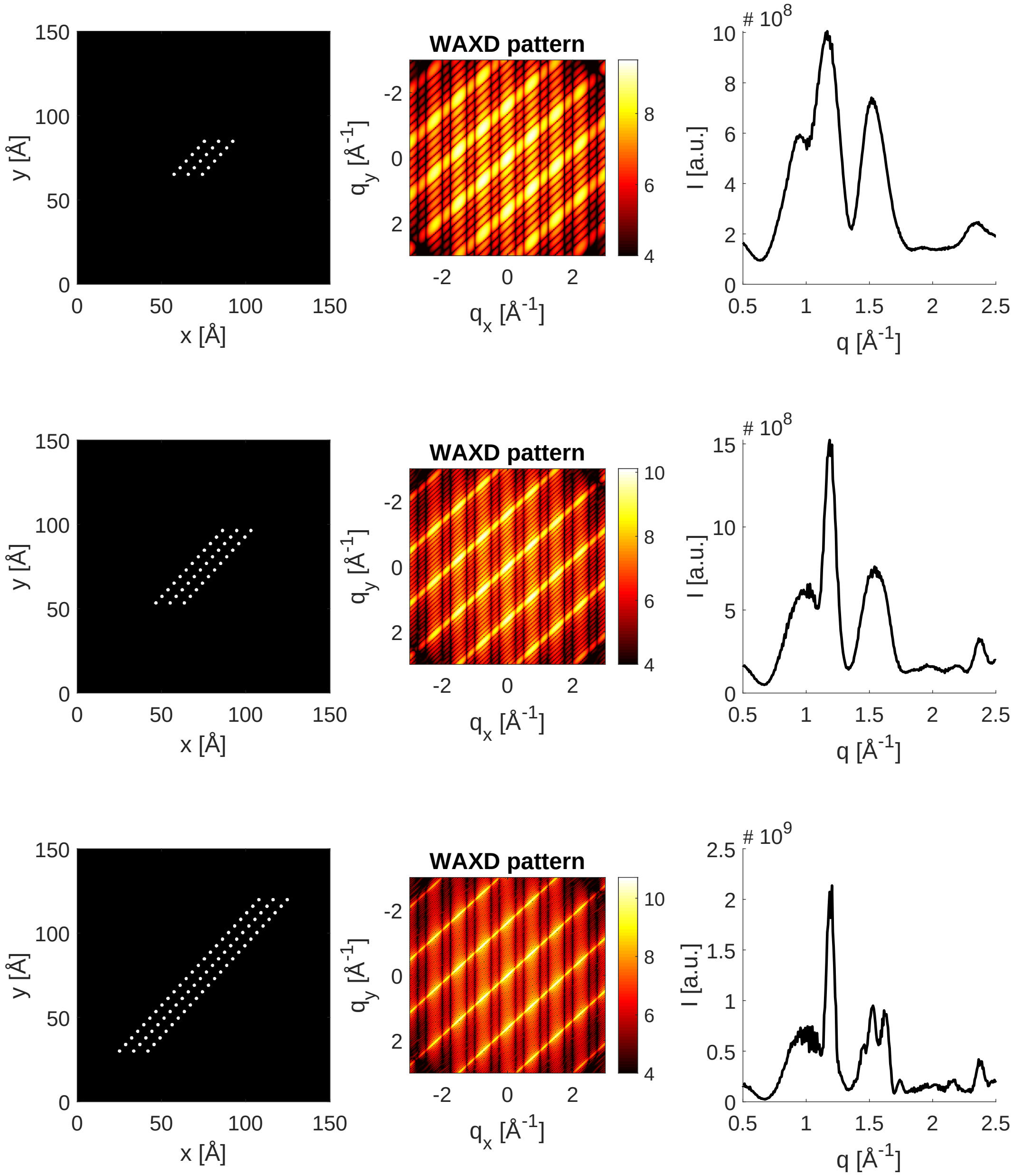


Sample #1

Vol% 1x1: 4.7

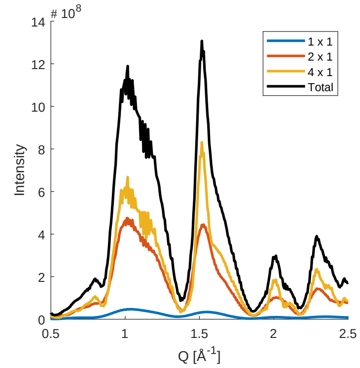
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: Rh2

Aggregation direction: (010)

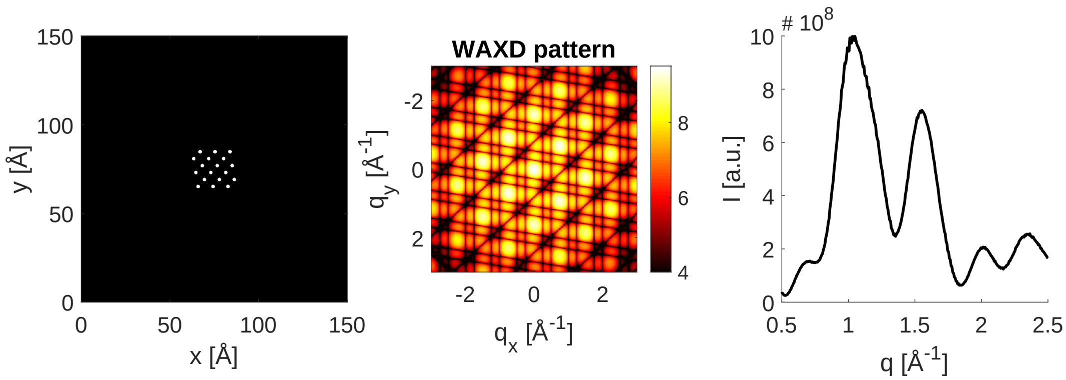


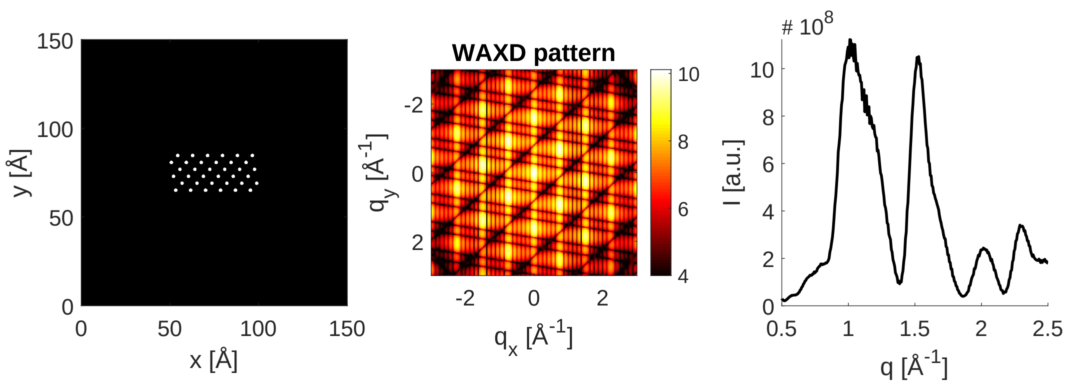
Sample #1

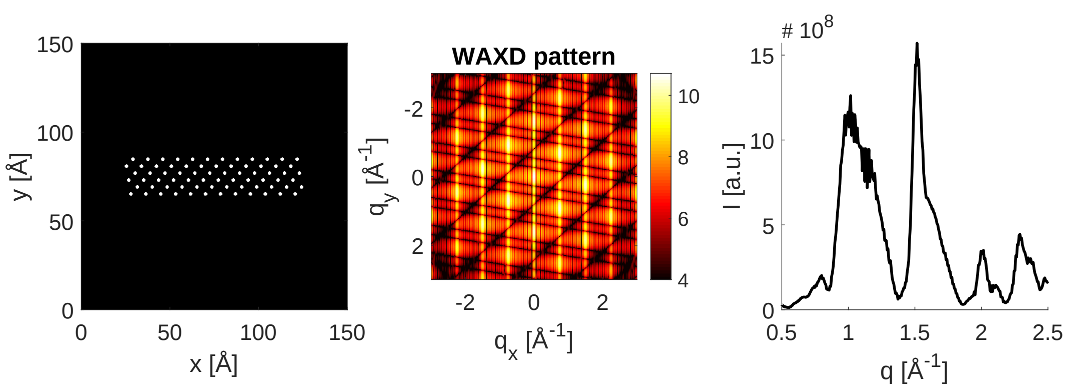
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

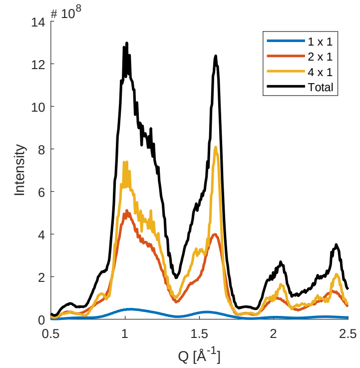






Model: Rh2

Aggregation direction: (200)

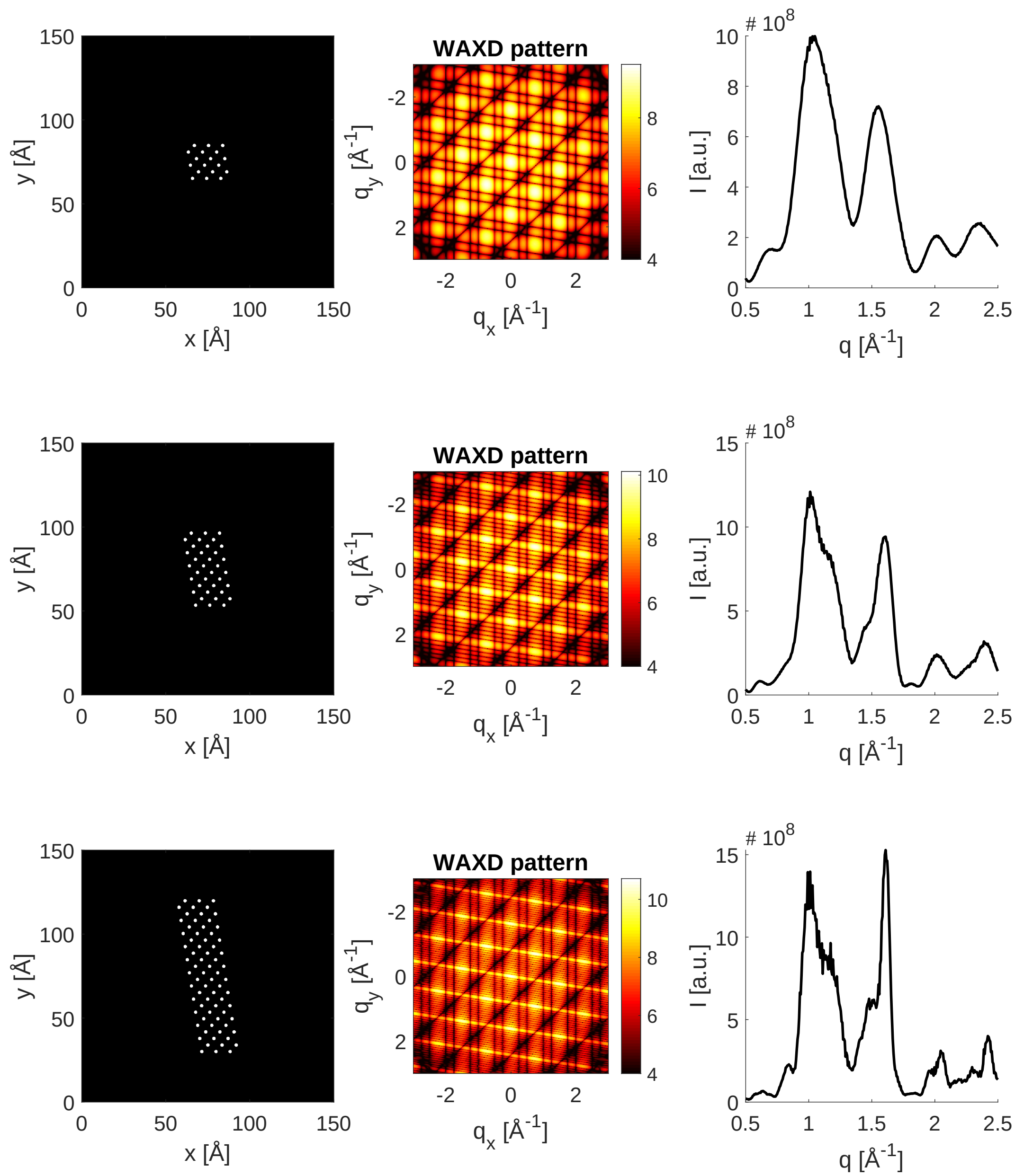


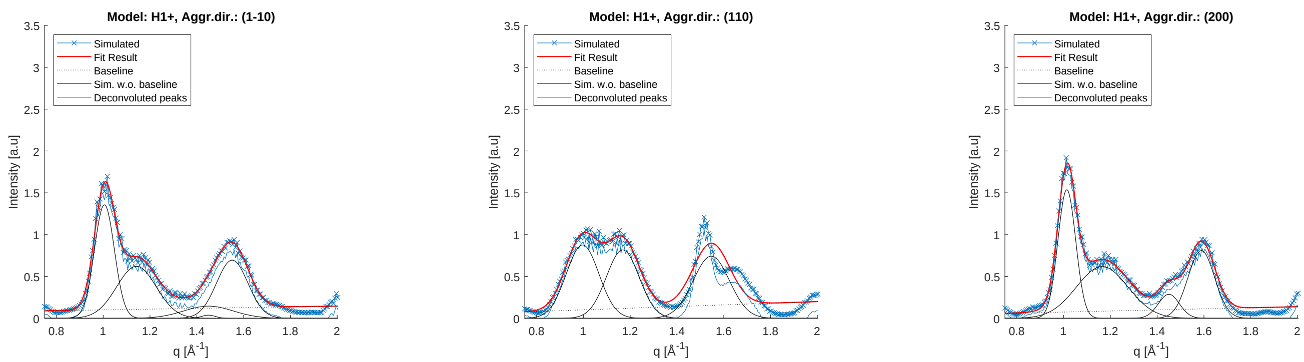
Sample #1

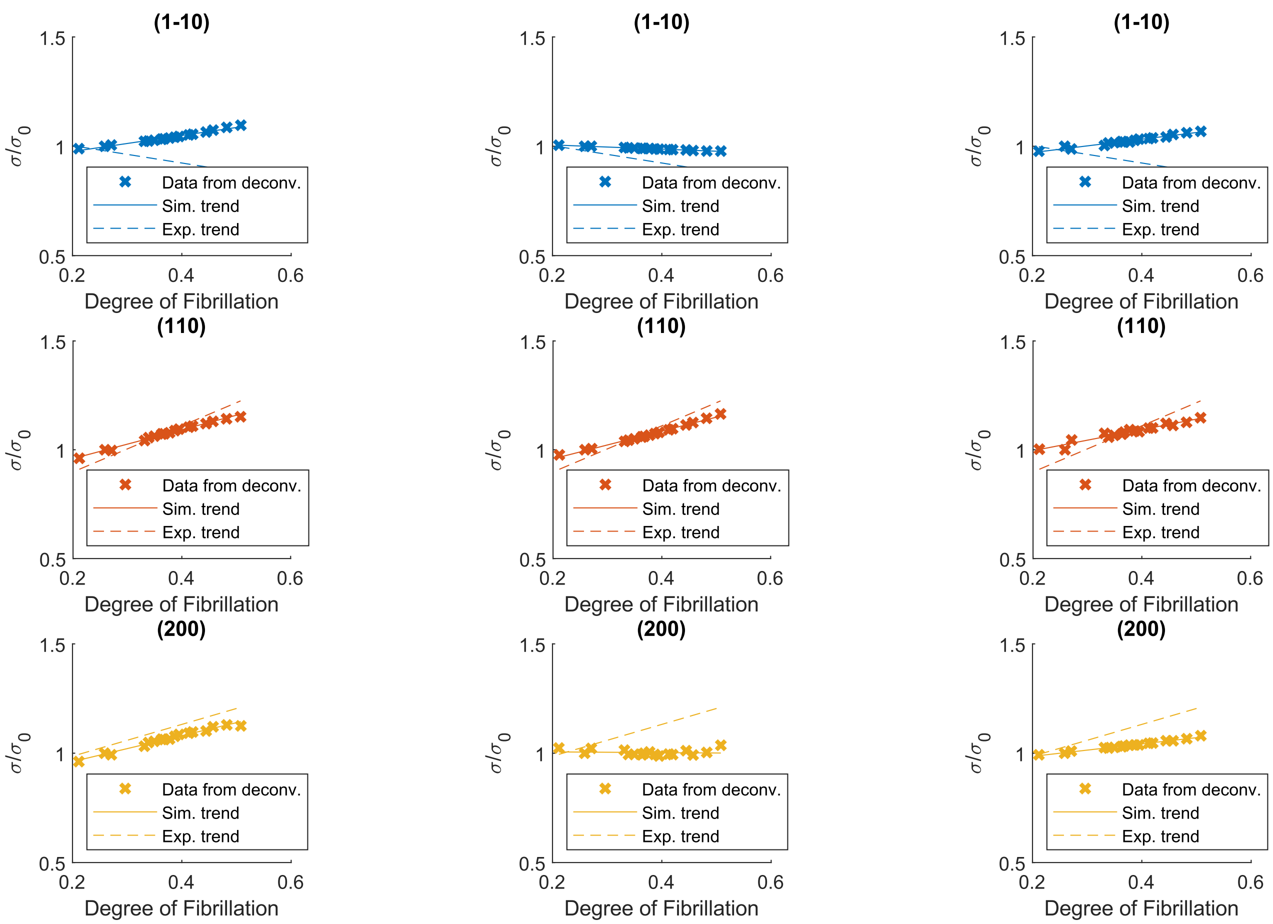
Vol% 1x1: 4.7

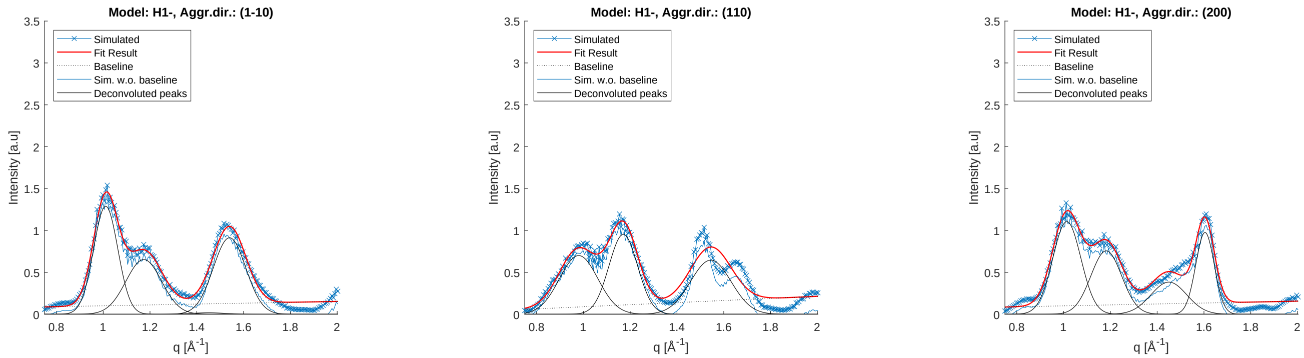
Vol% 2x1: 42.3

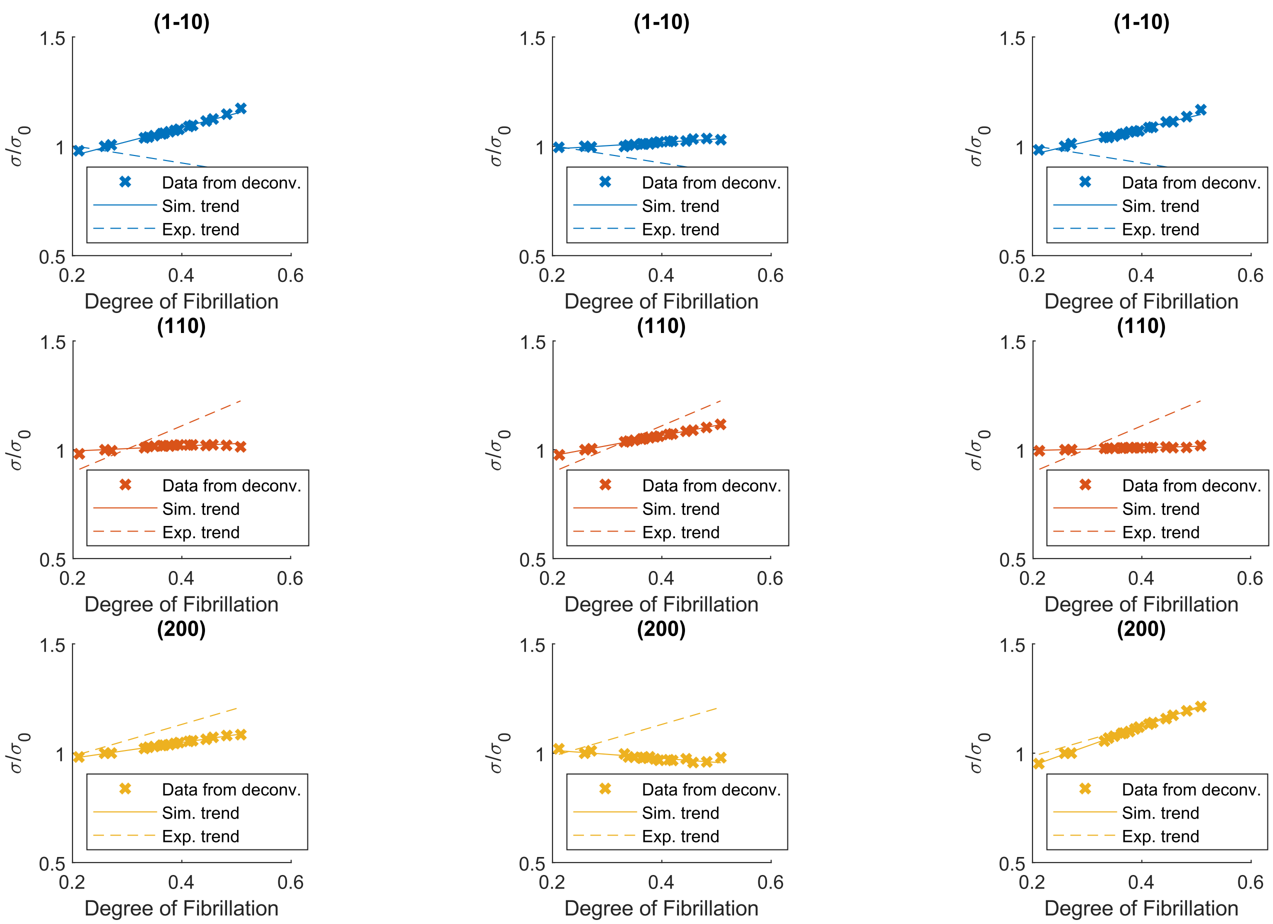
Vol% 4x1: 53.0

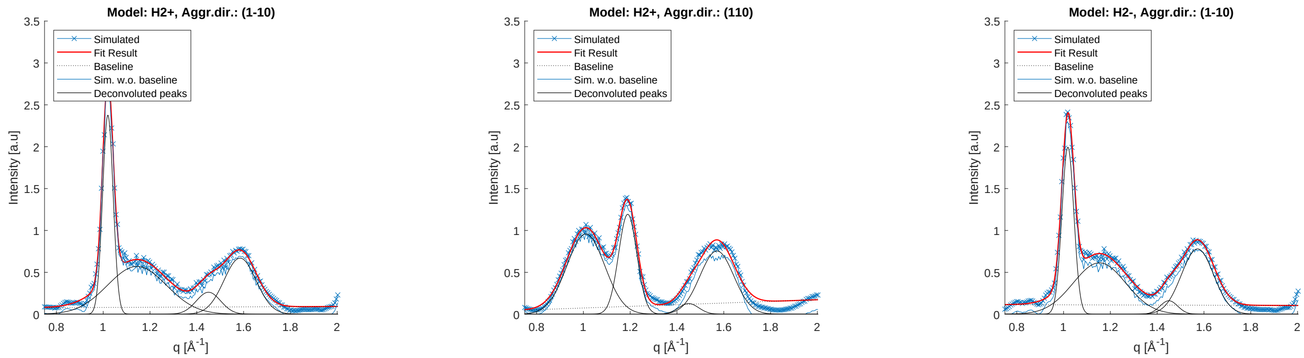


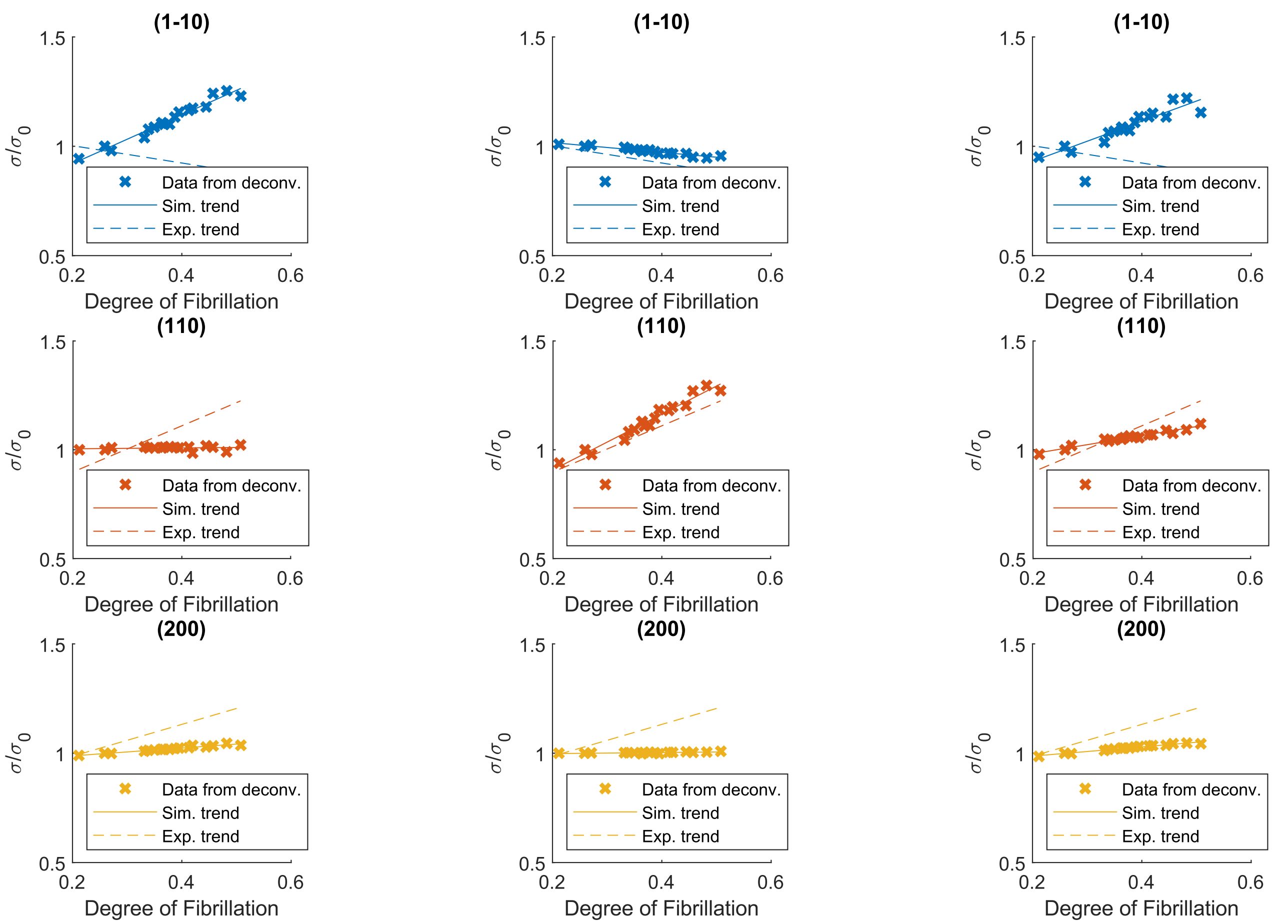

Model: H1+, Aggr.dir.: (1-10)
Model: H1+, Aggr.dir.: (110)
Model: H1+, Aggr.dir.: (200)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^{-1}]

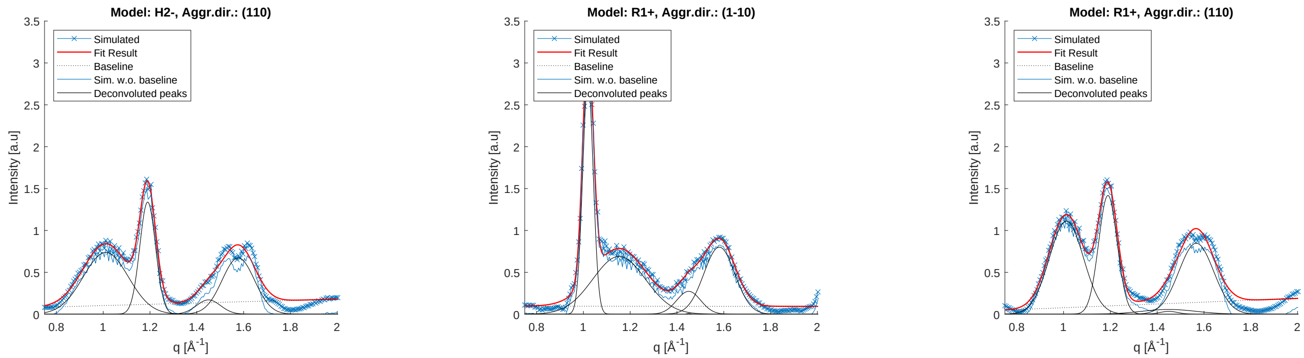

(1-10)
(110)
(200)
σ/σ_0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation

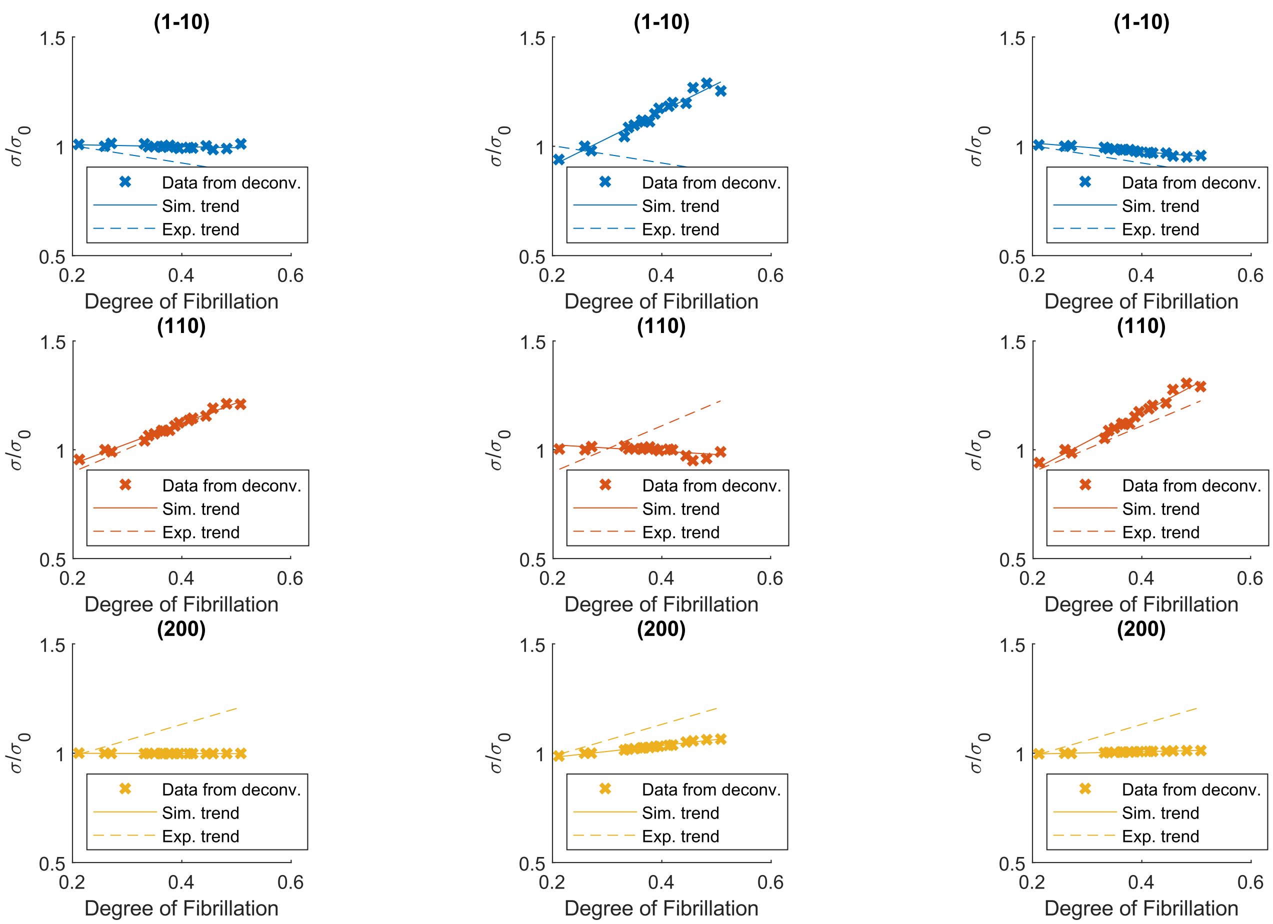

Model: H1-, Aggr.dir.: (1-10)
Model: H1-, Aggr.dir.: (110)
Model: H1-, Aggr.dir.: (200)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^{-1}]

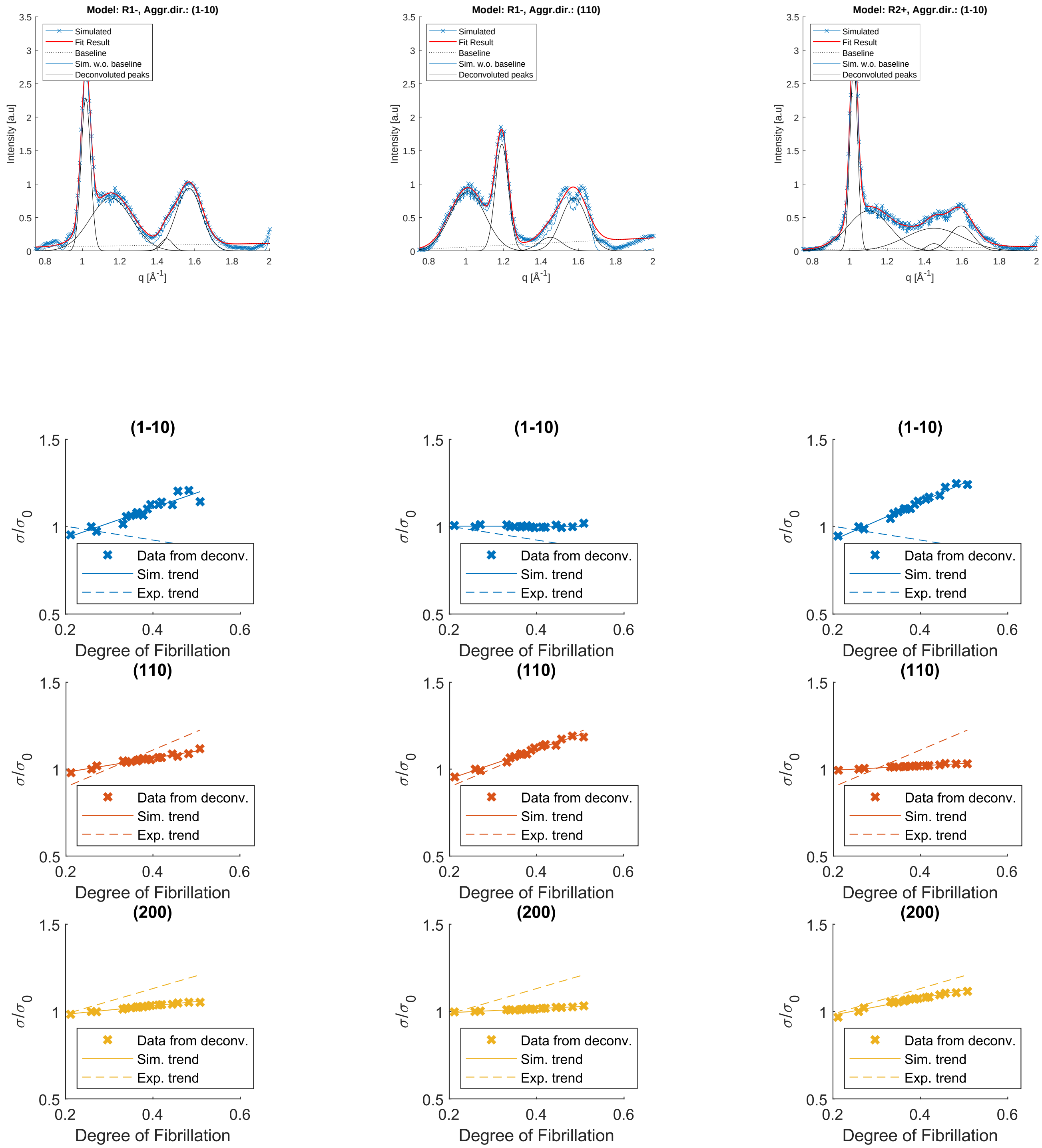

(1-10)
(110)
(200)
σ/σ_0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation

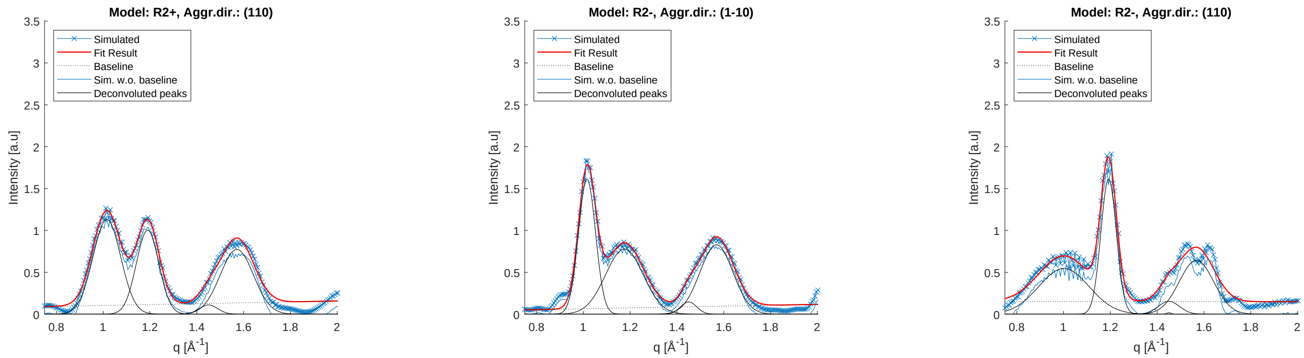

Model: H2+, Aggr.dir.: (1-10)
Model: H2+, Aggr.dir.: (110)
Model: H2-, Aggr.dir.: (1-10)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^{-1}]

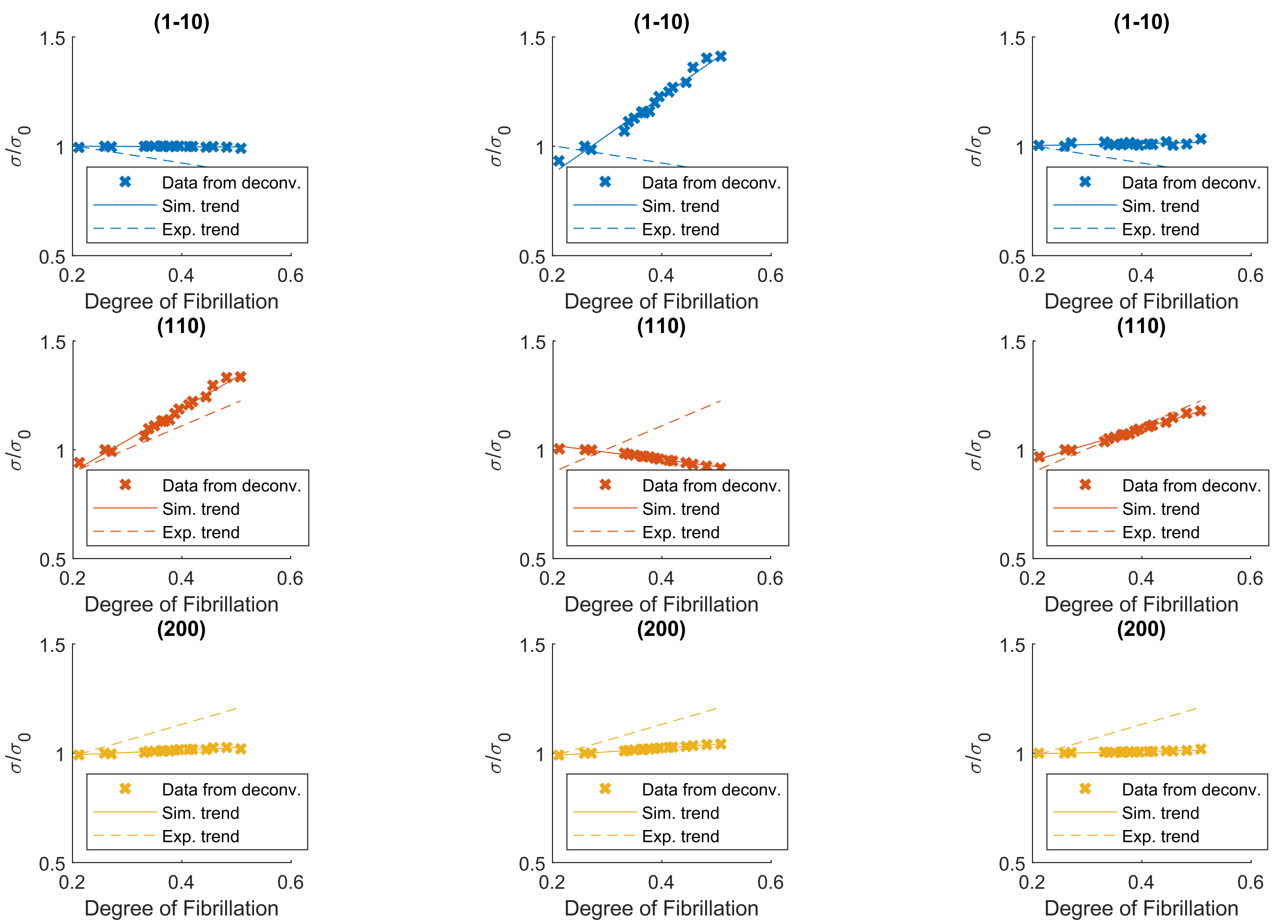

(1-10)
(110)
(200)
σ/σ_0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation

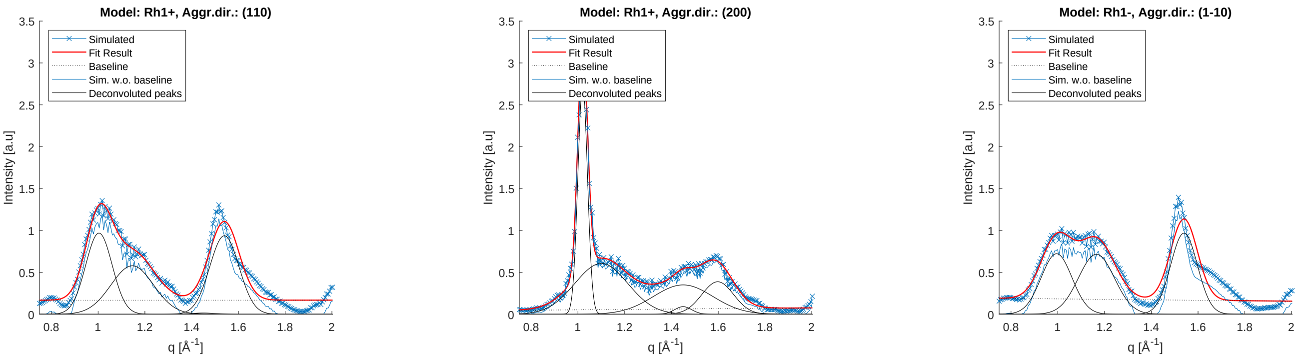

Model: H2-, Aggr.dir.: (110)
Model: R1+, Aggr.dir.: (1-10)
Model: R1+, Aggr.dir.: (110)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^{-1}]

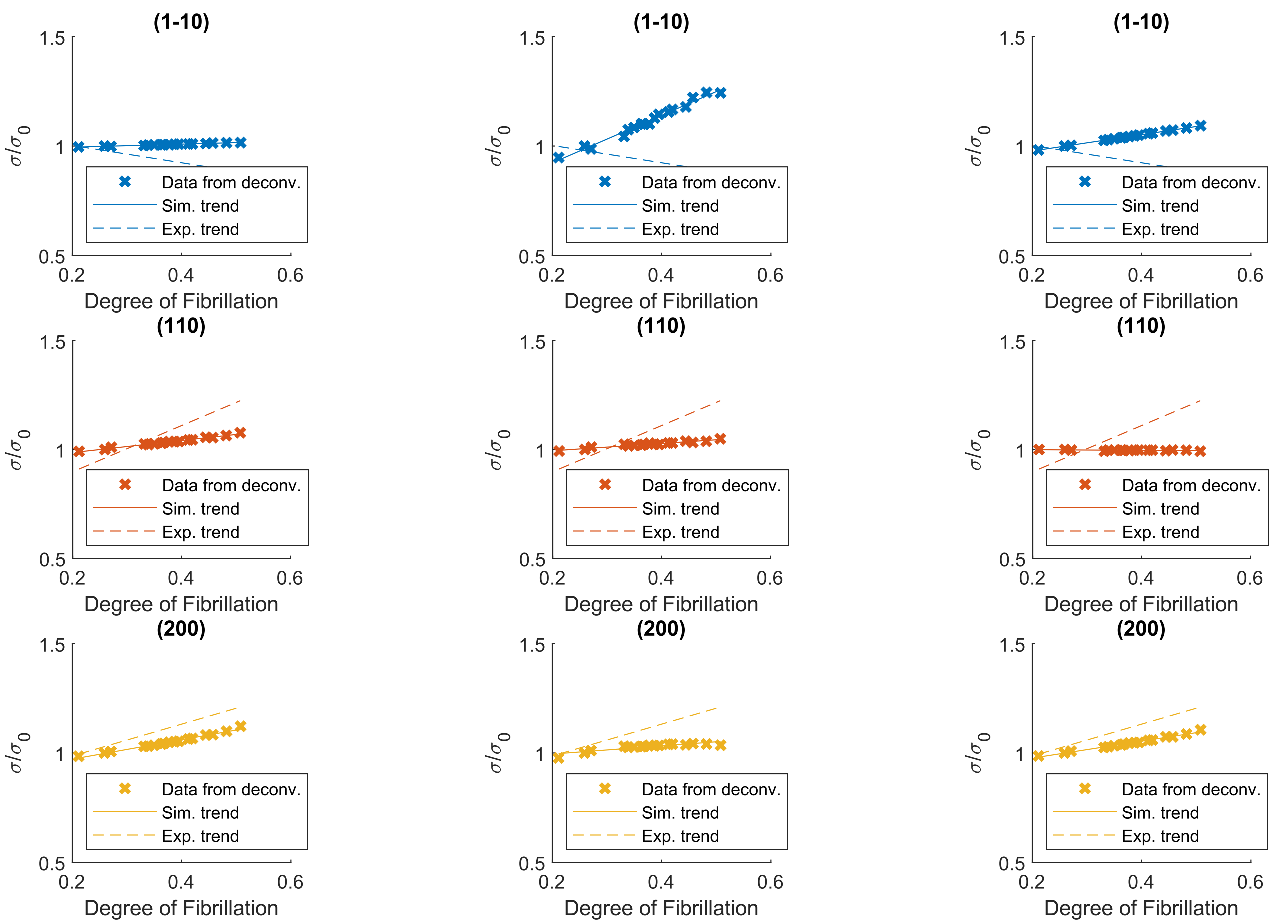

(1-10)
(110)
(200)
Data from deconv.
Sim. trend
Exp. trend
σ/σ_0
Degree of Fibrillation

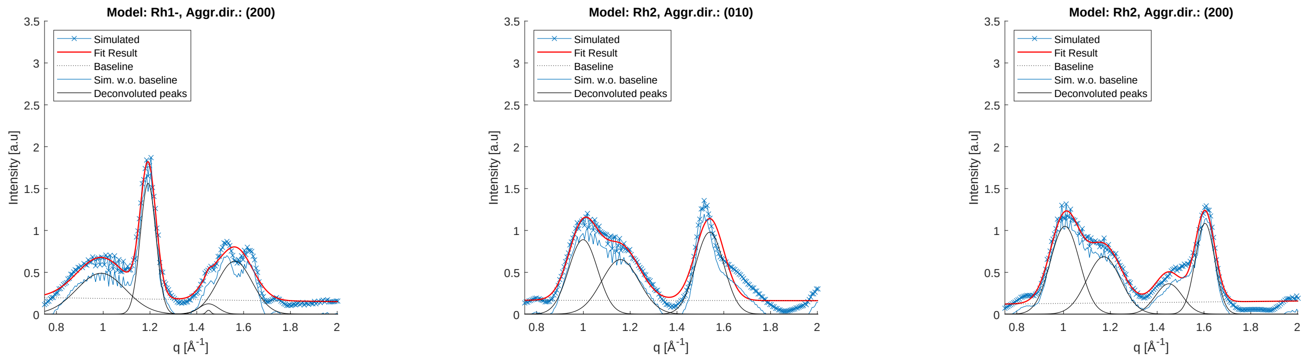

Model: R1-, Aggr.dir.: (1-10)
Model: R1-, Aggr.dir.: (110)
Model: R2+, Aggr.dir.: (1-10)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å⁻¹]
(1-10)
(110)
(200)
σ/σ0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation


Model: R2+, Aggr.dir.: (110)
Model: R2-, Aggr.dir.: (1-10)
Model: R2-, Aggr.dir.: (110)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^-1]

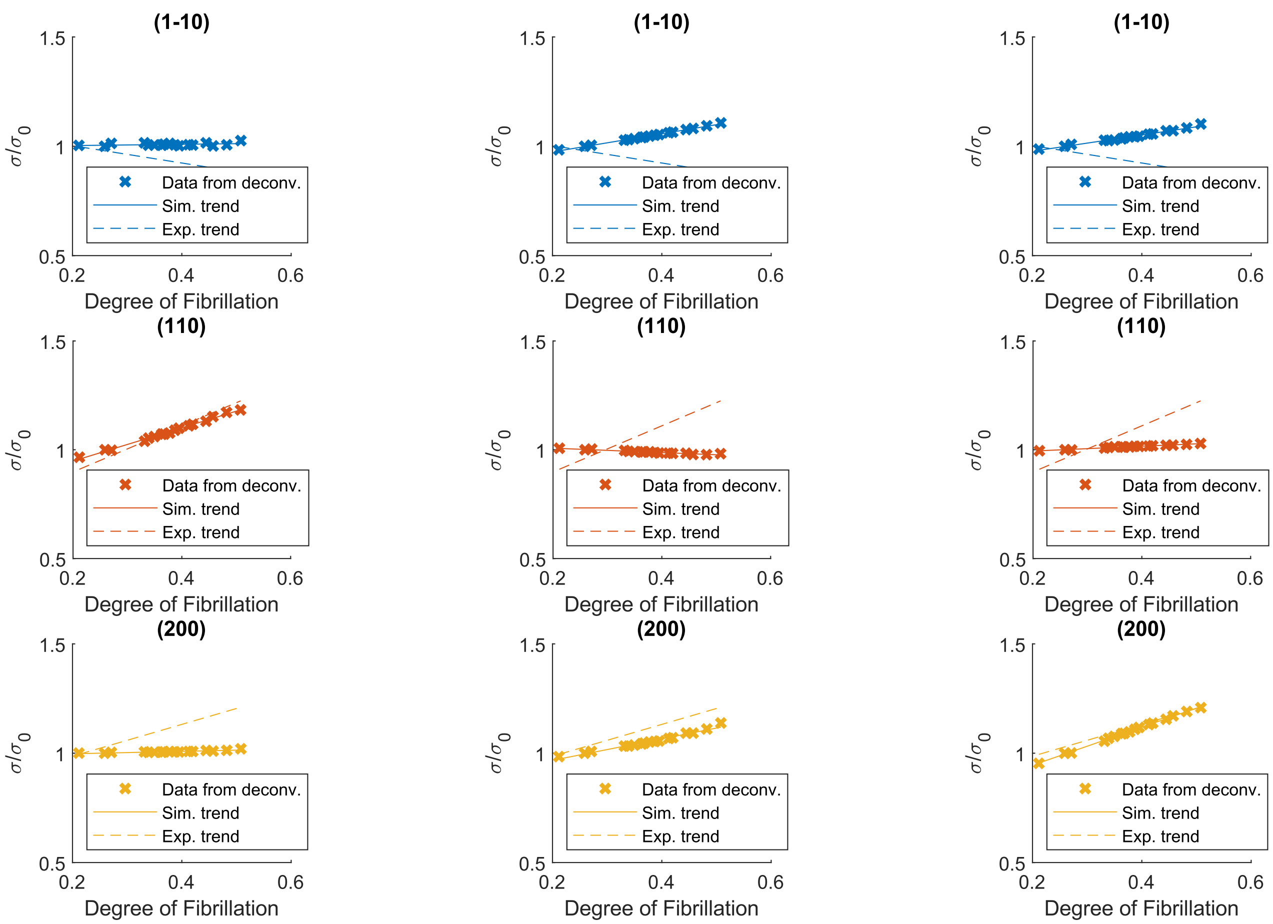

(1-10)
(110)
(200)
σ/σ0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation


Model: Rh1+, Aggr.dir.: (110)
Model: Rh1+, Aggr.dir.: (200)
Model: Rh1-, Aggr.dir.: (1-10)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^-1]


(1-10)
(110)
(200)
σ/σ0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation



Model: Rh1-, Aggr.dir.: (200)
Model: Rh2, Aggr.dir.: (010)
Model: Rh2, Aggr.dir.: (200)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^{-1}]



(1-10)
(110)
(200)
σ/σ_0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation

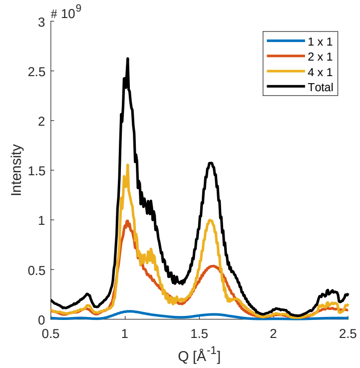
WAXD simulations: Results

Form factor of a CNF chain with semi-axes

2 Å x 0.75 Å

Model: H1+

Aggregation direction: (1-10)

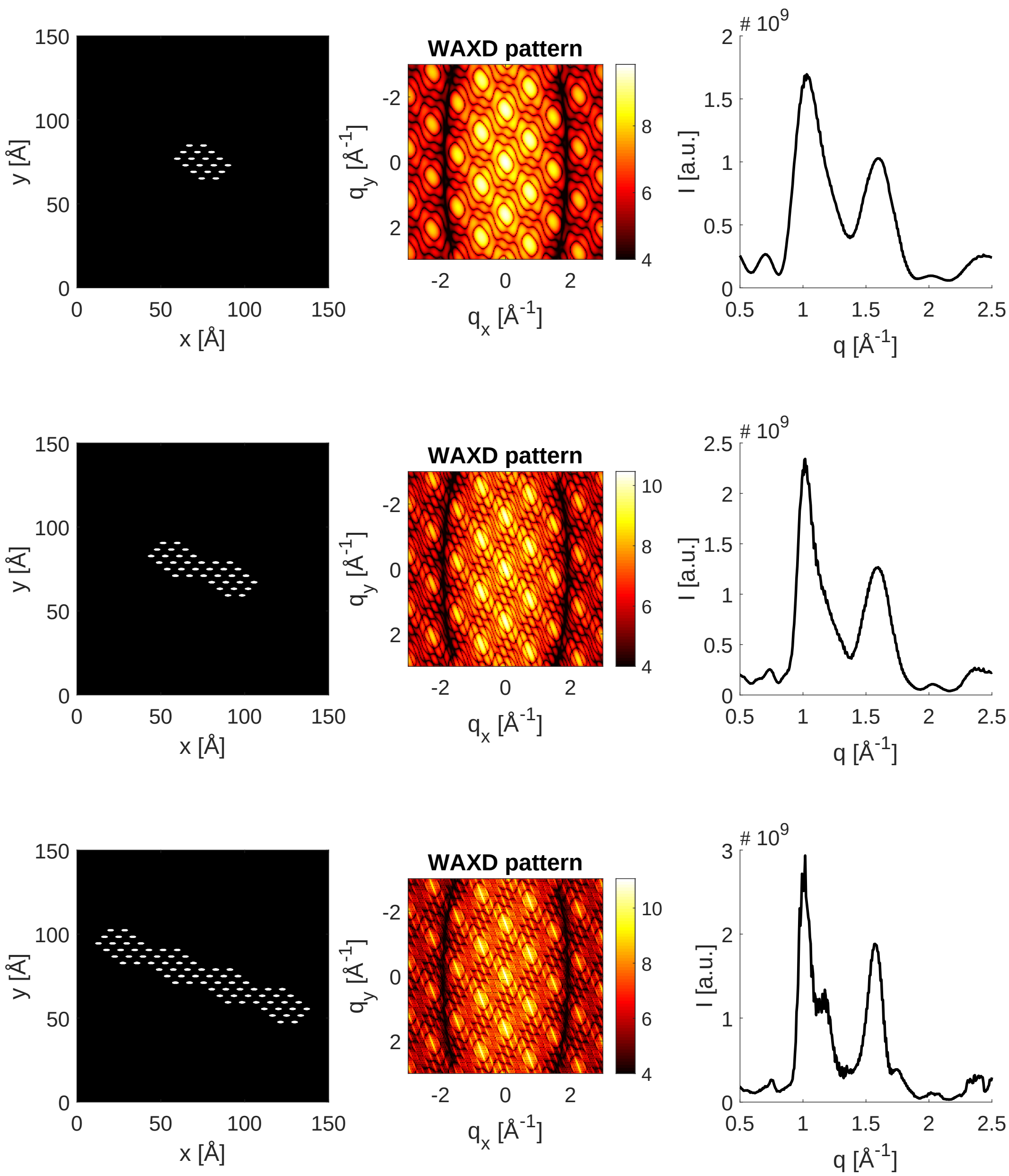


Sample #1

Vol% 1x1: 4.7

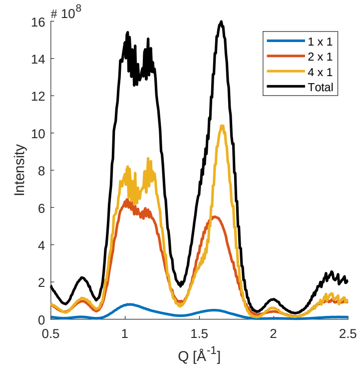
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: H1+

Aggregation direction: (110)

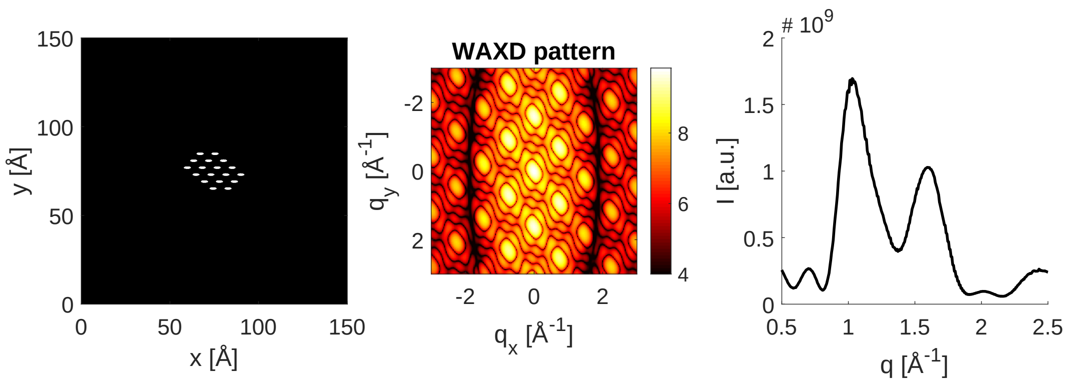


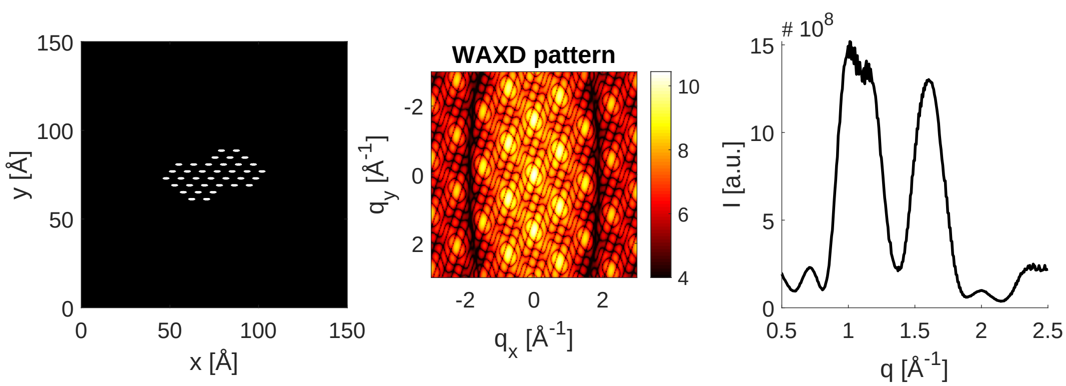
Sample #1

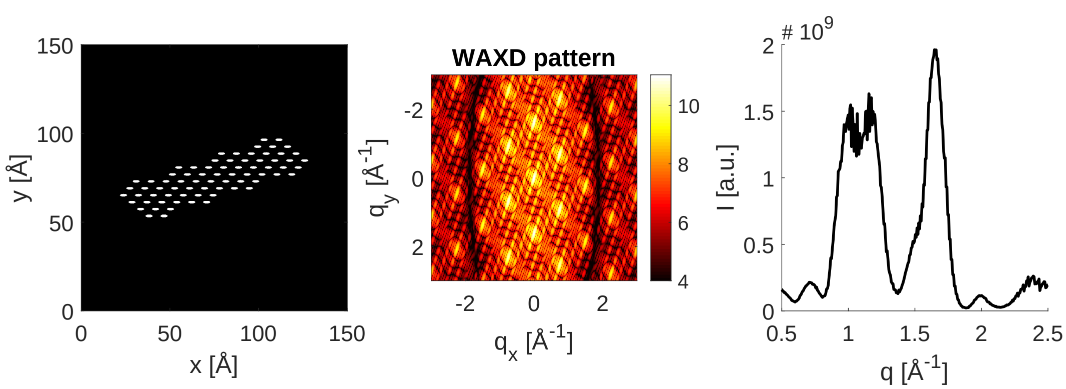
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

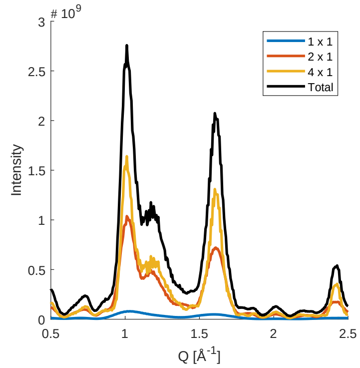






Model: H1+

Aggregation direction: (200)

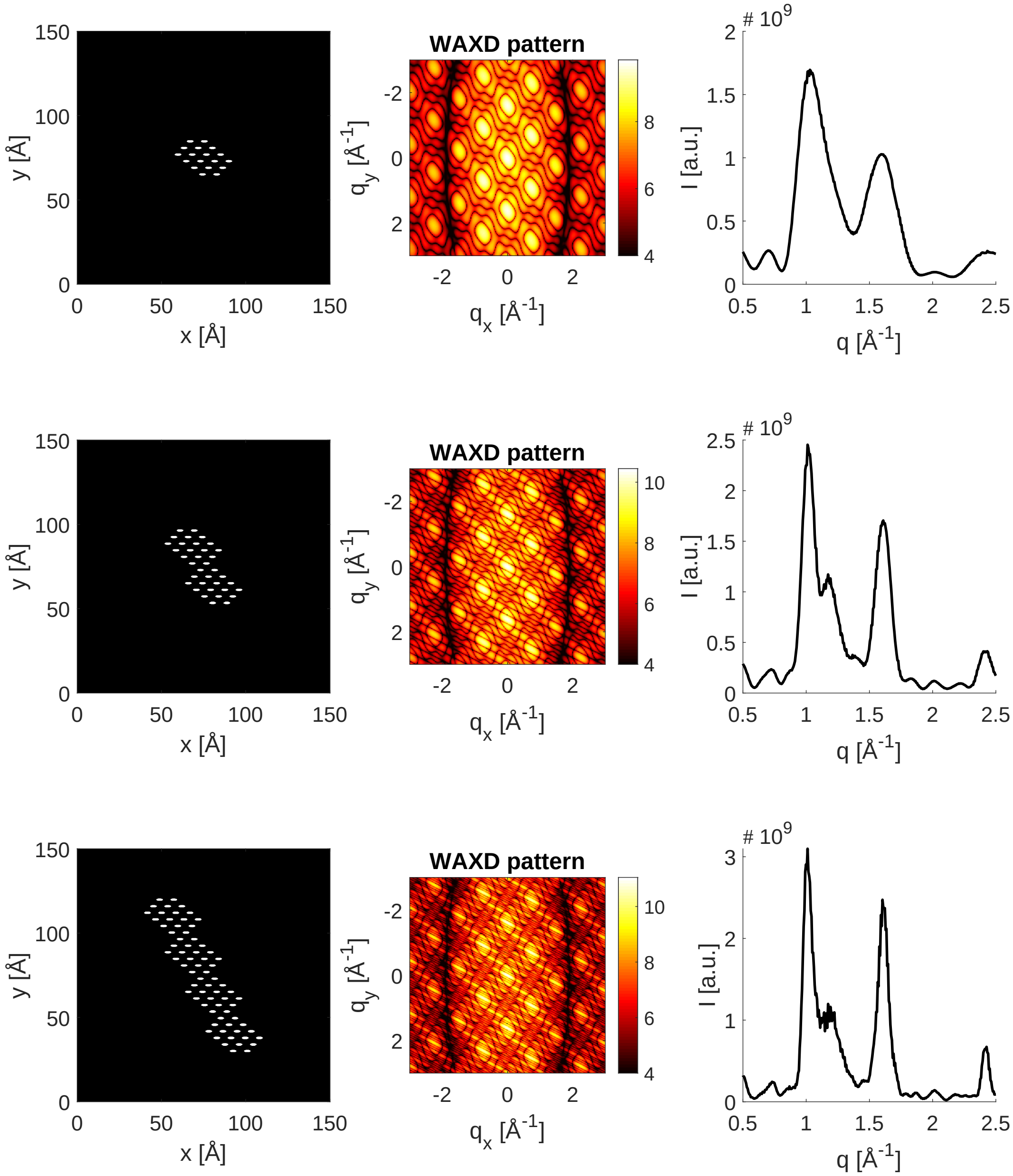


Sample #1

Vol% 1x1: 4.7

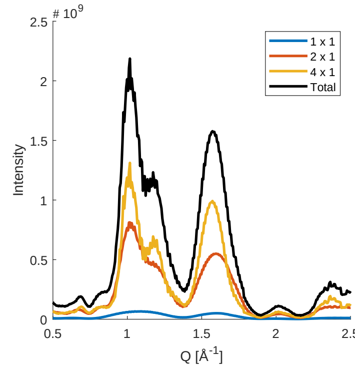
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: H1-

Aggregation direction: (1-10)

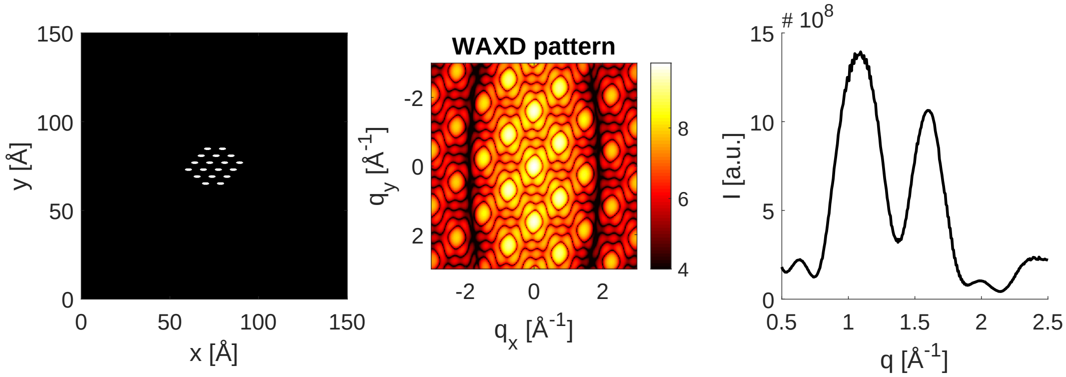


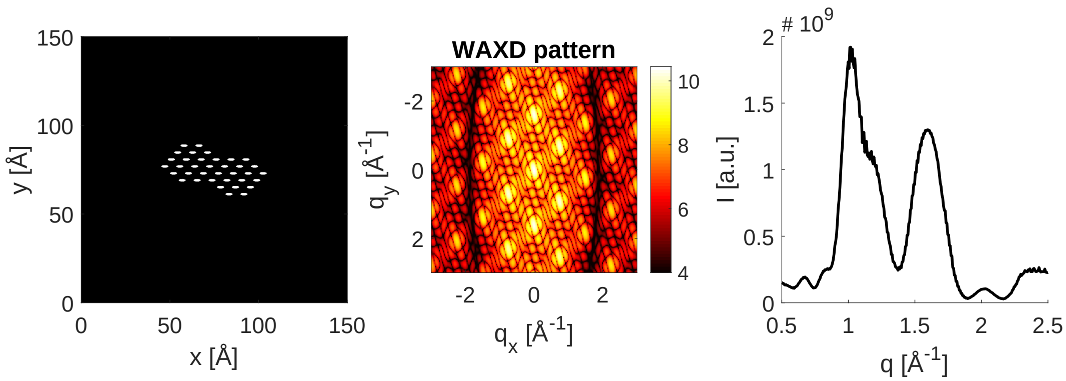
Sample #1

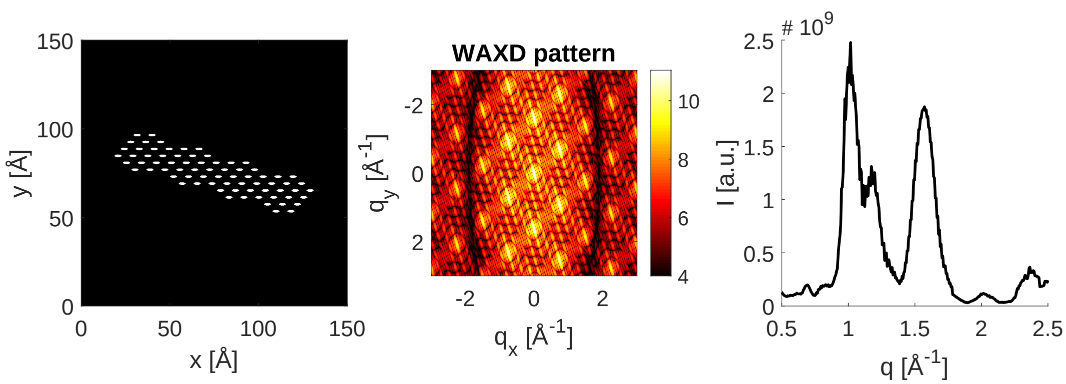
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

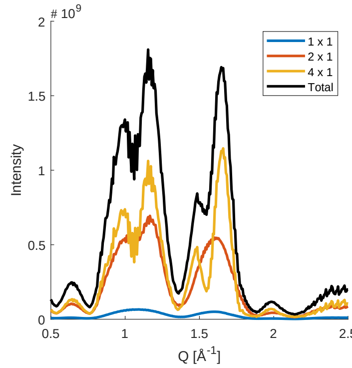






Model: H1-

Aggregation direction: (110)

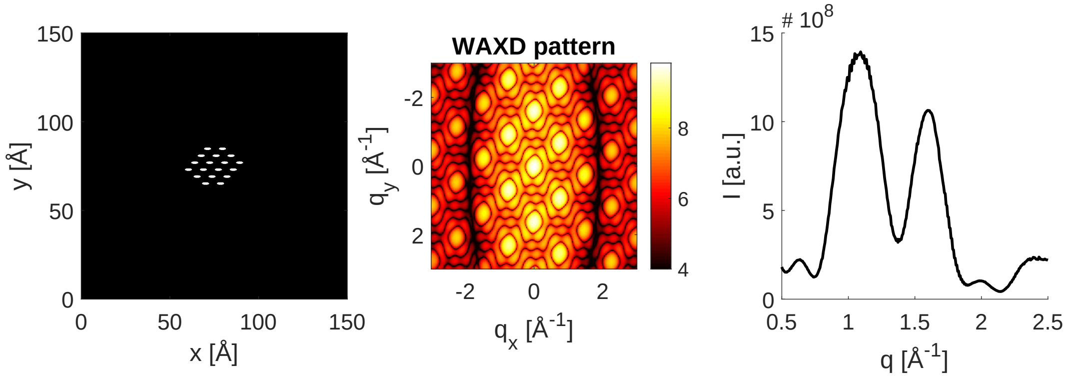


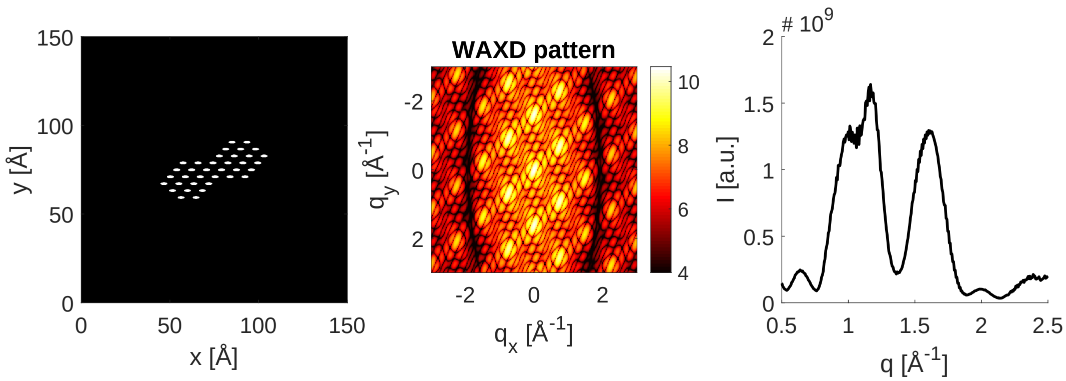
Sample #1

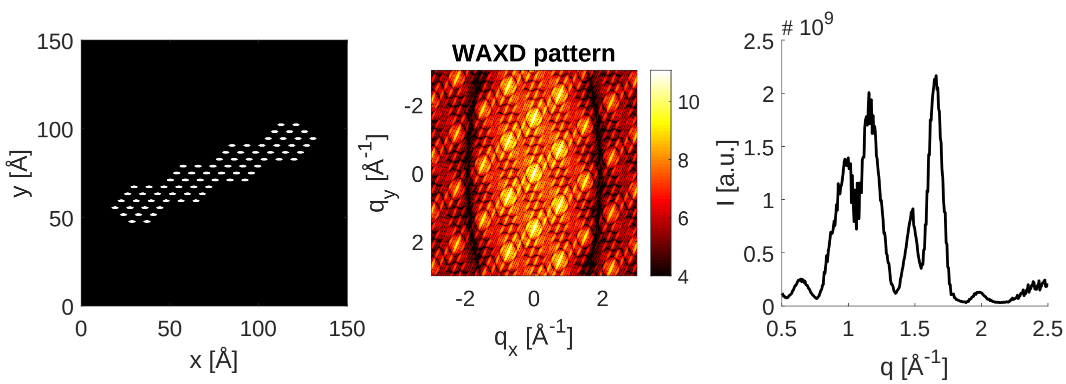
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

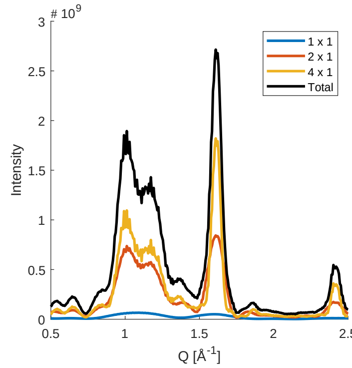






Model: H1-

Aggregation direction: (200)

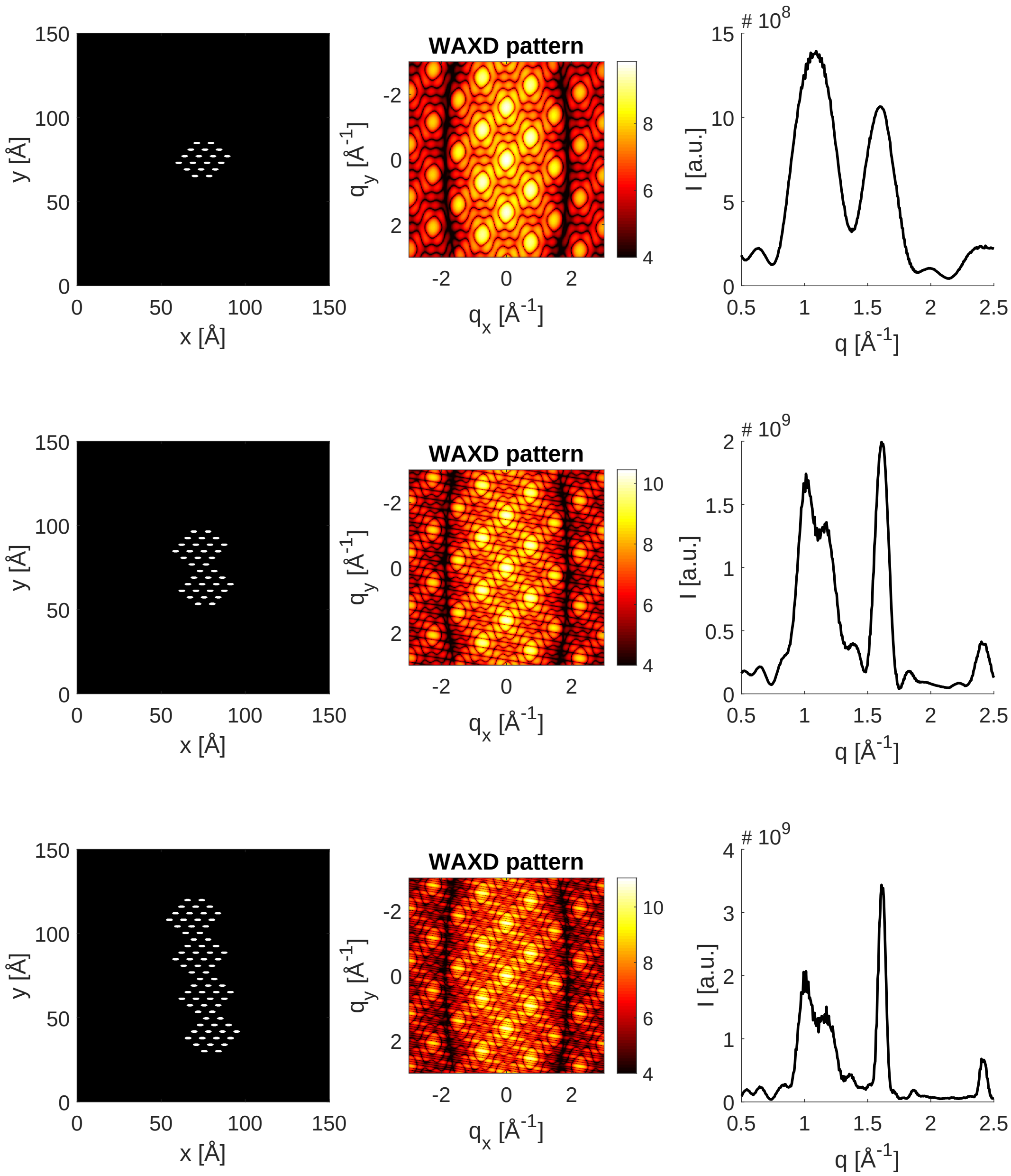


Sample #1

Vol% 1x1: 4.7

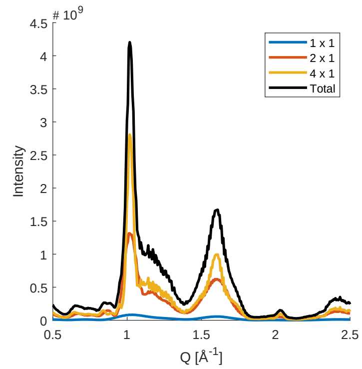
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: H2+

Aggregation direction: (1-10)

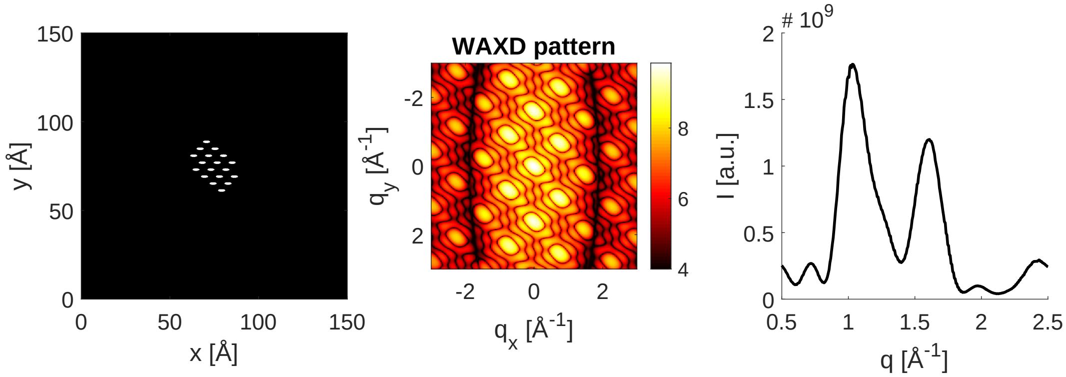


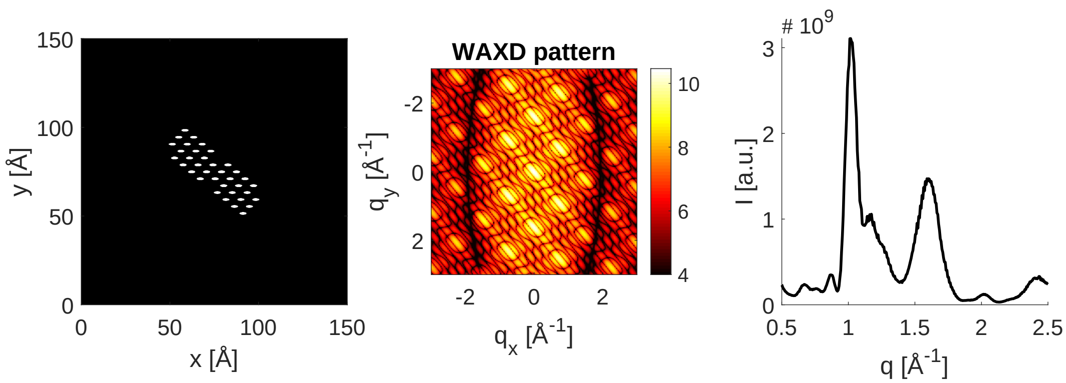
Sample #1

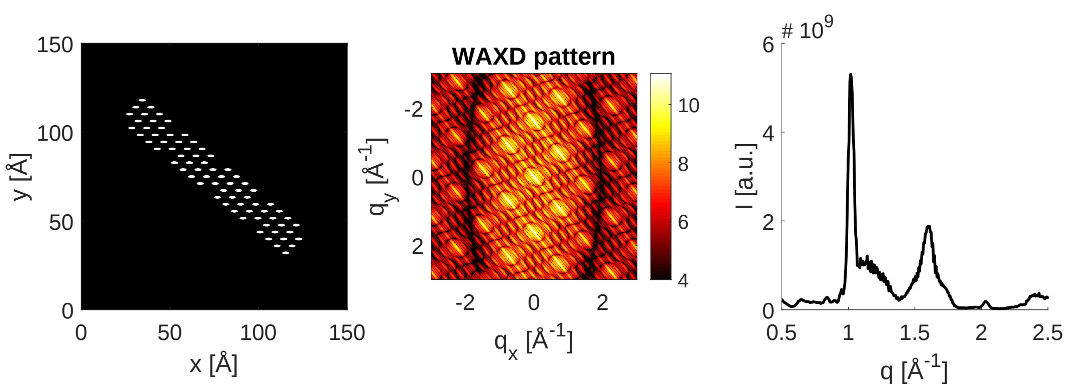
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

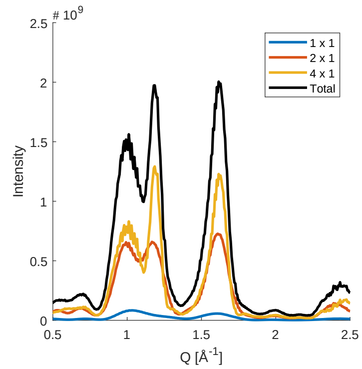






Model: H2+

Aggregation direction: (110)

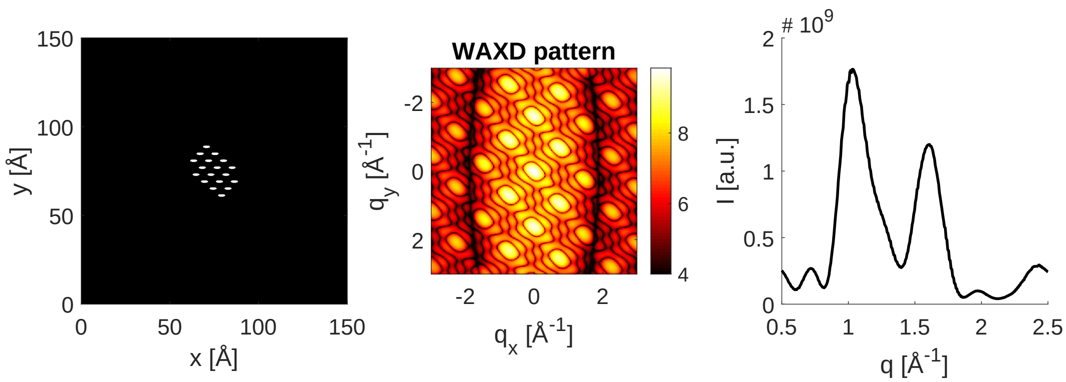


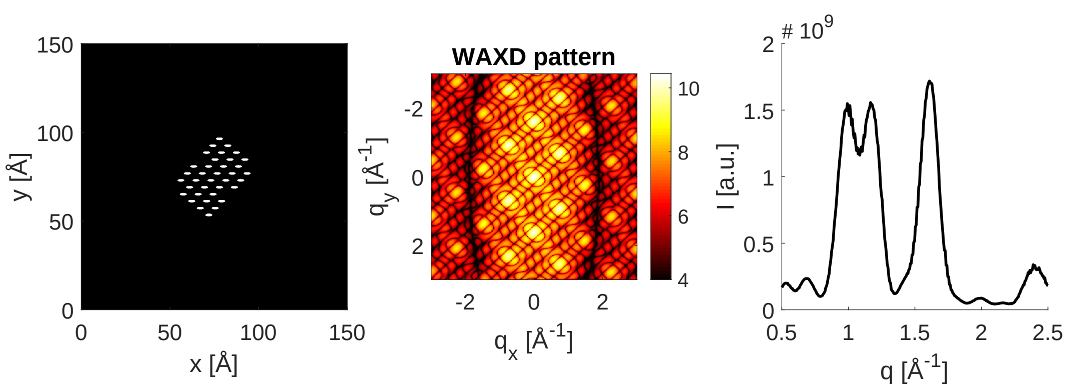
Sample #1

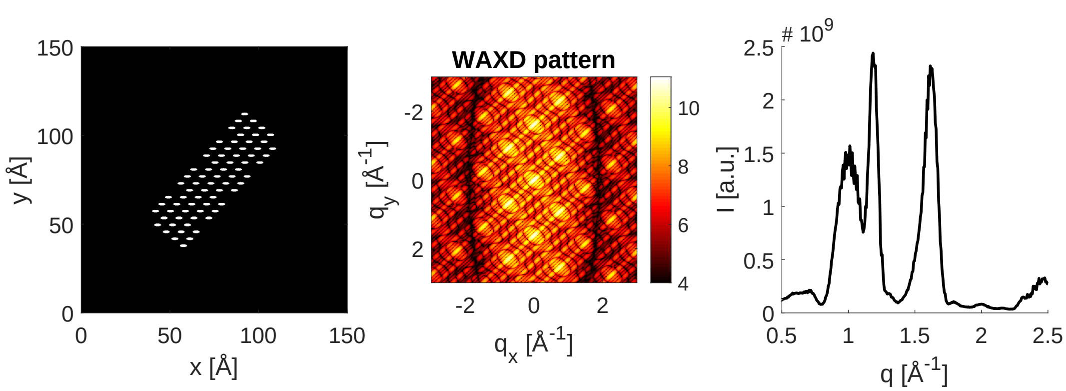
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

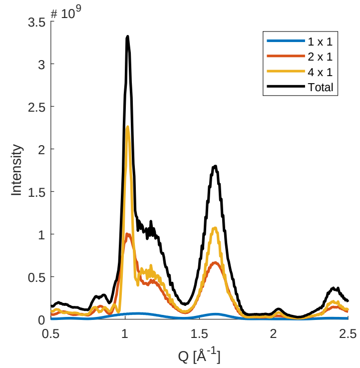






Model: H2-

Aggregation direction: (1-10)

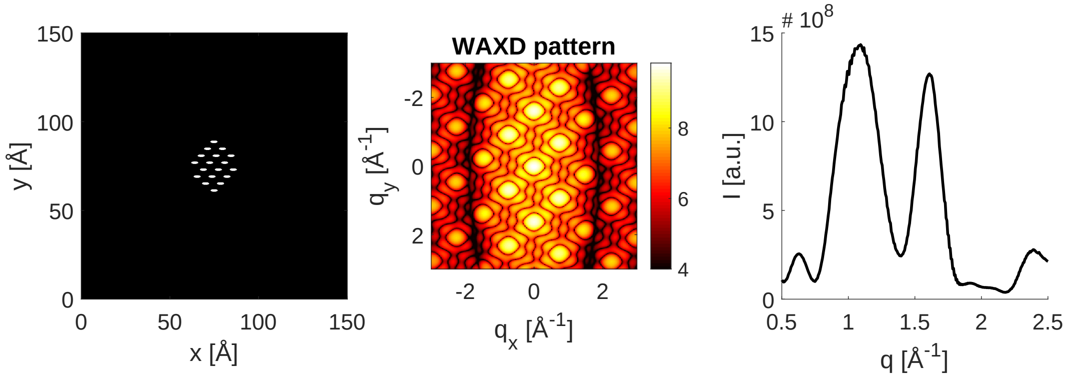


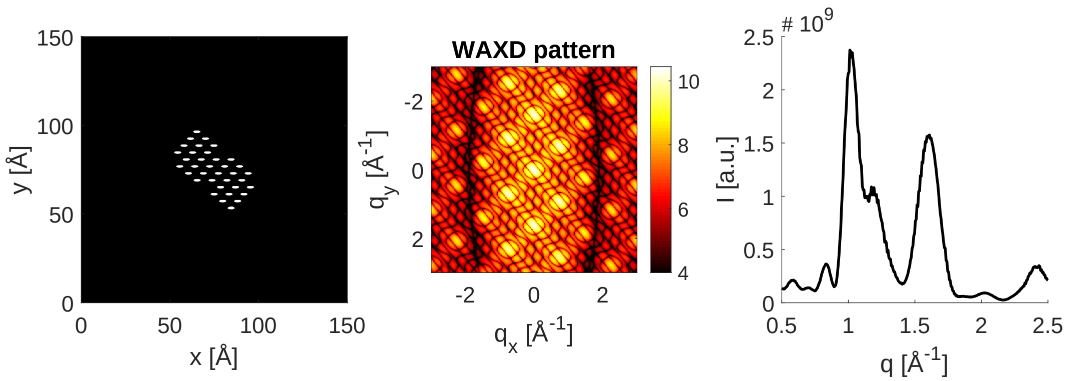
Sample #1

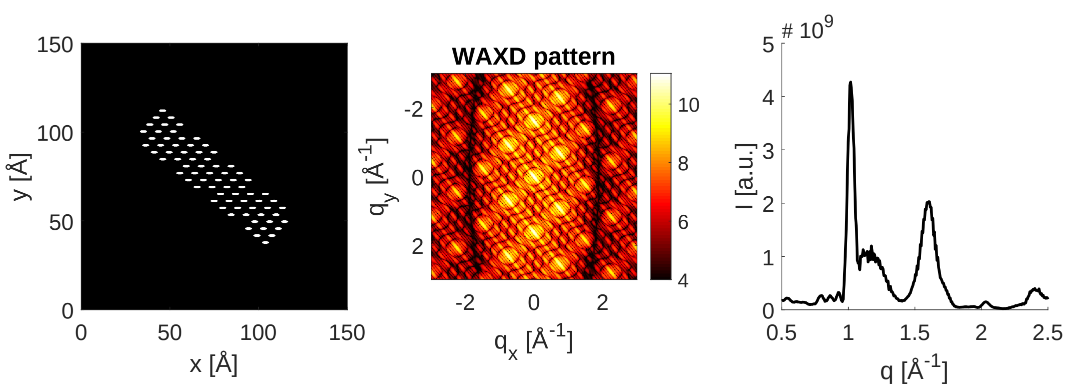
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

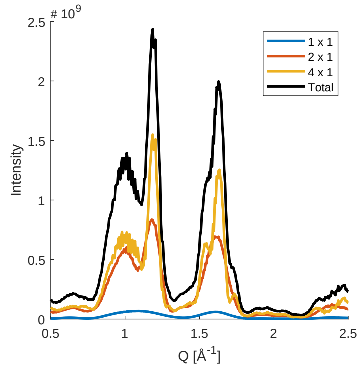






Model: H2-

Aggregation direction: (110)

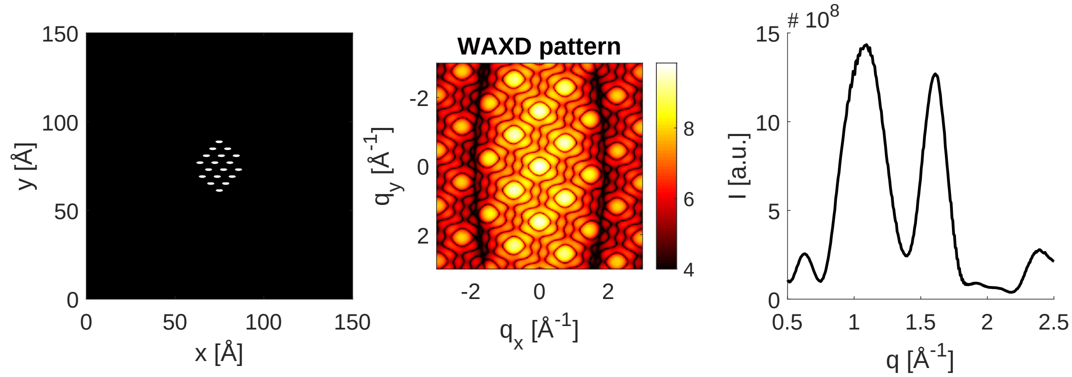


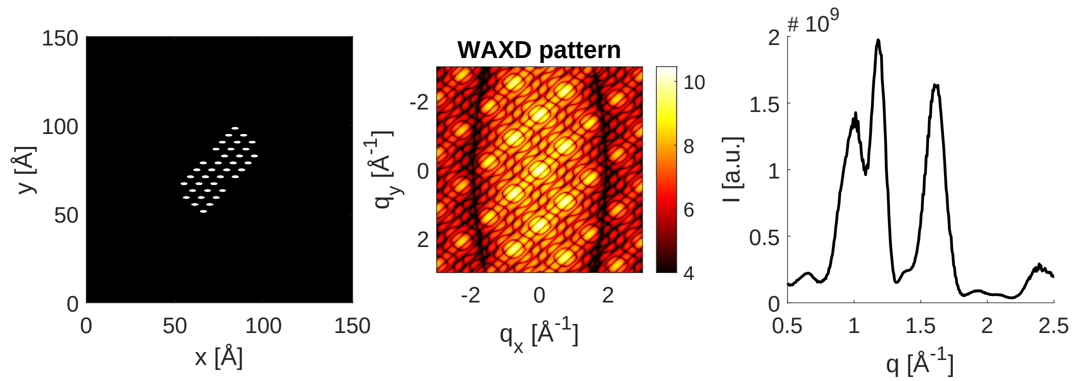
Sample #1

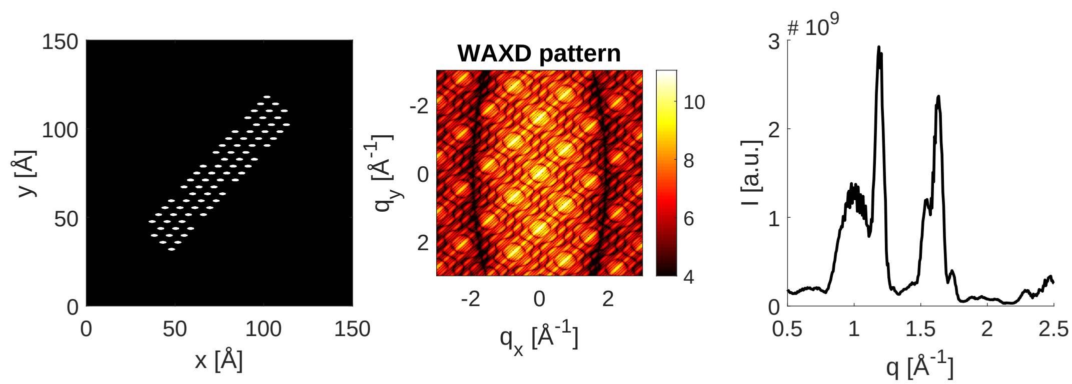
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

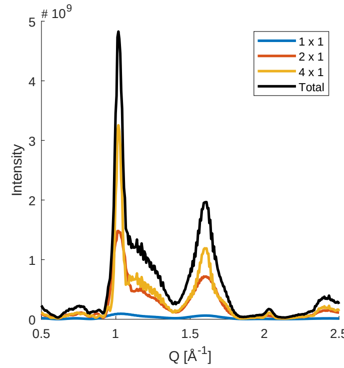






Model: R1+

Aggregation direction: (1-10)

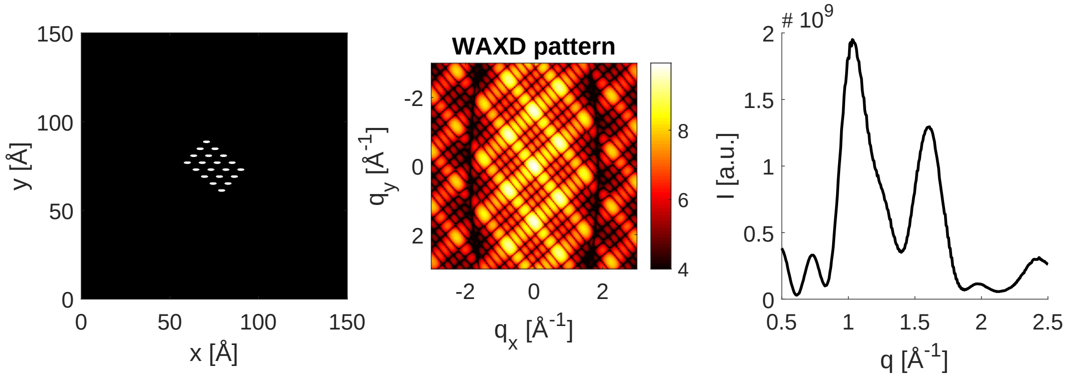


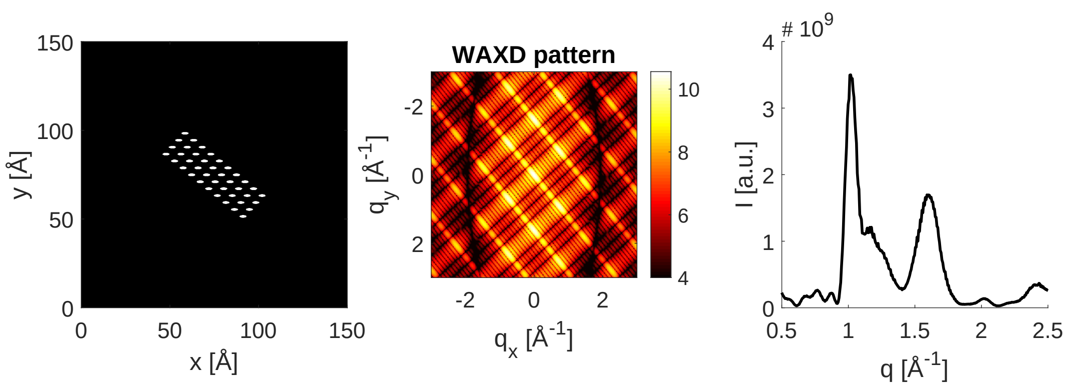
Sample #1

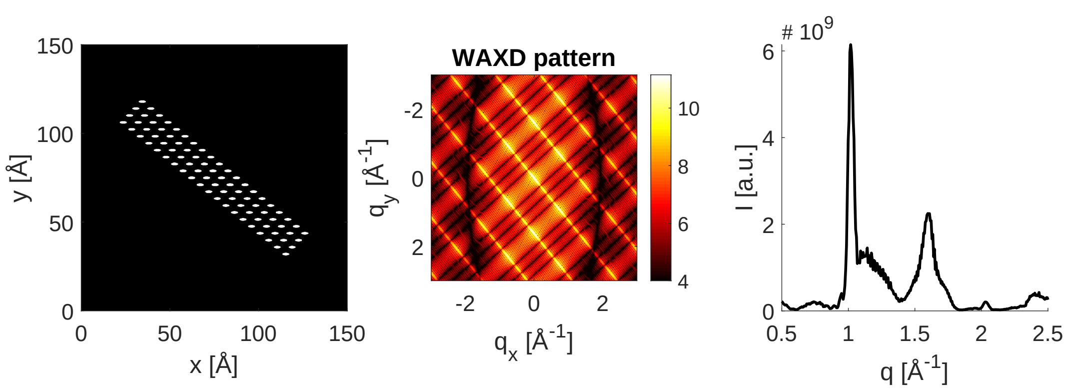
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

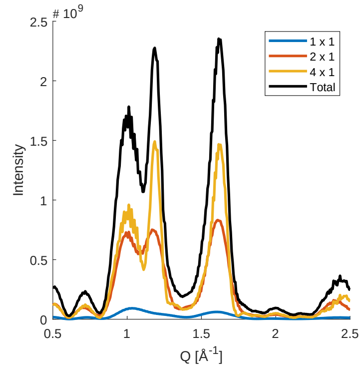






Model: R1+

Aggregation direction: (110)

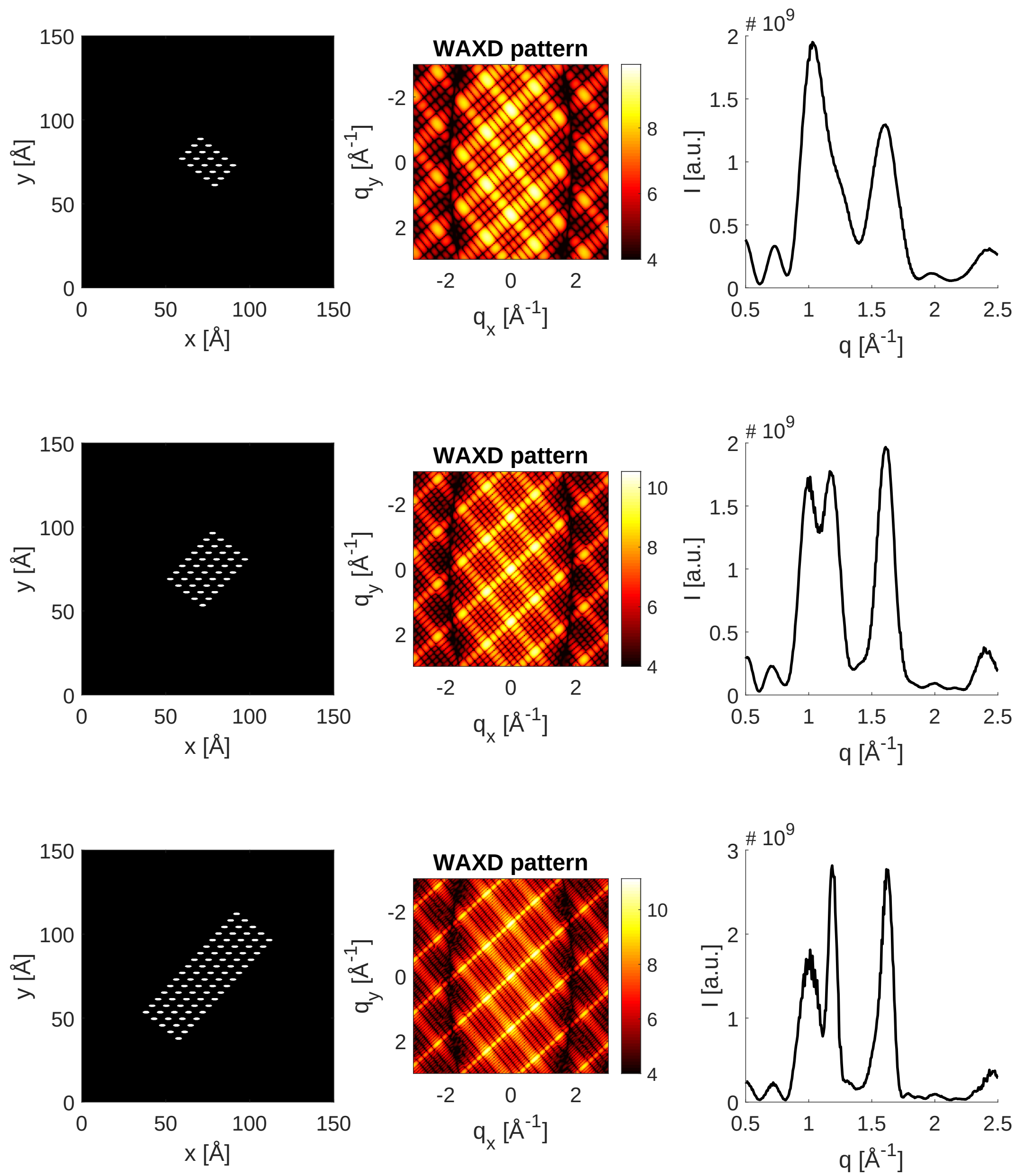


Sample #1

Vol% 1x1: 4.7

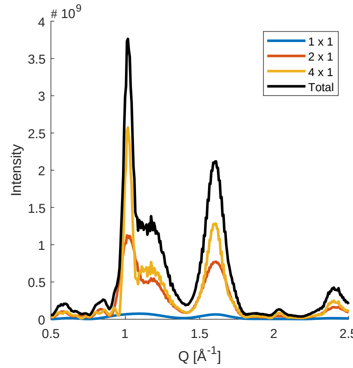
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: R1-

Aggregation direction: (1-10)

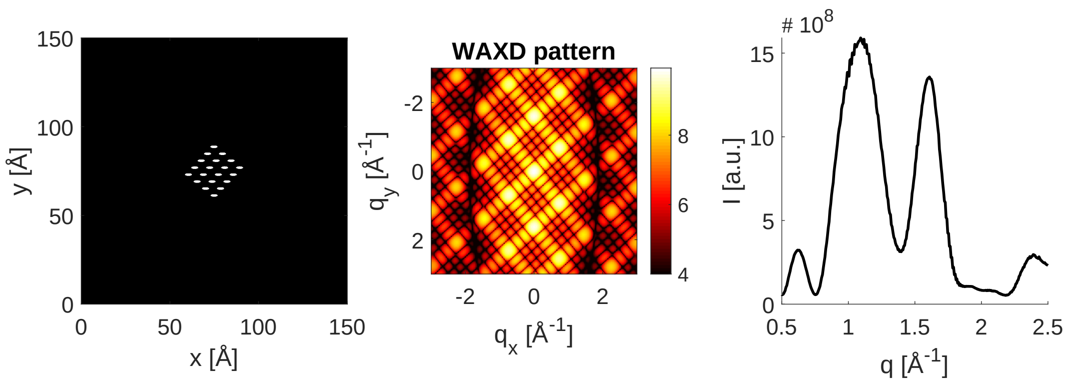


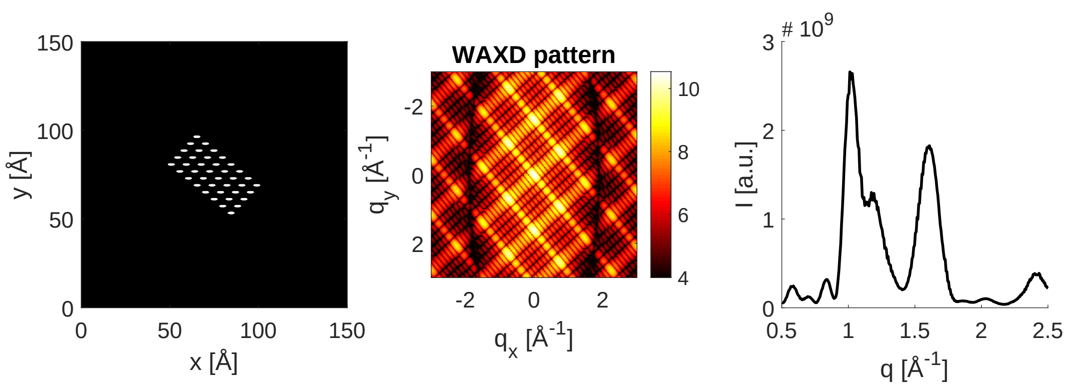
Sample #1

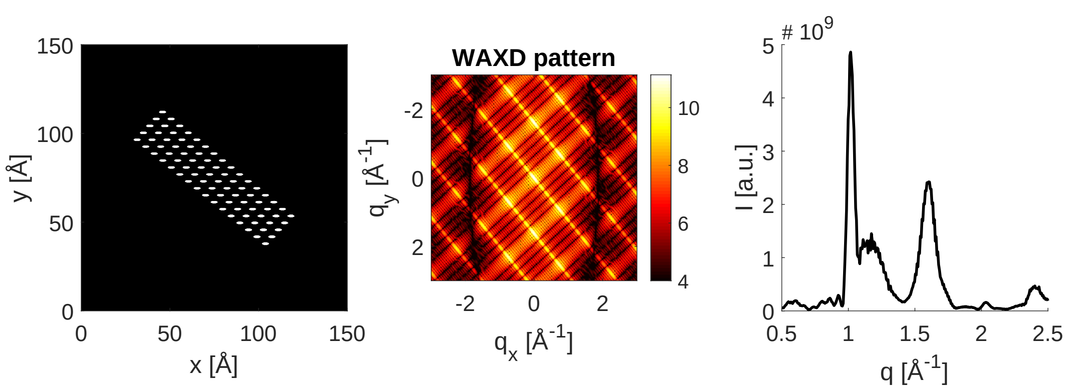
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

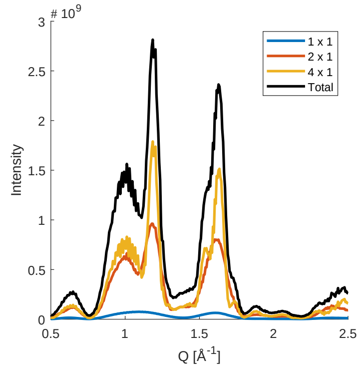






Model: R1-

Aggregation direction: (110)

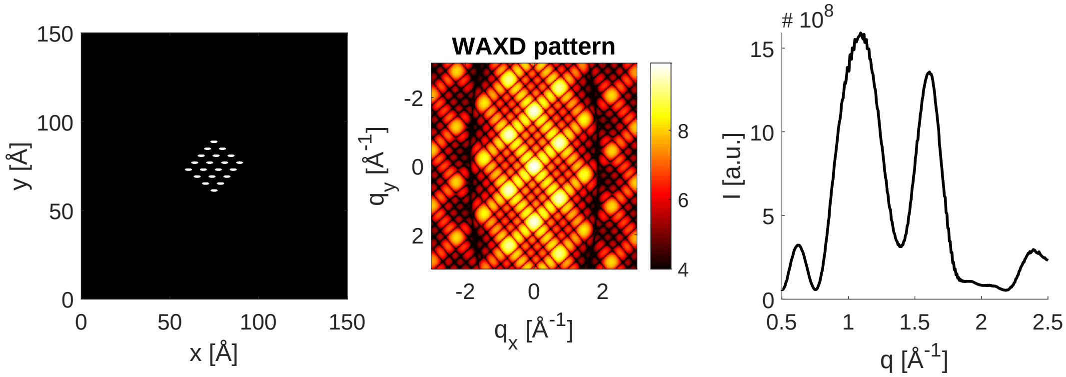


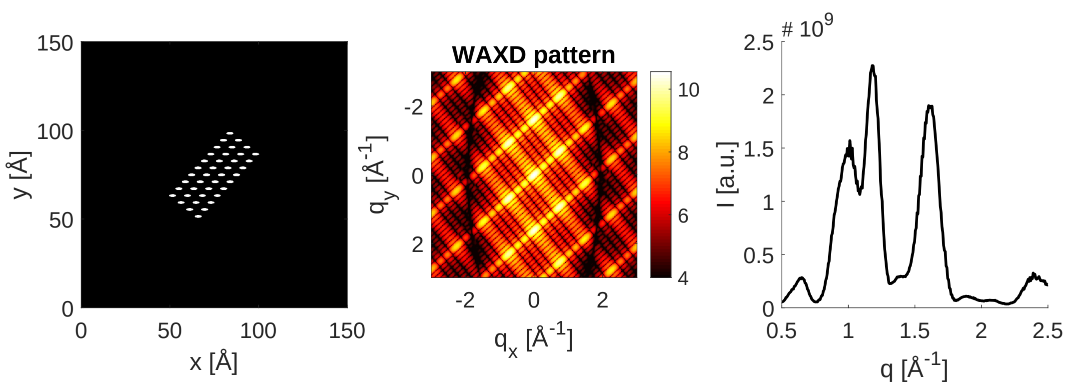
Sample #1

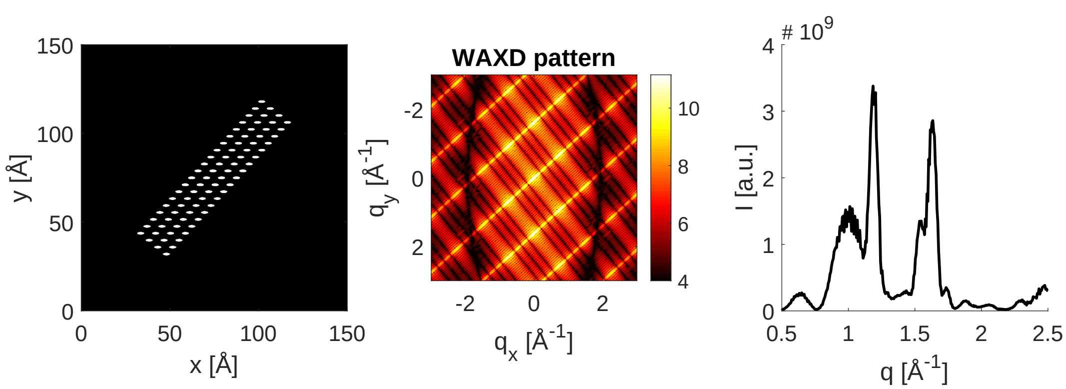
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

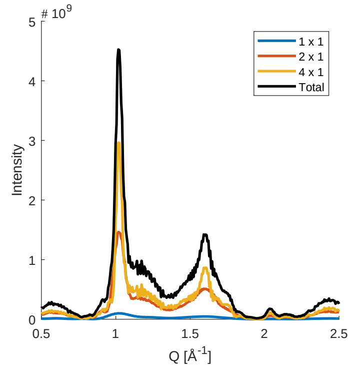






Model: R2+

Aggregation direction: (1-10)

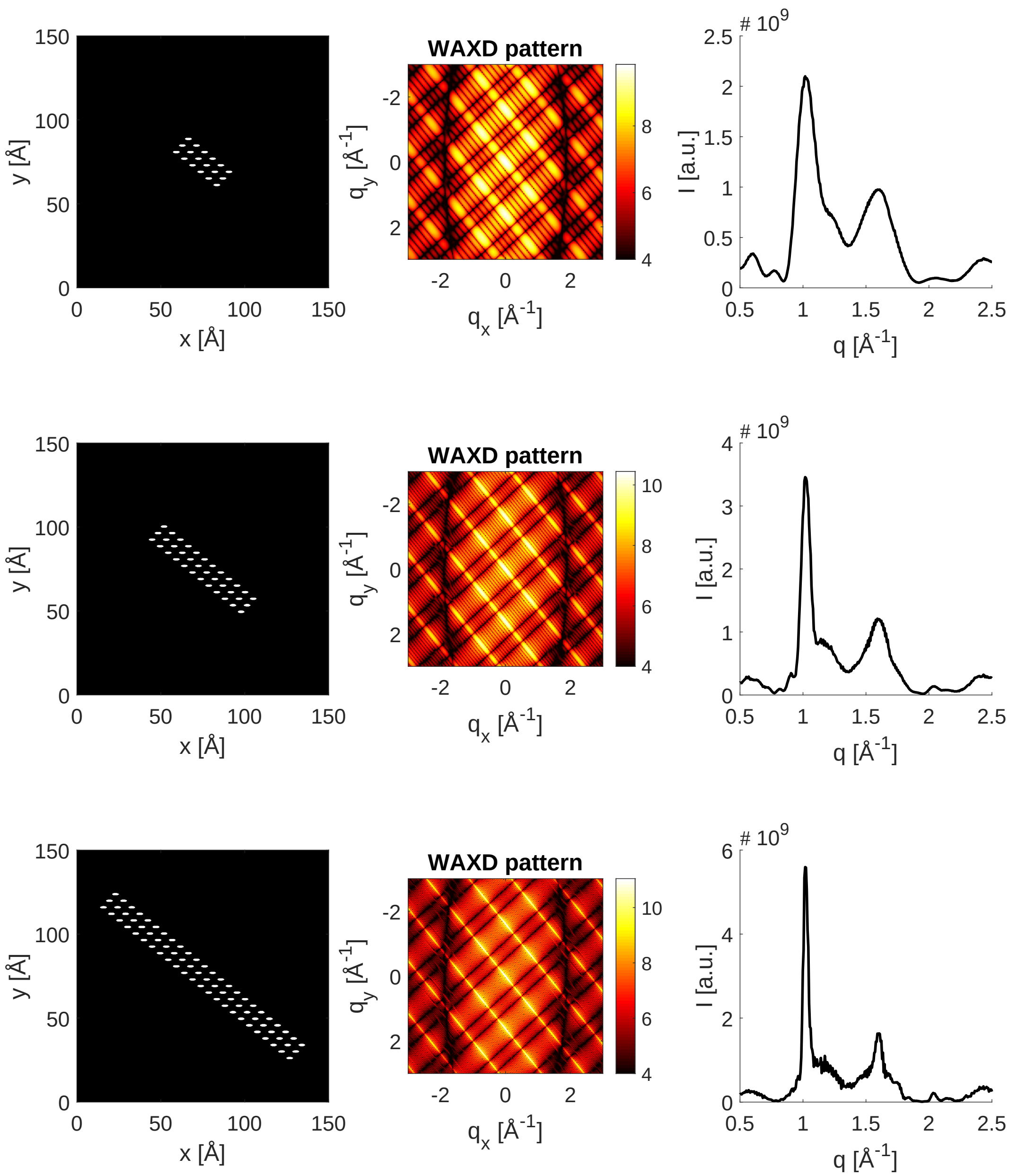


Sample #1

Vol% 1x1: 4.7

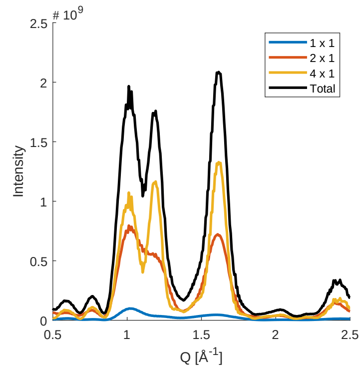
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: R2+

Aggregation direction: (110)

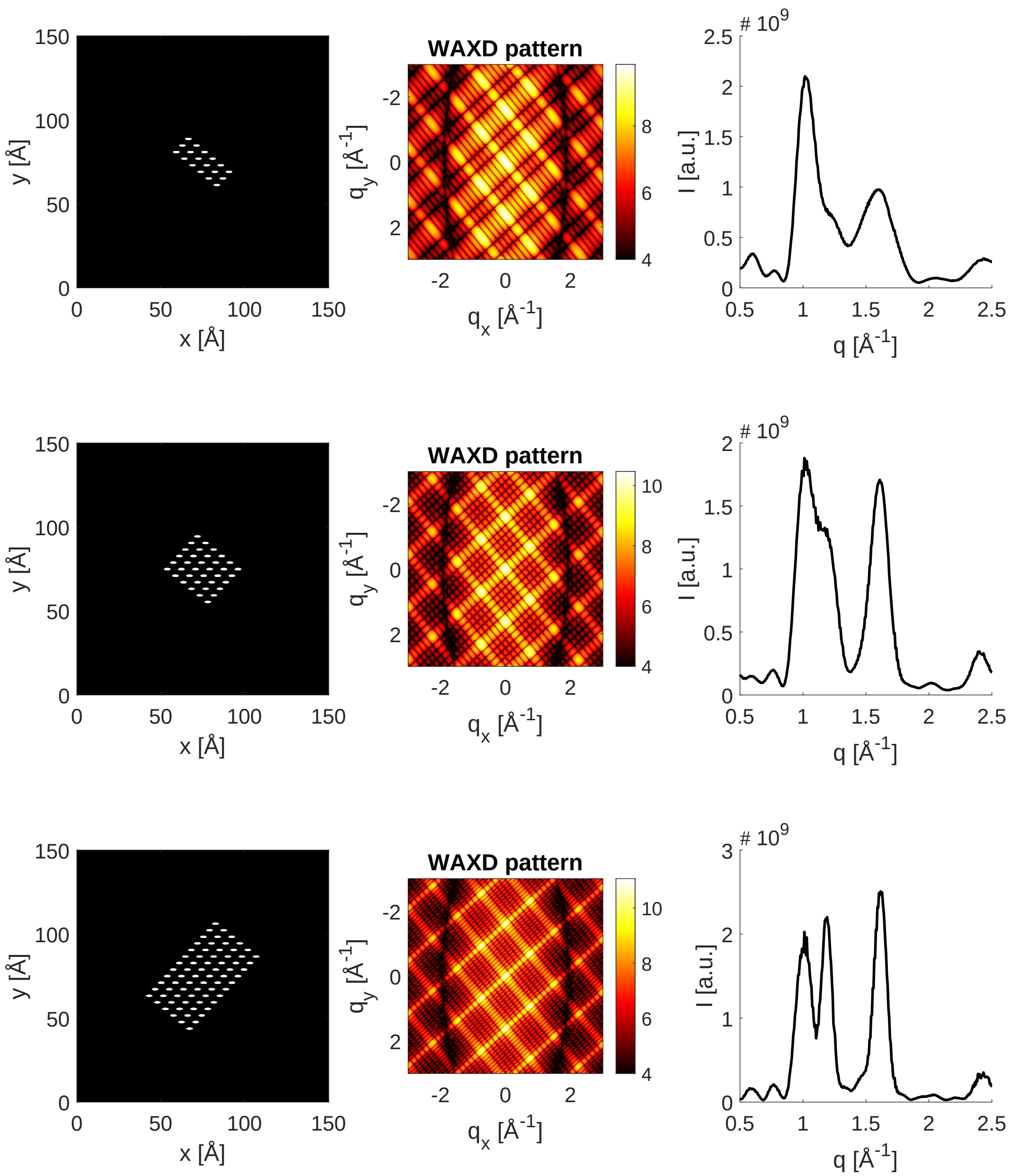


Sample #1

Vol% 1x1: 4.7

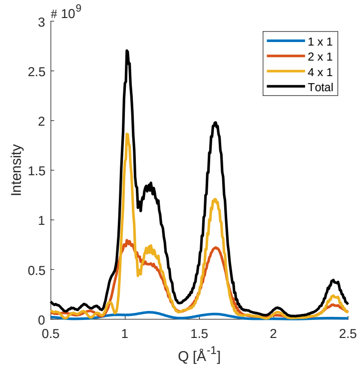
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: R2-

Aggregation direction: (1-10)

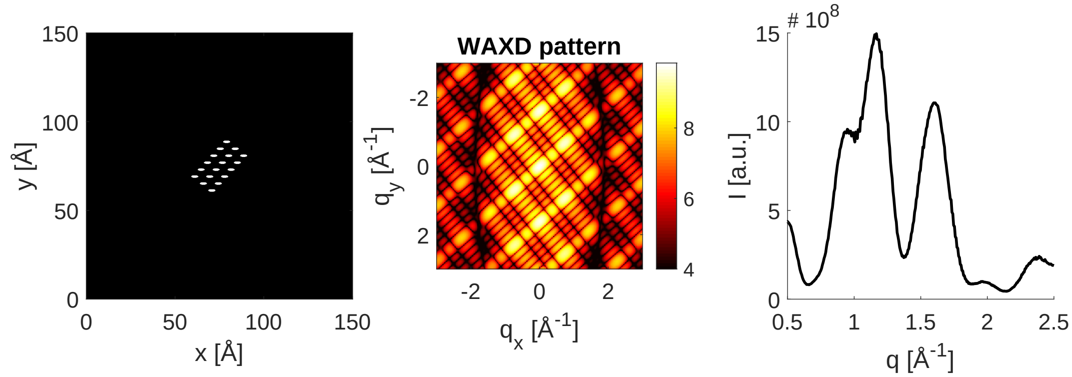


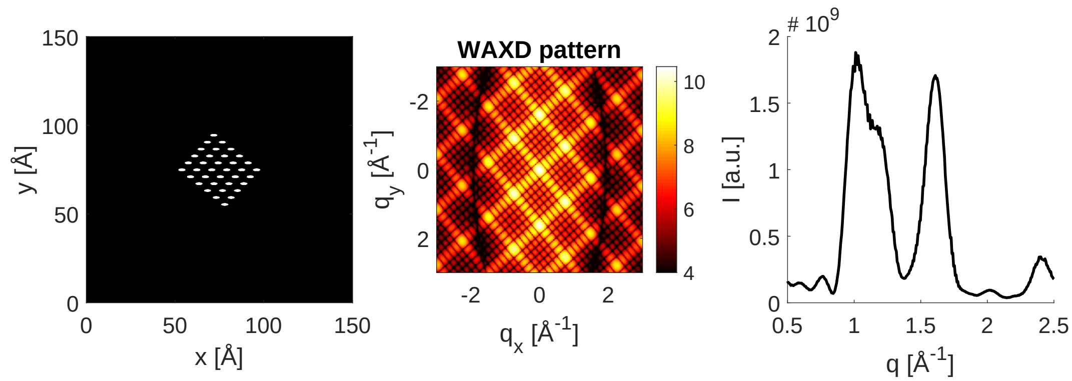
Sample #1

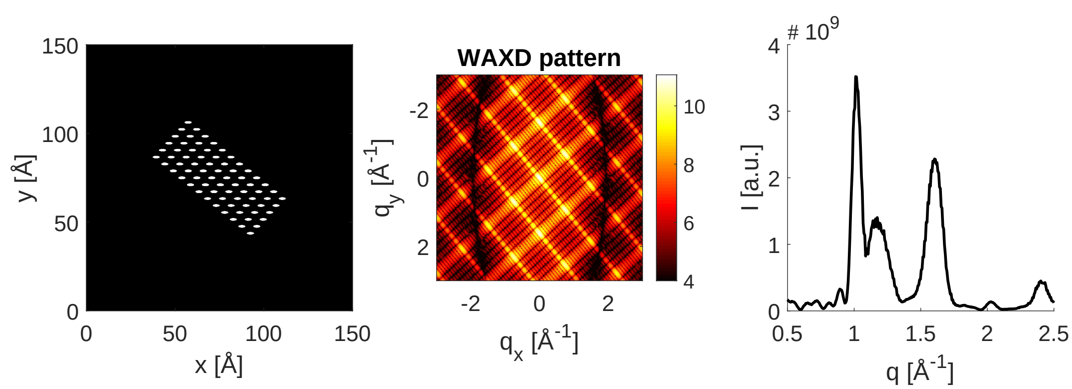
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

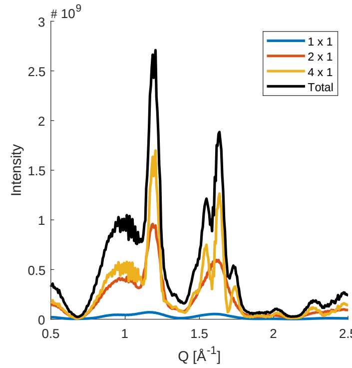






Model: R2-

Aggregation direction: (110)

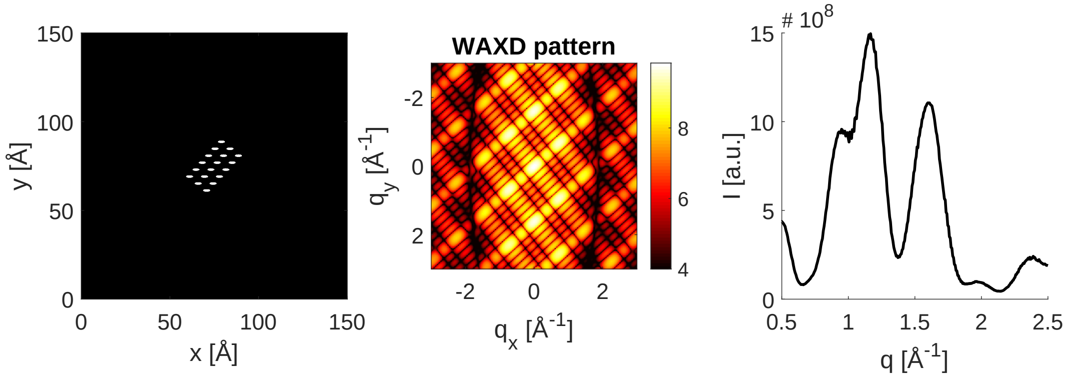


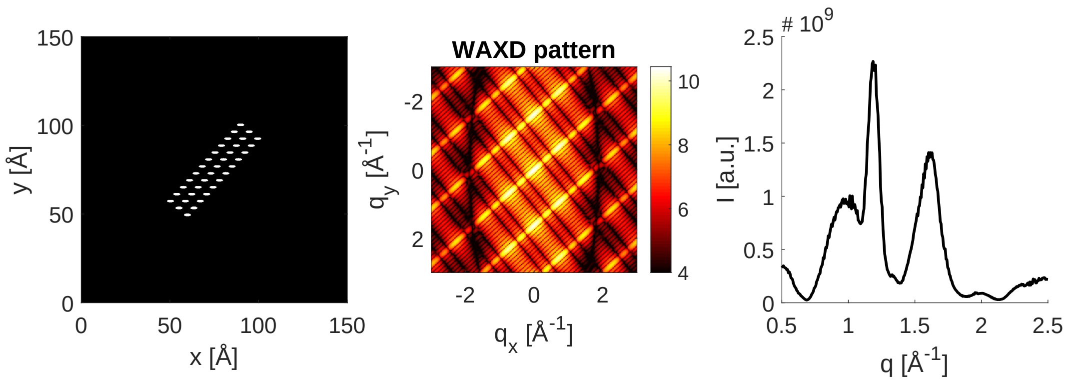
Sample #1

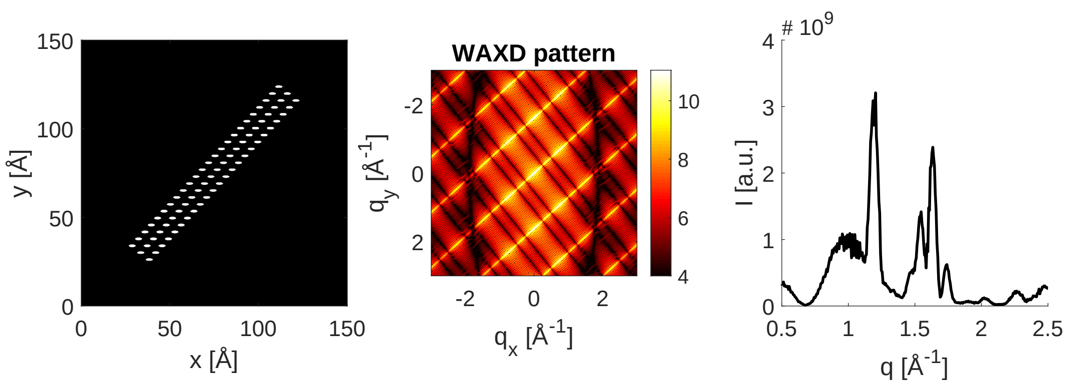
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

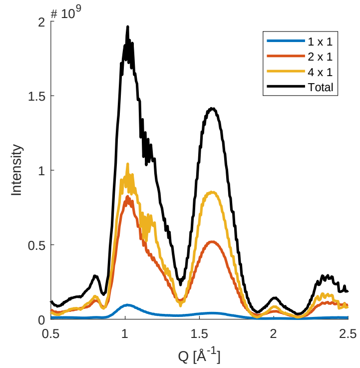






Model: Rh1+

Aggregation direction: (110)

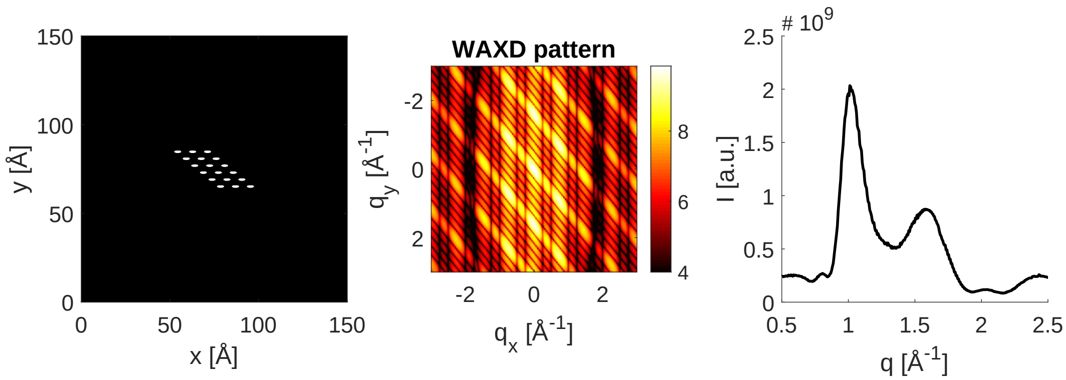


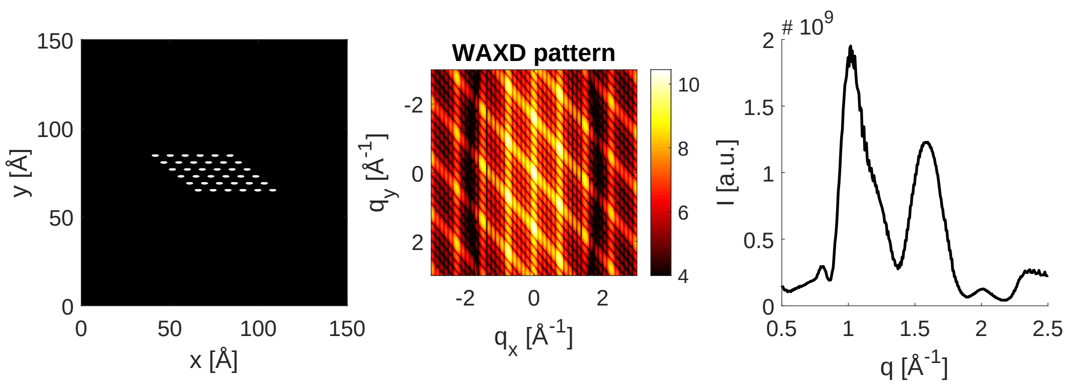
Sample #1

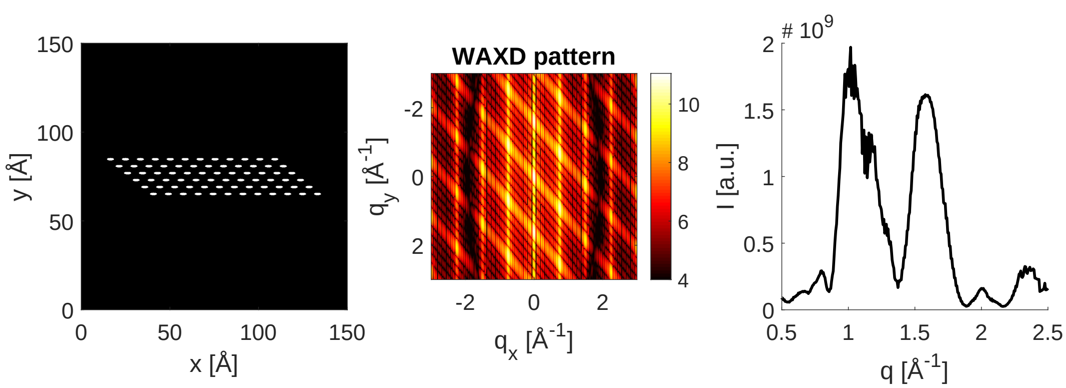
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

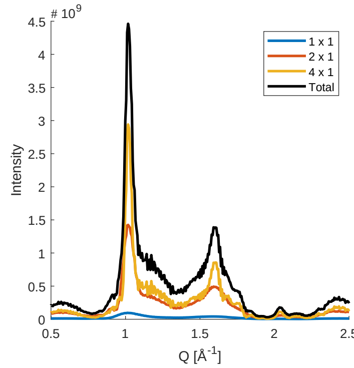






Model: Rh1+

Aggregation direction: (200)

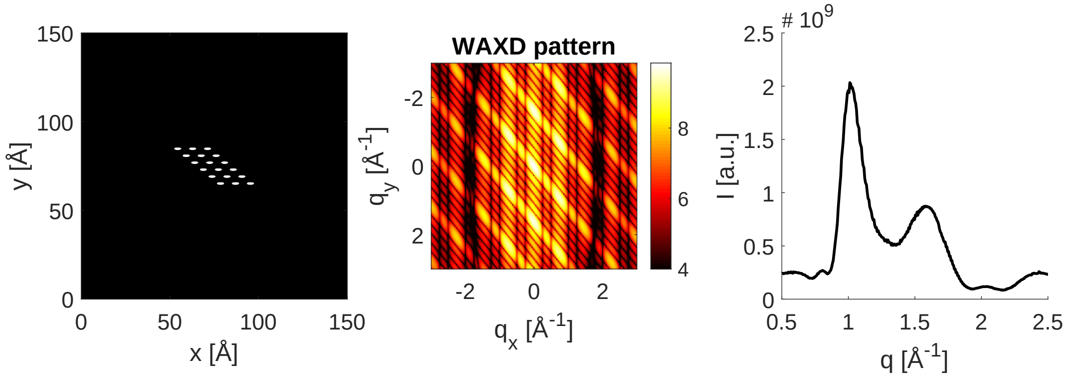


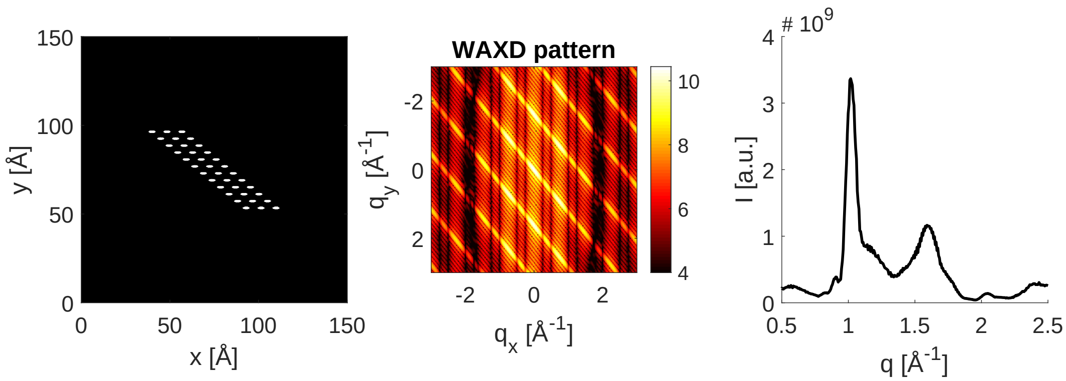
Sample #1

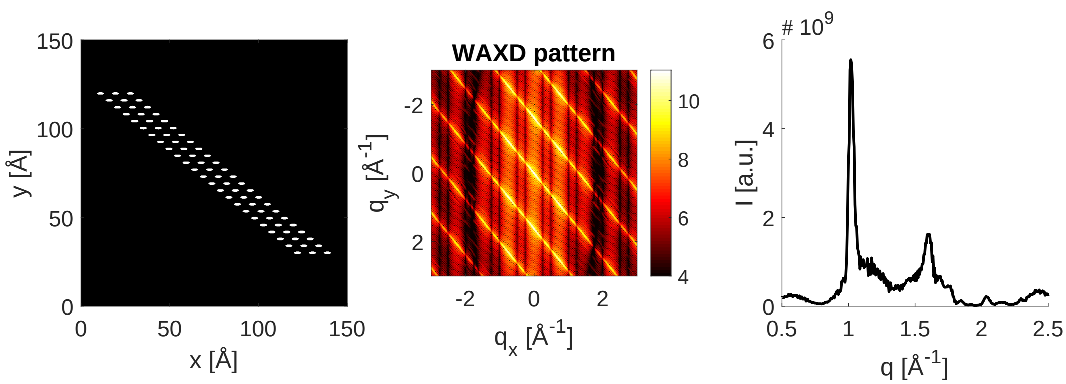
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

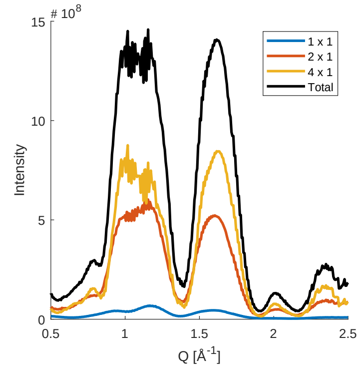






Model: Rh1-

Aggregation direction: (1-10)

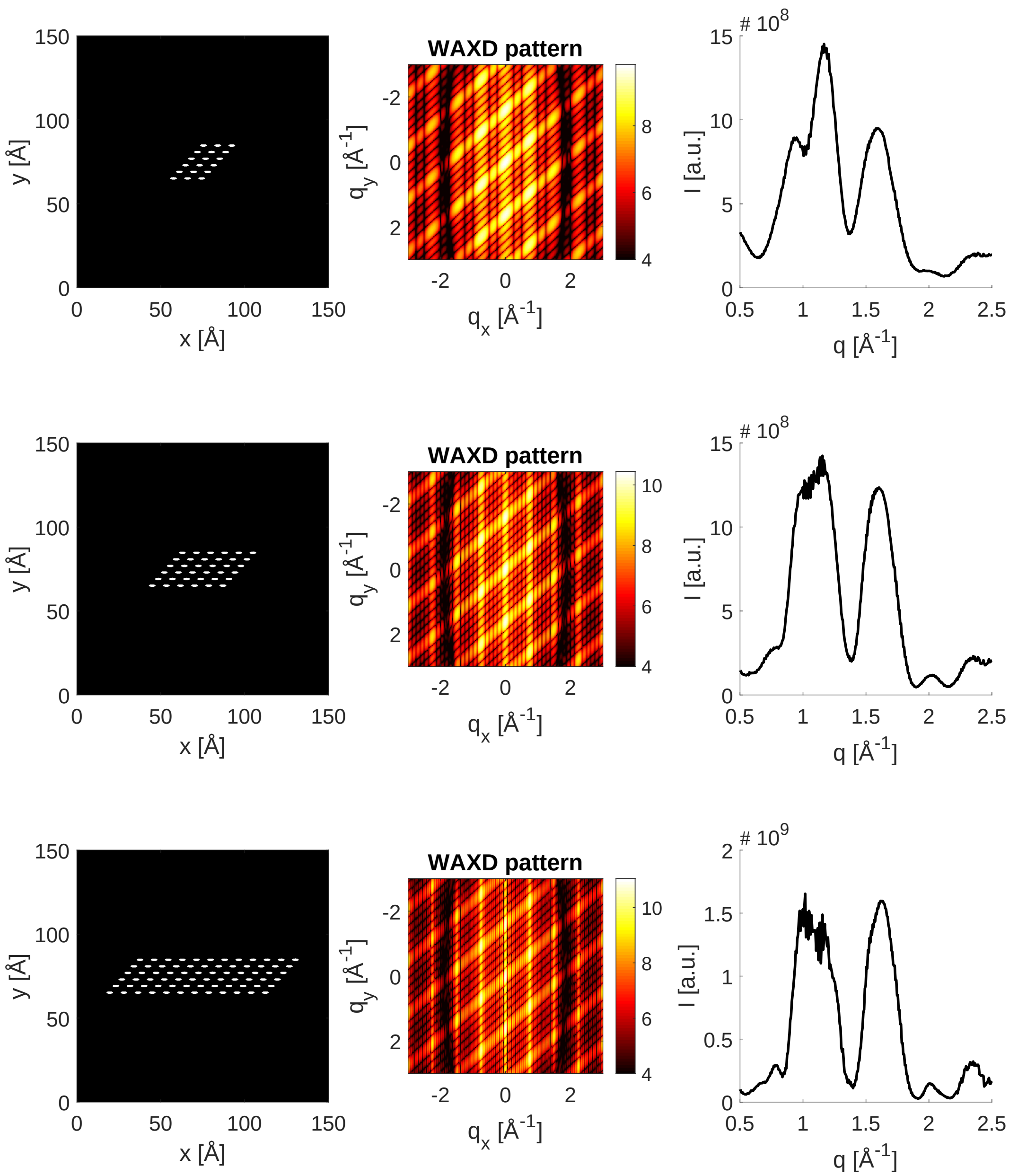


Sample #1

Vol% 1x1: 4.7

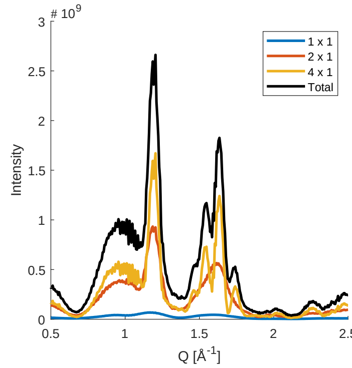
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: Rh1-

Aggregation direction: (200)

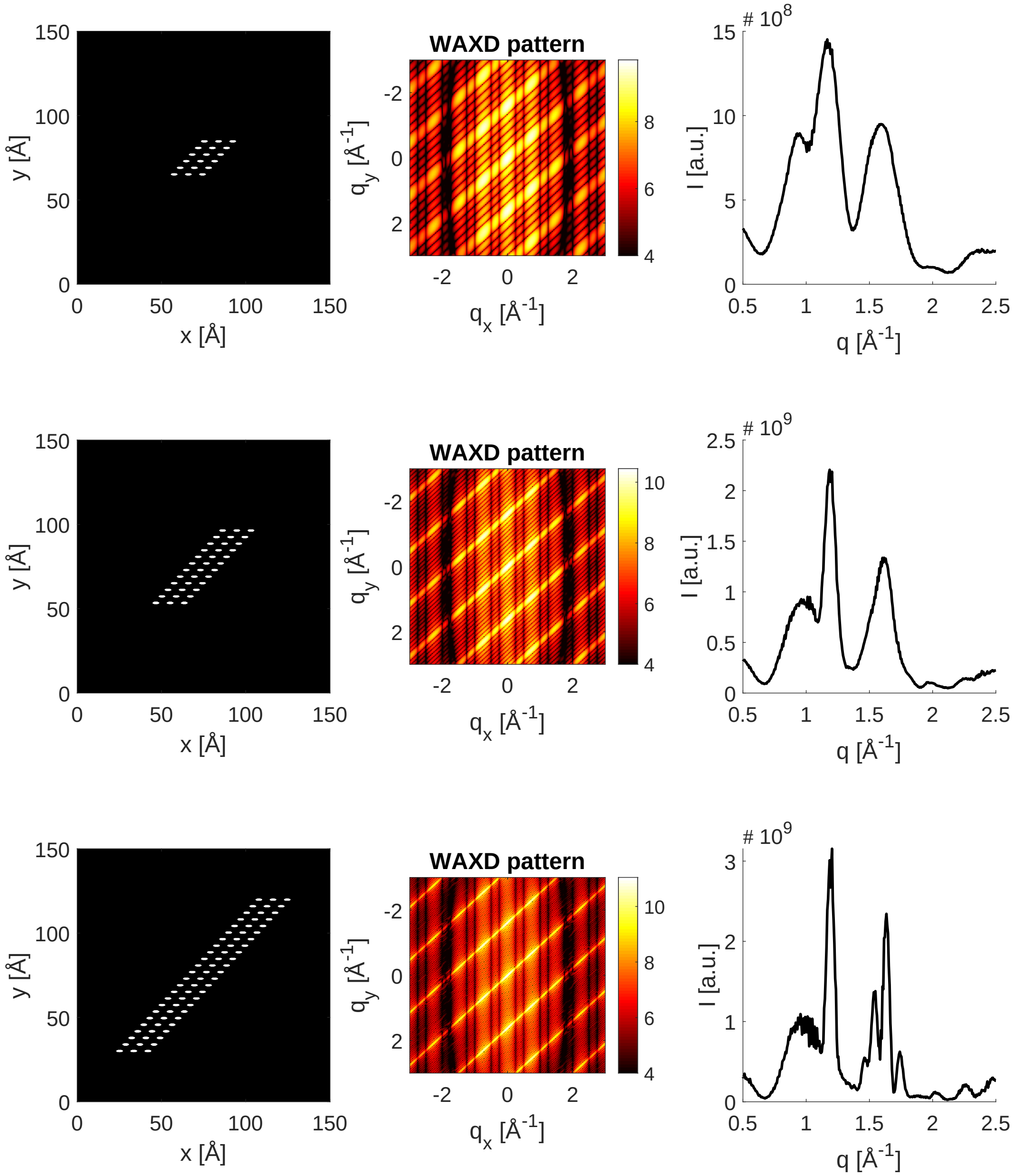


Sample #1

Vol% 1x1: 4.7

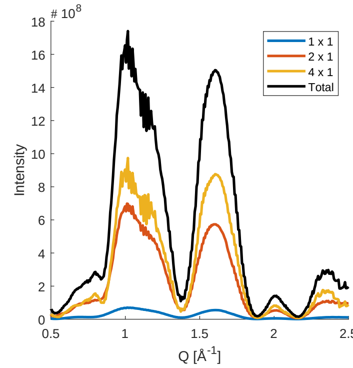
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: Rh2

Aggregation direction: (010)

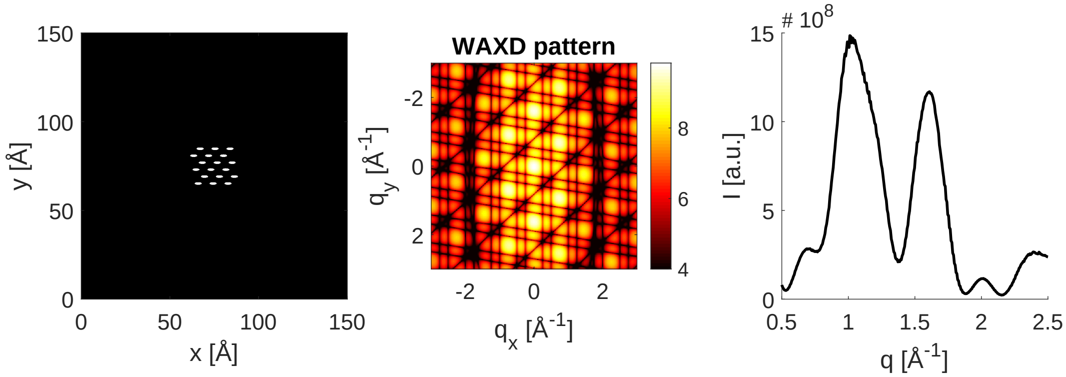


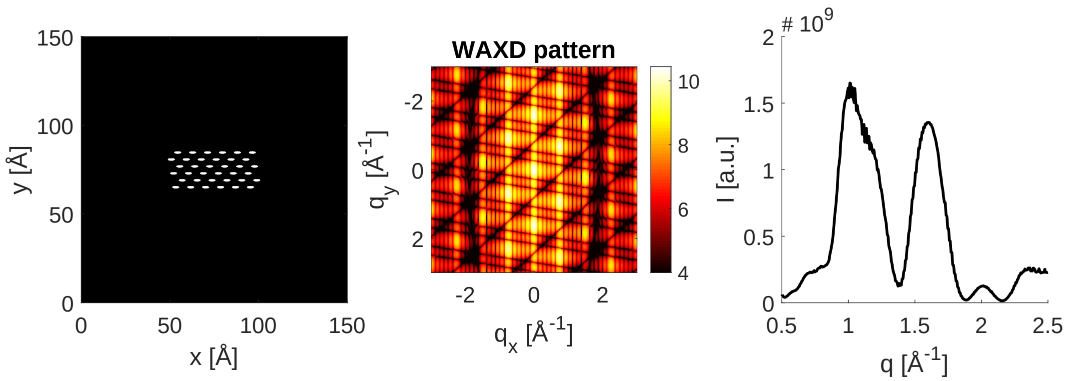
Sample #1

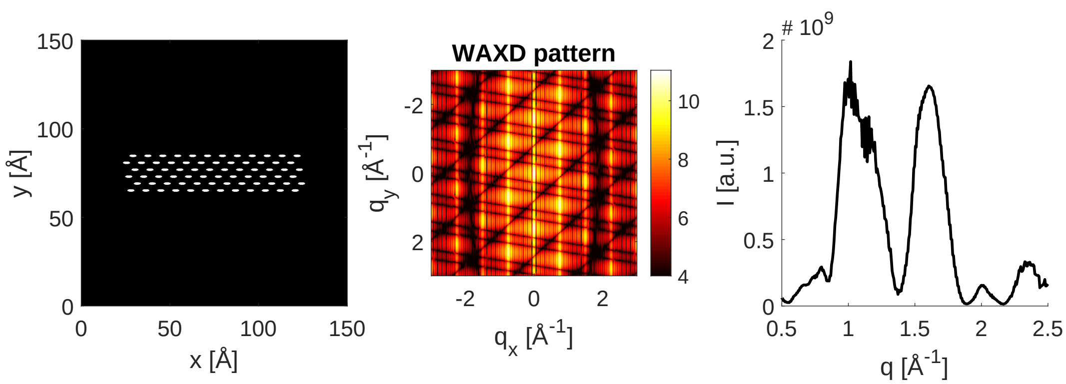
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

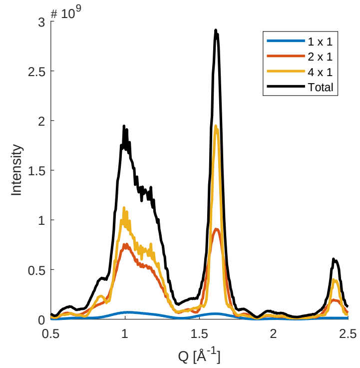






Model: Rh2

Aggregation direction: (200)

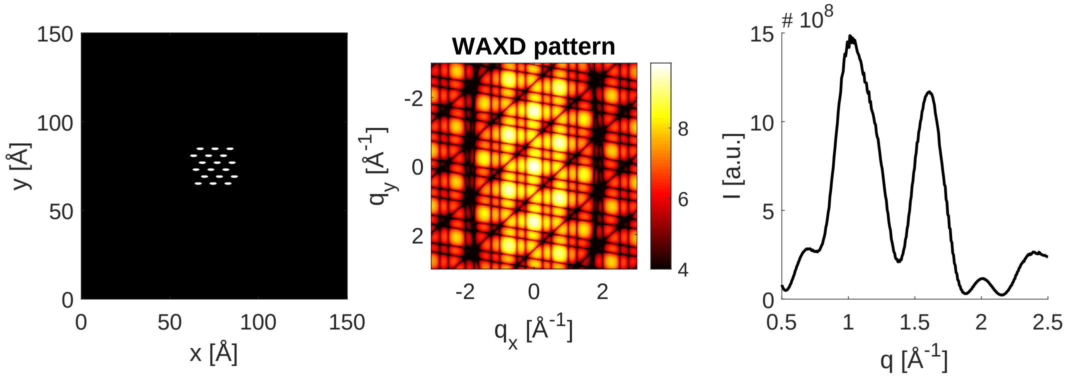


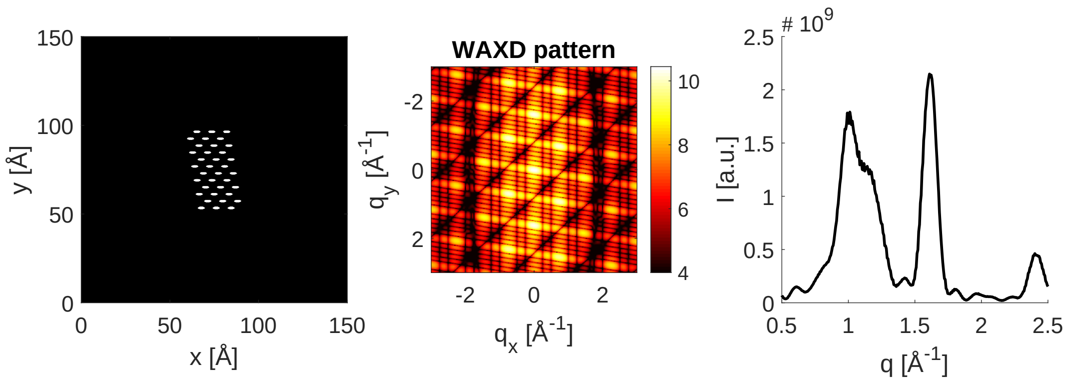
Sample #1

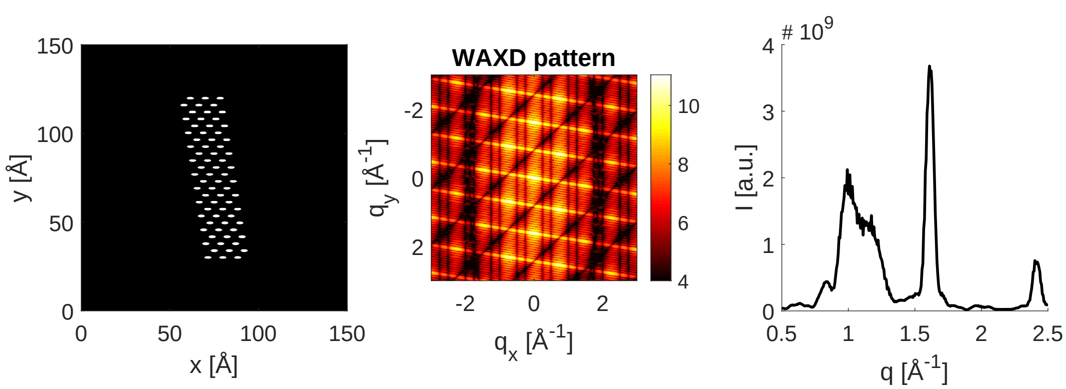
Vol% 1x1: 4.7

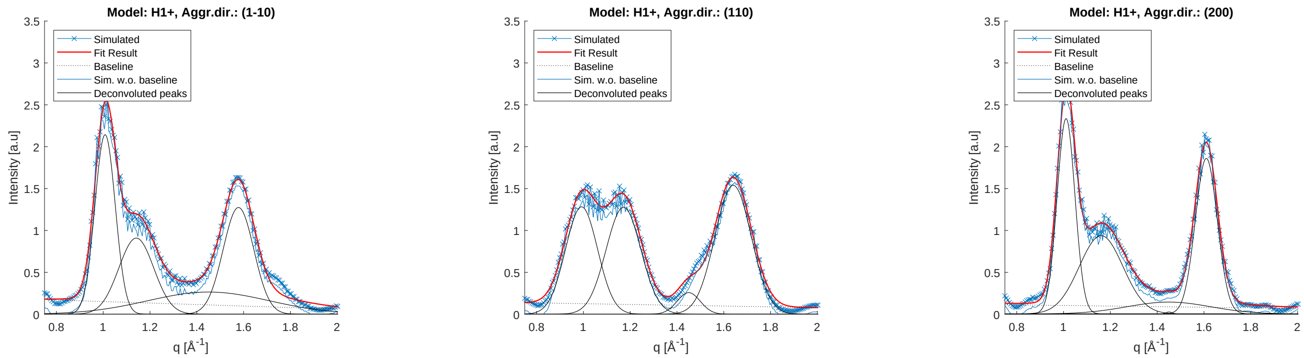
Vol% 2x1: 42.3

Vol% 4x1: 53.0

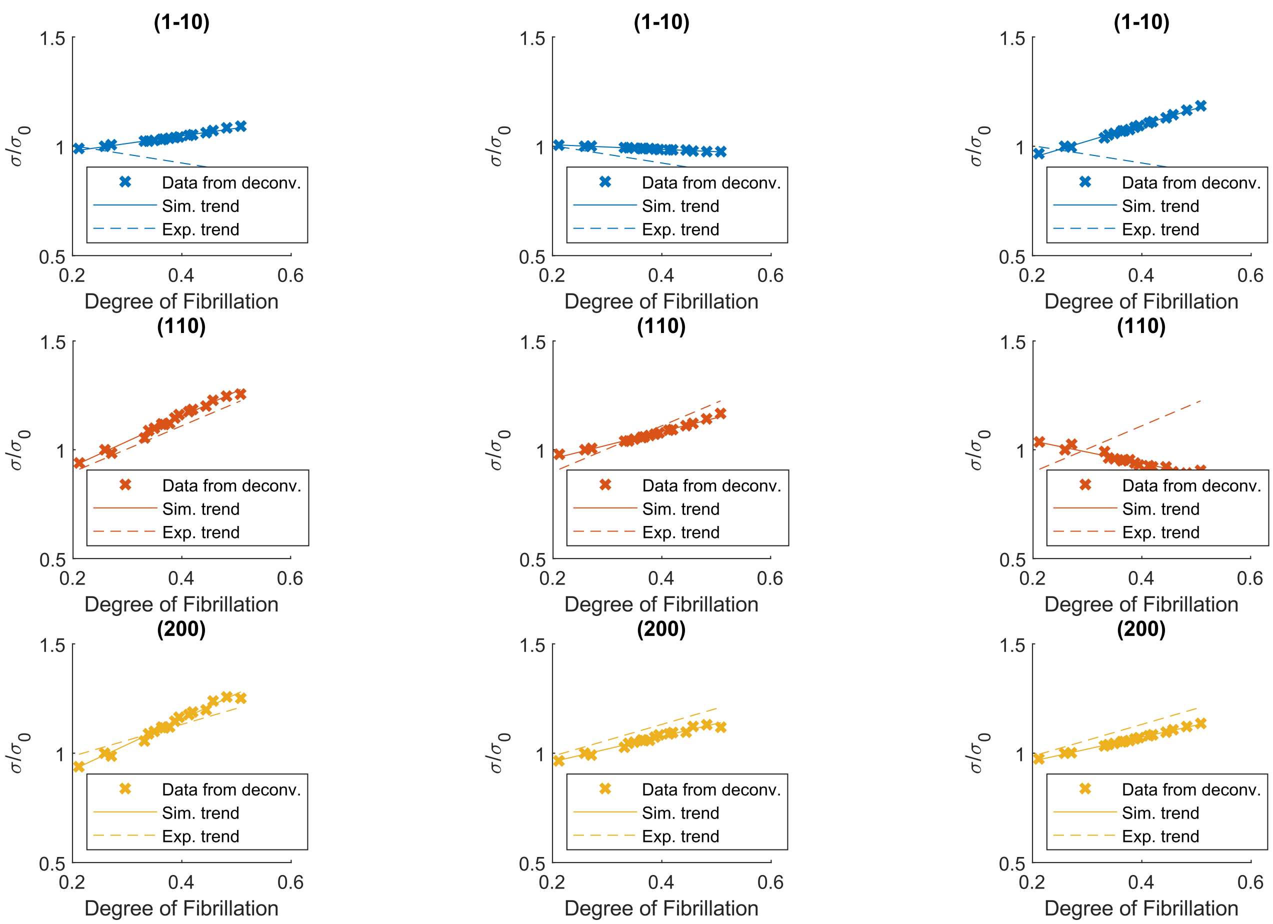




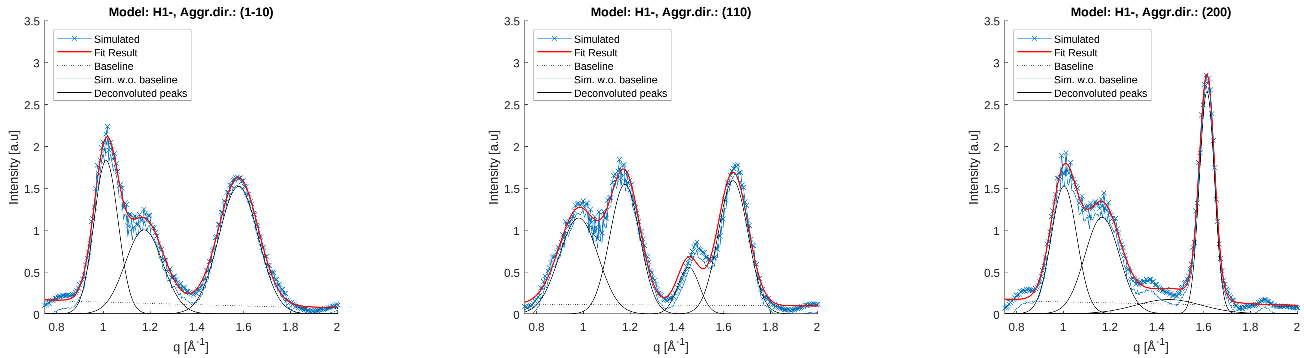


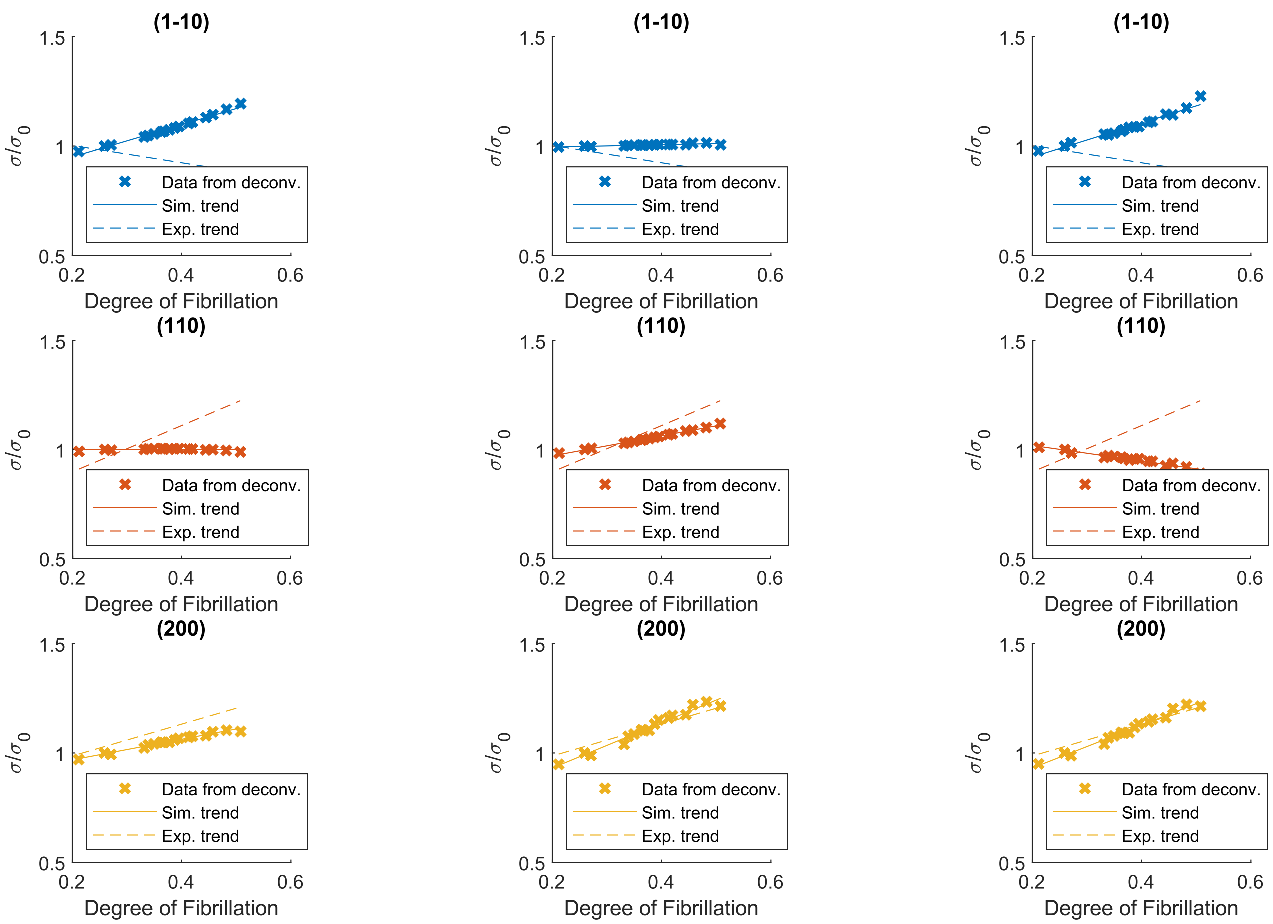


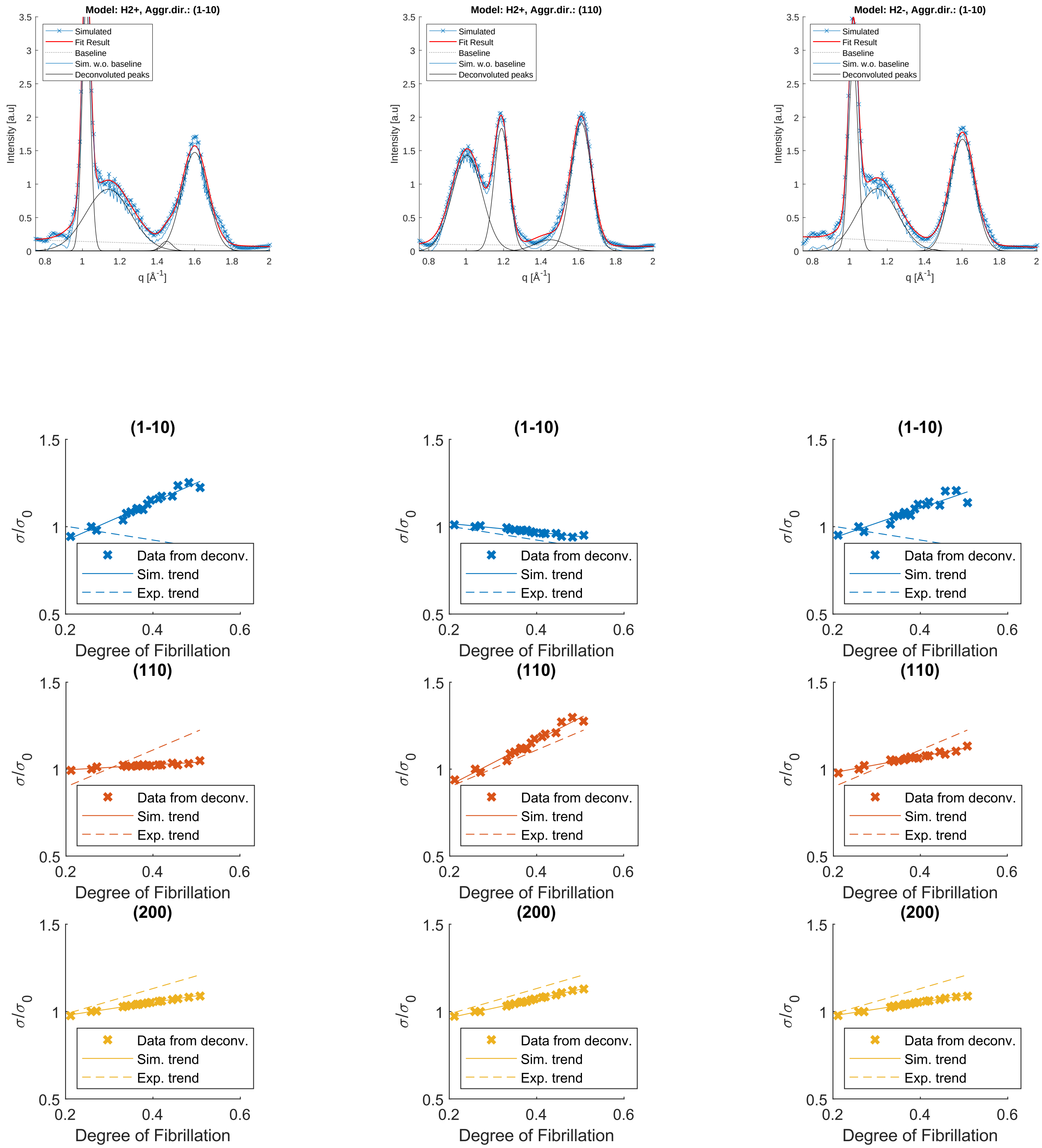
Model: H1+, Aggr.dir.: (1-10)
Model: H1+, Aggr.dir.: (110)
Model: H1+, Aggr.dir.: (200)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^-1]

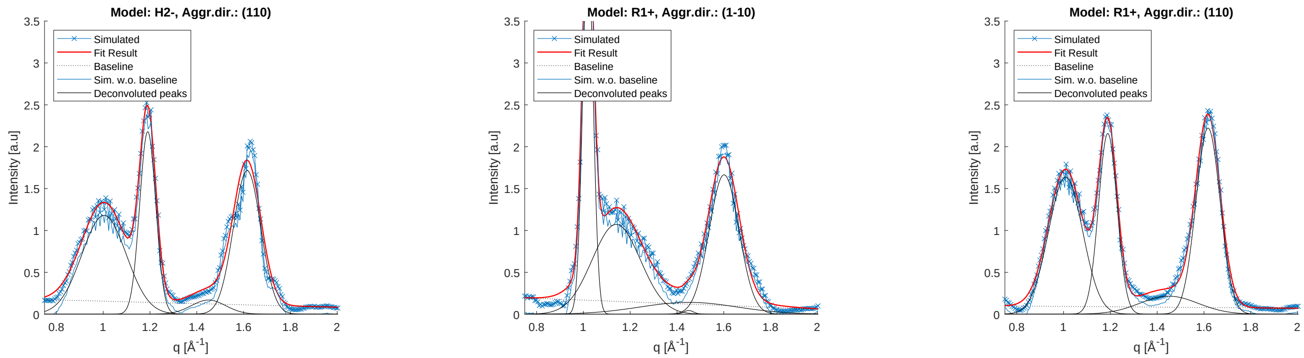


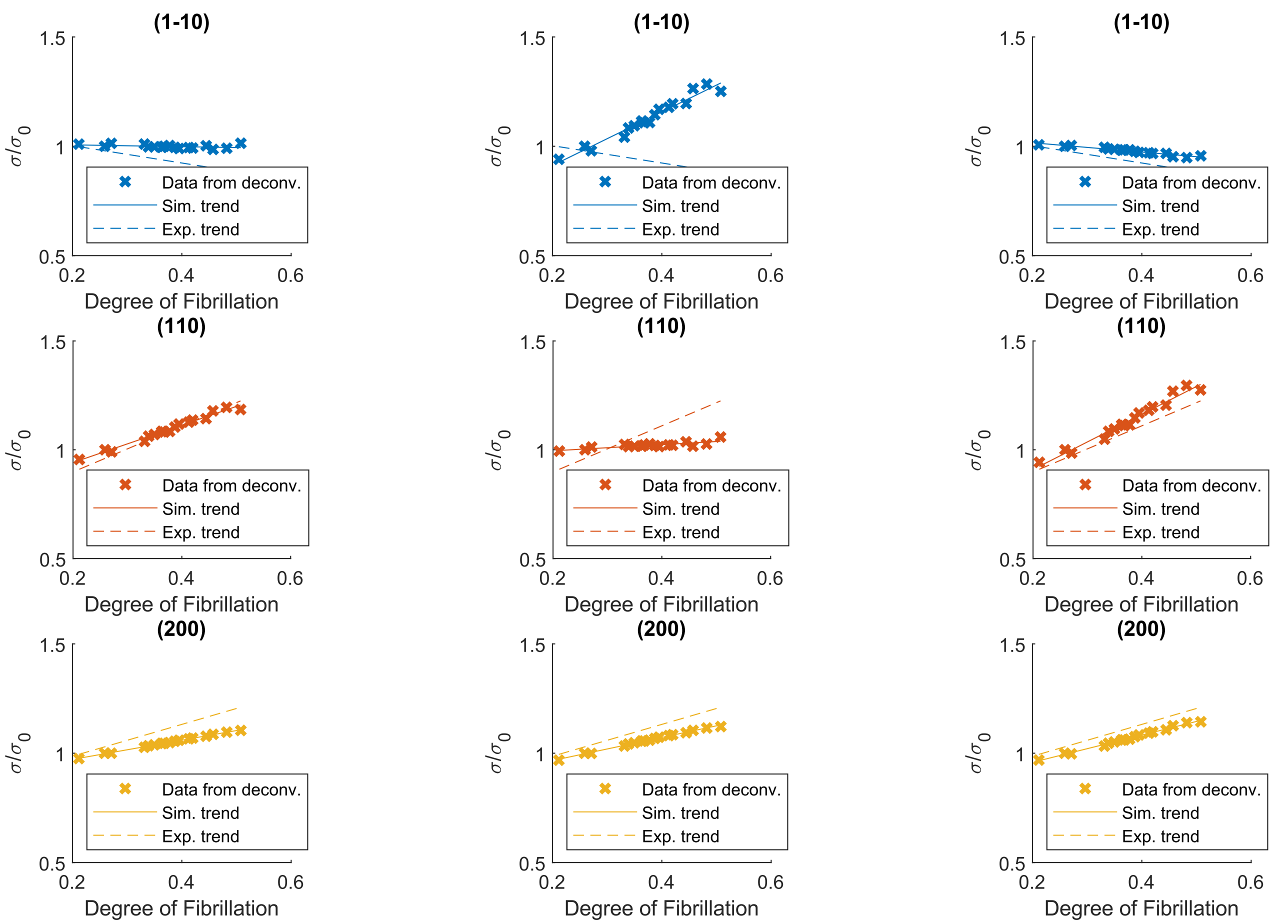
(1-10)
(110)
(200)
σ/σ0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation

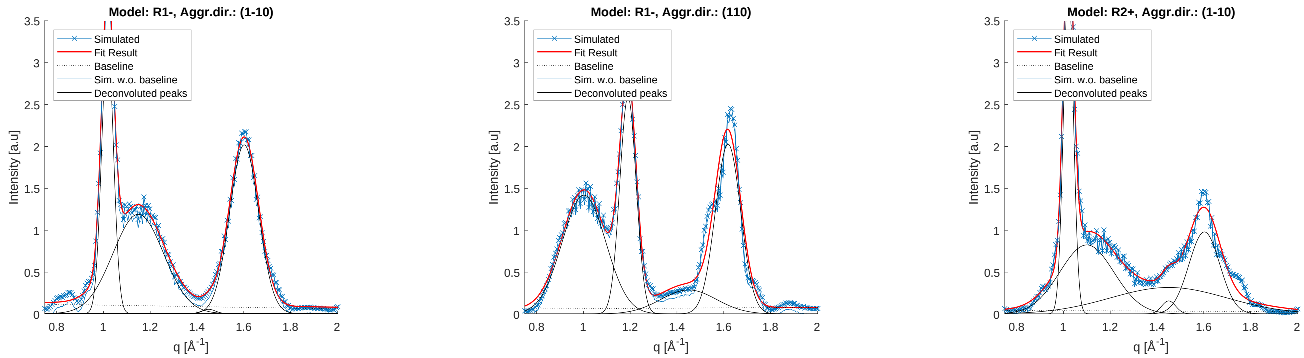

Model: H1-, Aggr.dir.: (1-10)
Model: H1-, Aggr.dir.: (110)
Model: H1-, Aggr.dir.: (200)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^{-1}]


(1-10)
(110)
(200)
σ/σ_0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation

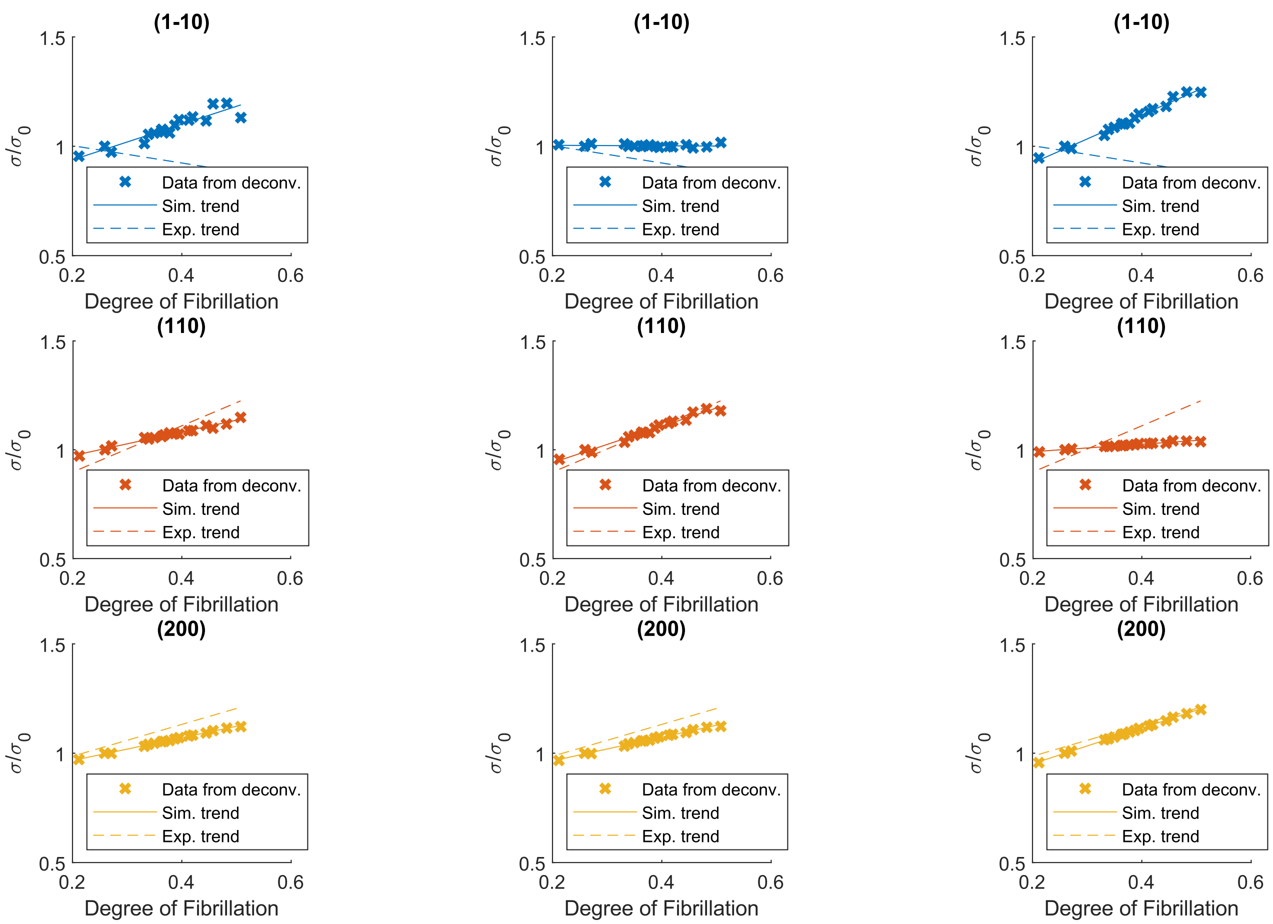

Model: H2+, Aggr.dir.: (1-10)
Model: H2+, Aggr.dir.: (110)
Model: H2-, Aggr.dir.: (1-10)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å-1]
(1-10)
(110)
(200)
σ/σ0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation


Model: H2-, Aggr.dir.: (110)
Model: R1+, Aggr.dir.: (1-10)
Model: R1+, Aggr.dir.: (110)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å-1]

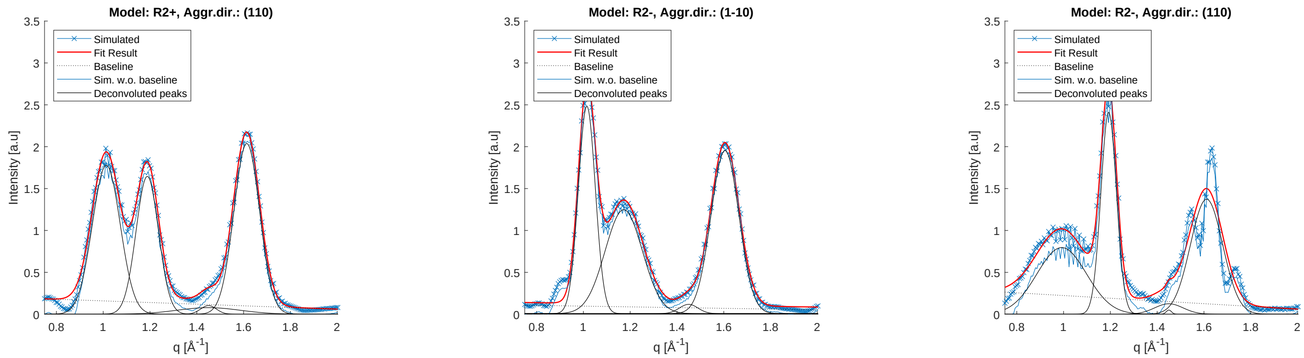

(1-10)
(110)
(200)
σ/σ0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation

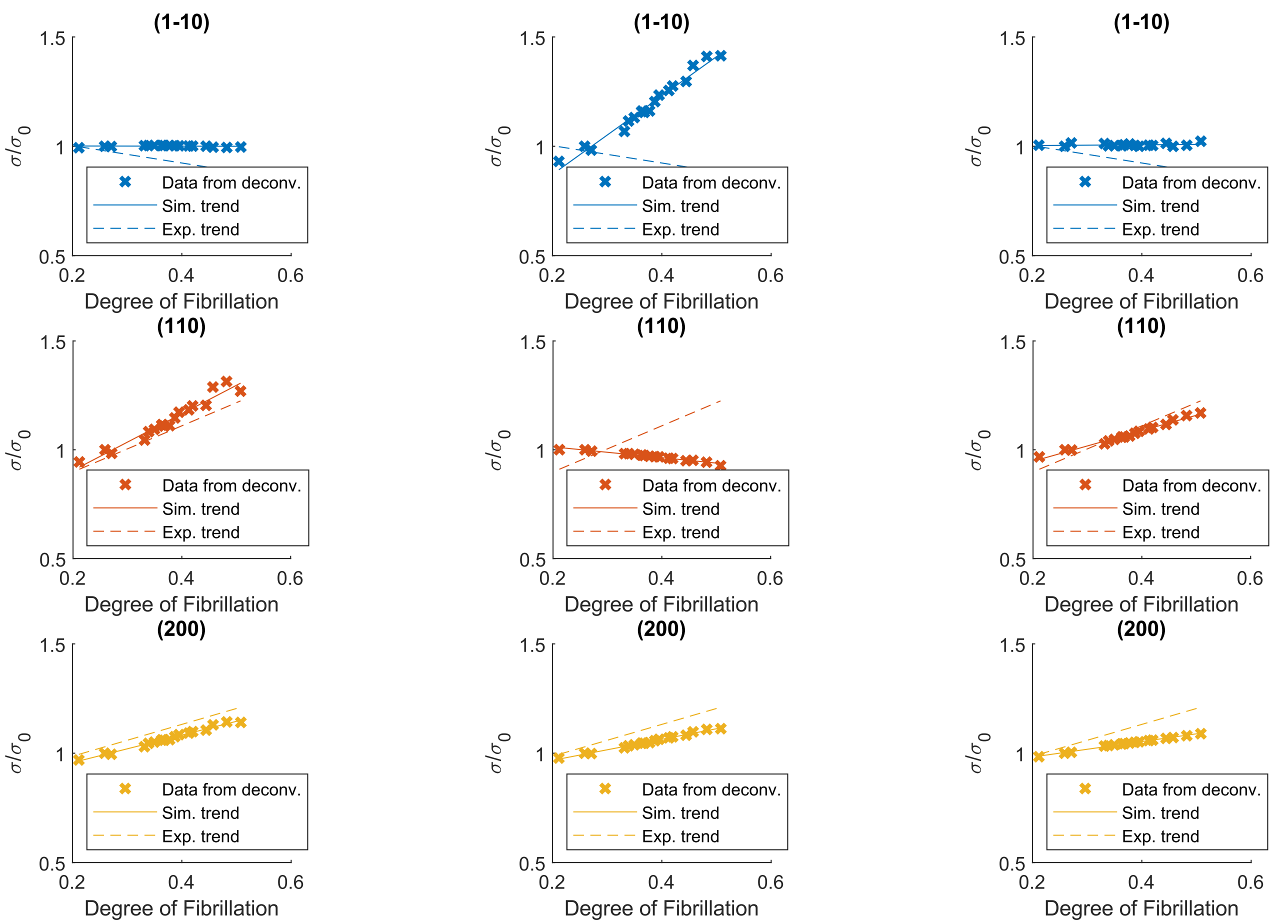


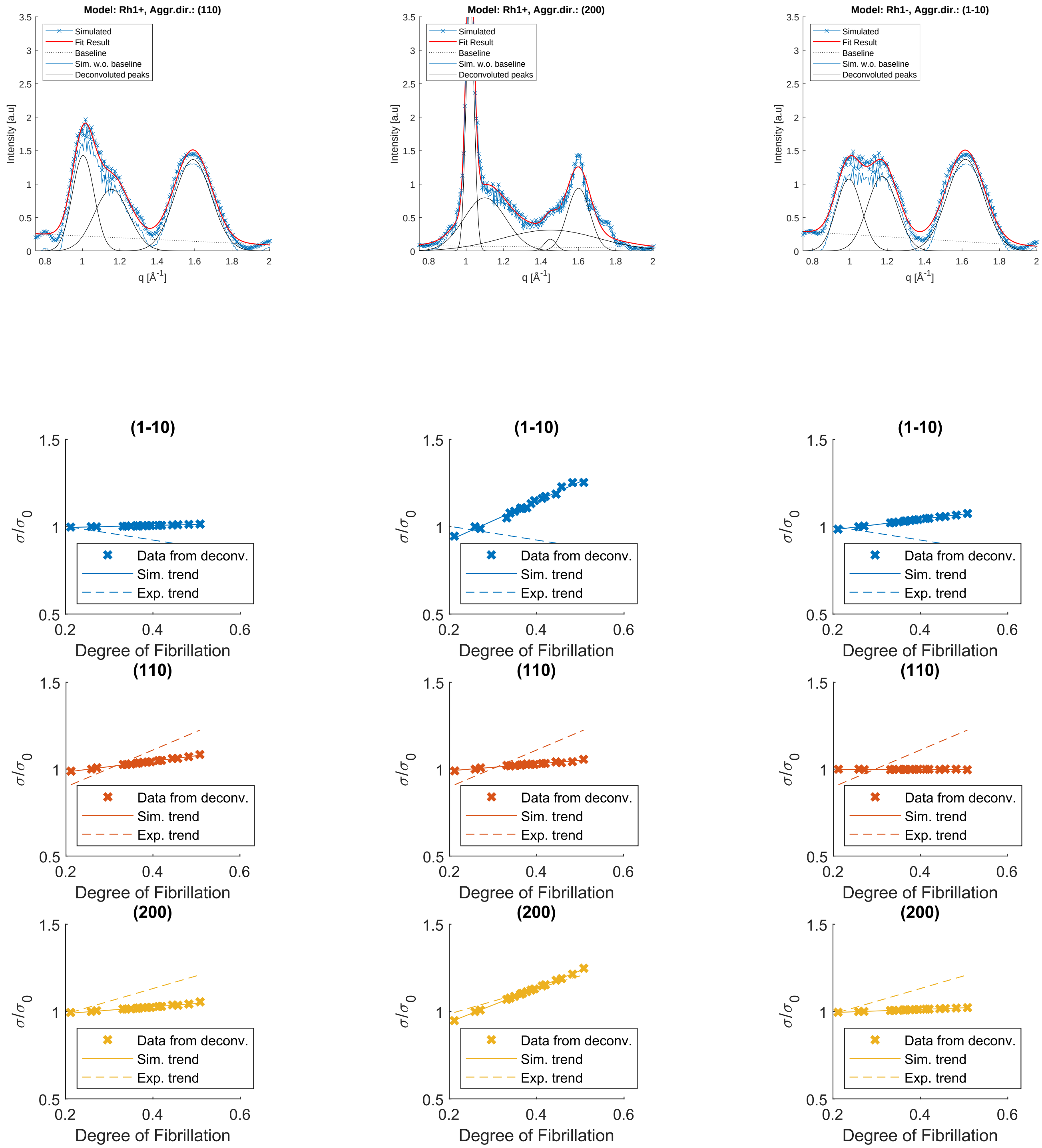
Model: R1-, Aggr.dir.: (1-10)
Model: R1-, Aggr.dir.: (110)
Model: R2+, Aggr.dir.: (1-10)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^{-1}]

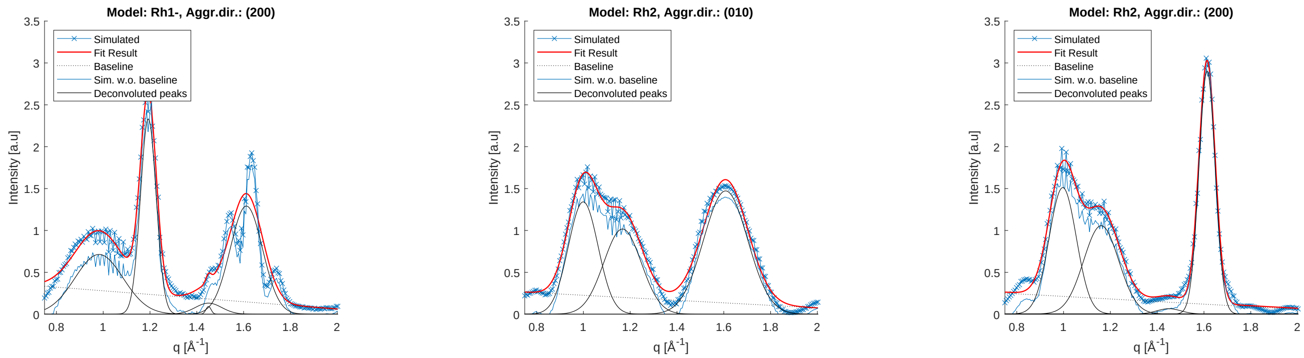


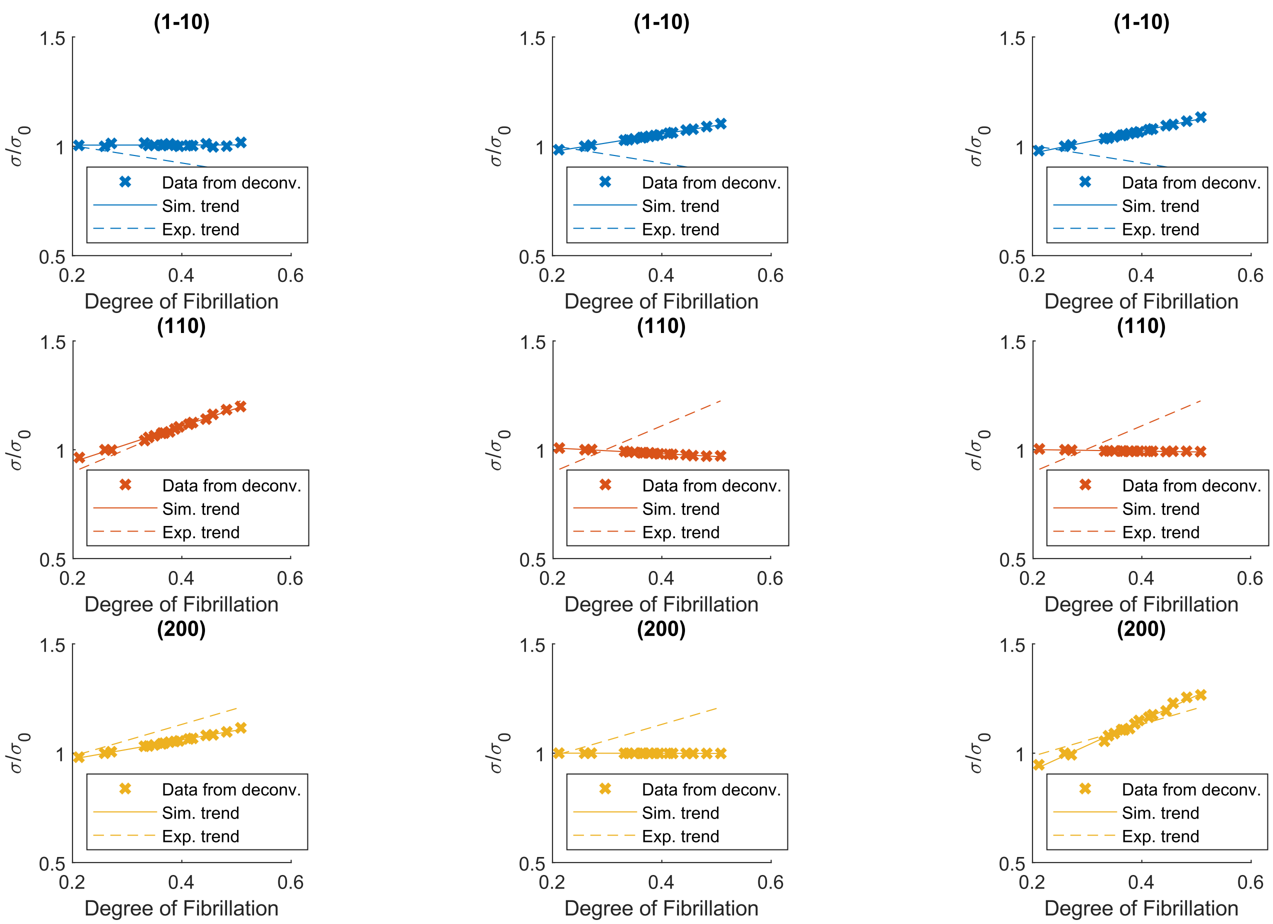
(1-10)
(110)
(200)
σ/σ_0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation


Model: R2+, Aggr.dir.: (110)
Model: R2-, Aggr.dir.: (1-10)
Model: R2-, Aggr.dir.: (110)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å-1]


(1-10)
(110)
(200)
Data from deconv.
Sim. trend
Exp. trend
σ/σ0
Degree of Fibrillation


Model: Rh1+, Aggr.dir.: (110)
Model: Rh1+, Aggr.dir.: (200)
Model: Rh1-, Aggr.dir.: (1-10)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^{-1}]
(1-10)
(110)
(200)
σ/σ_0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation


Model: Rh1-, Aggr.dir.: (200)
Model: Rh2, Aggr.dir.: (010)
Model: Rh2, Aggr.dir.: (200)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^-1]


(1-10)
(110)
(200)
Data from deconv.
Sim. trend
Exp. trend
σ/σ0
Degree of Fibrillation

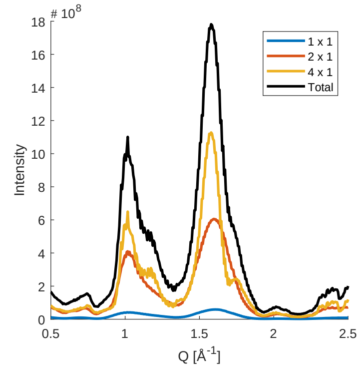
WAXD simulations: Results

Form factor of a CNF chain with semi-axes

3 Å x 0.5 Å

Model: H1+

Aggregation direction: (1-10)

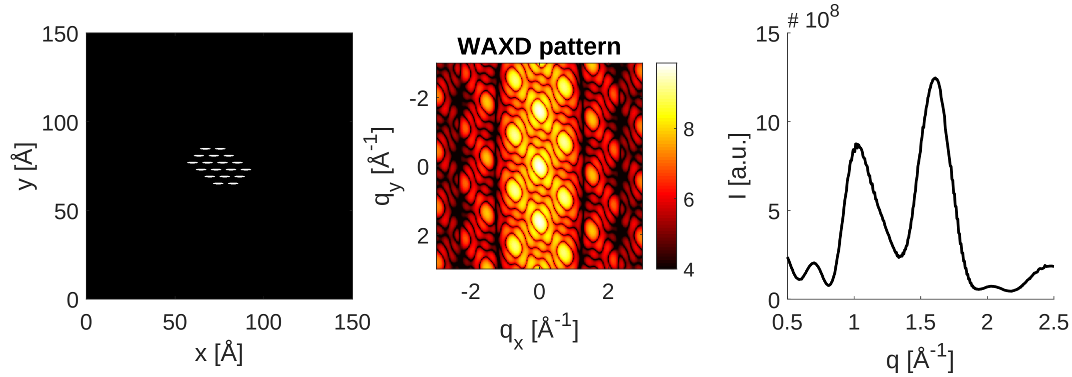


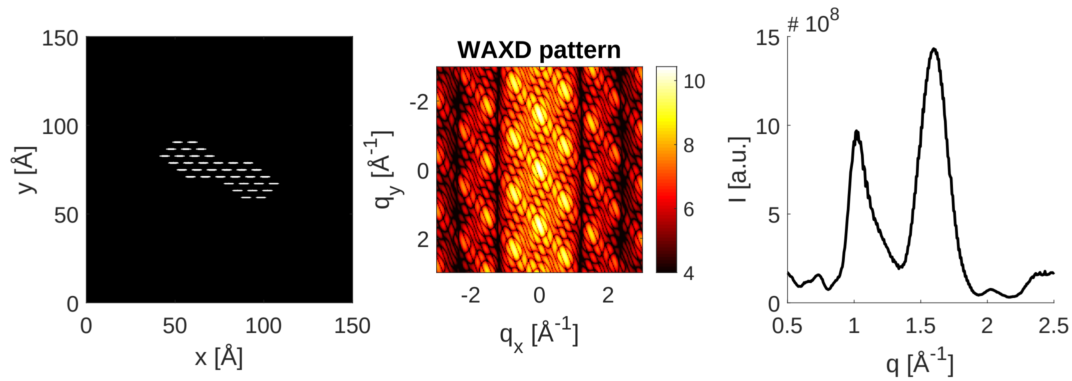
Sample #1

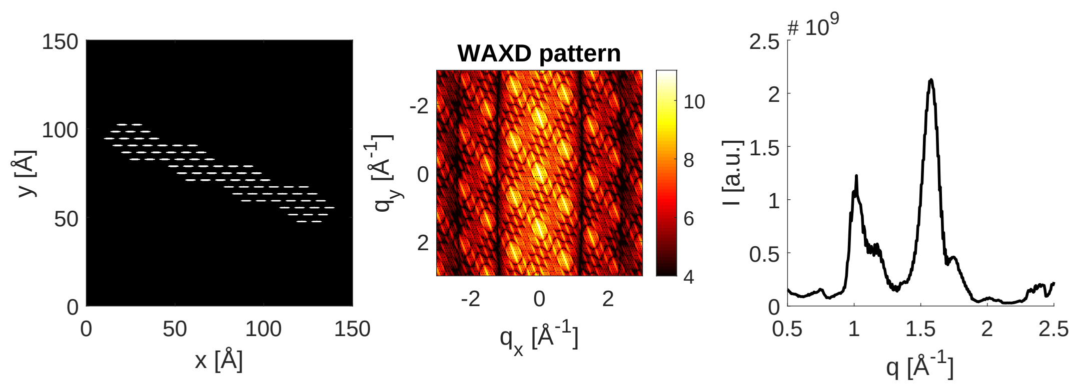
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

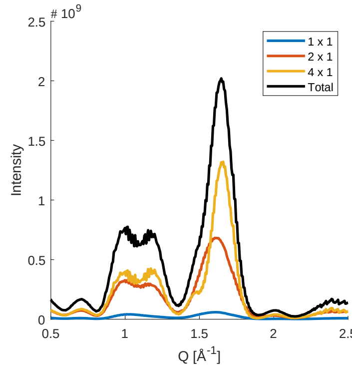






Model: H1+

Aggregation direction: (110)

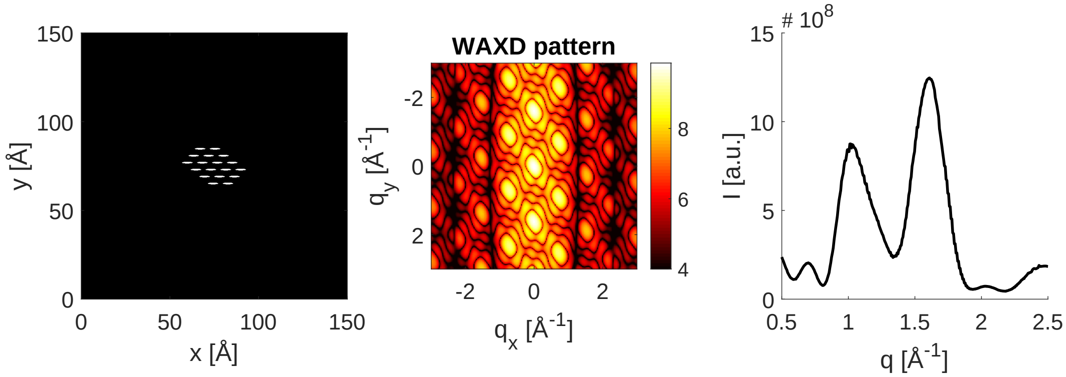


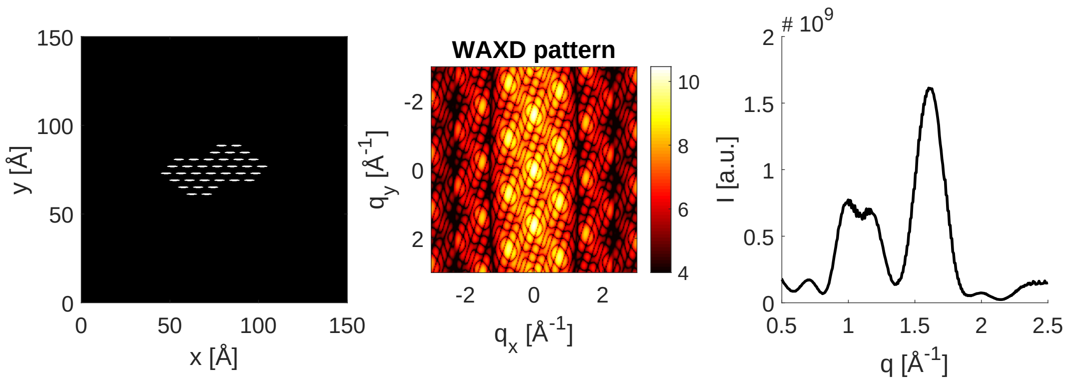
Sample #1

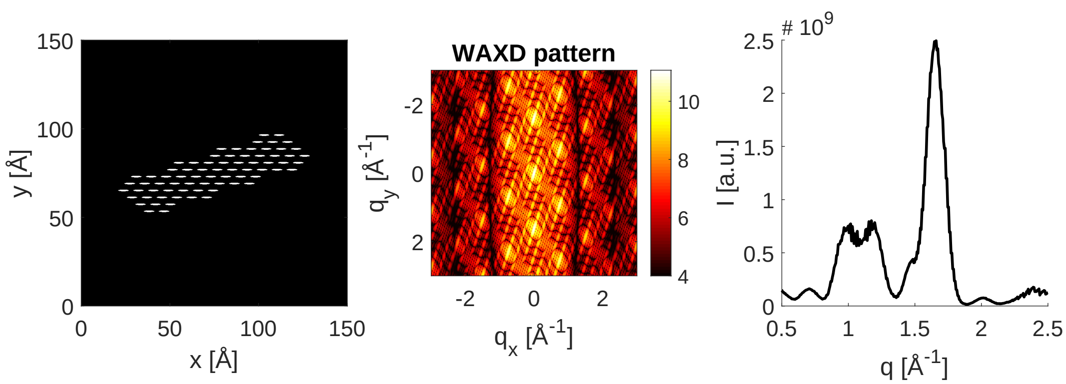
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

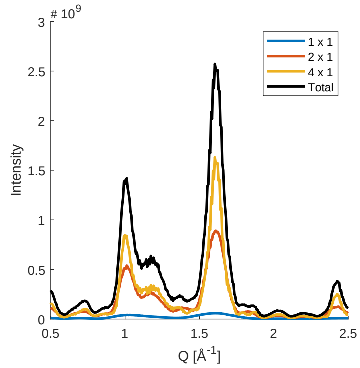






Model: H1+

Aggregation direction: (200)

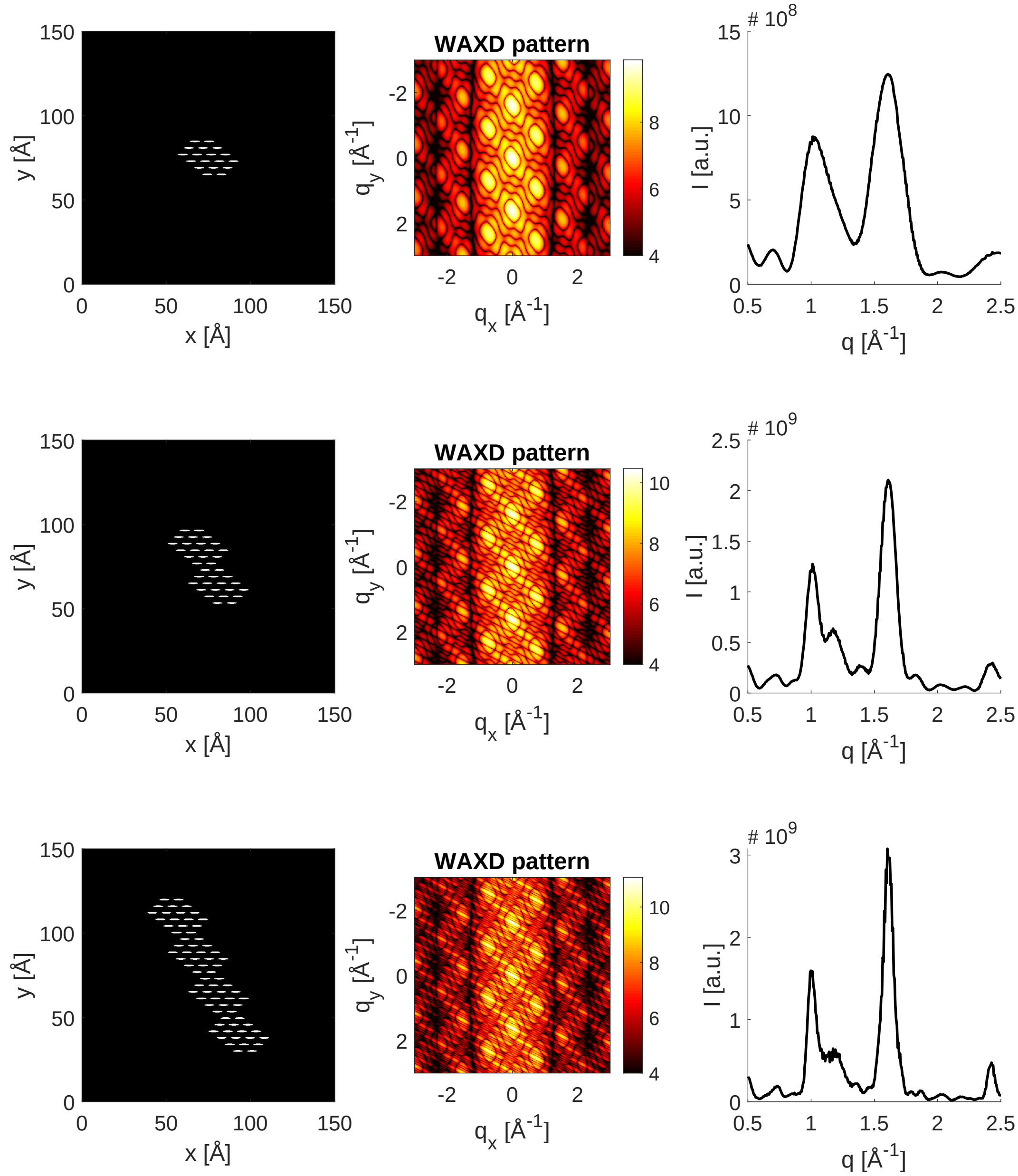


Sample #1

Vol% 1x1: 4.7

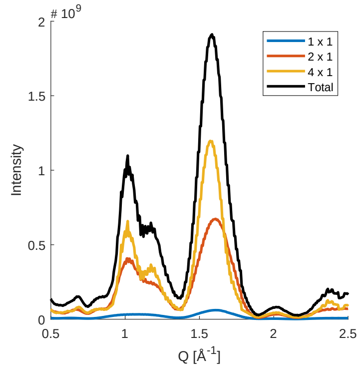
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: H1-

Aggregation direction: (1-10)

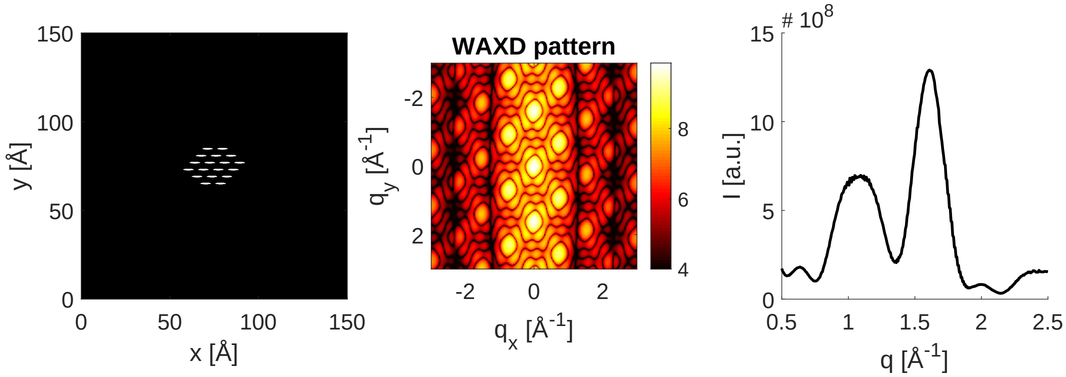


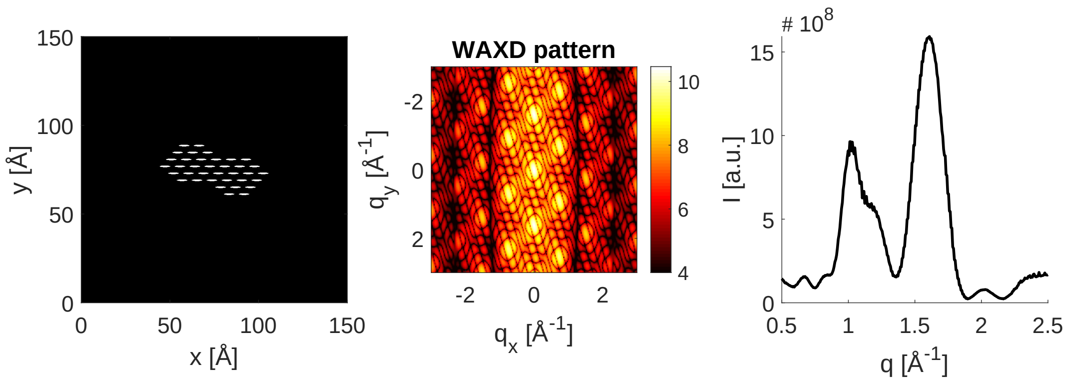
Sample #1

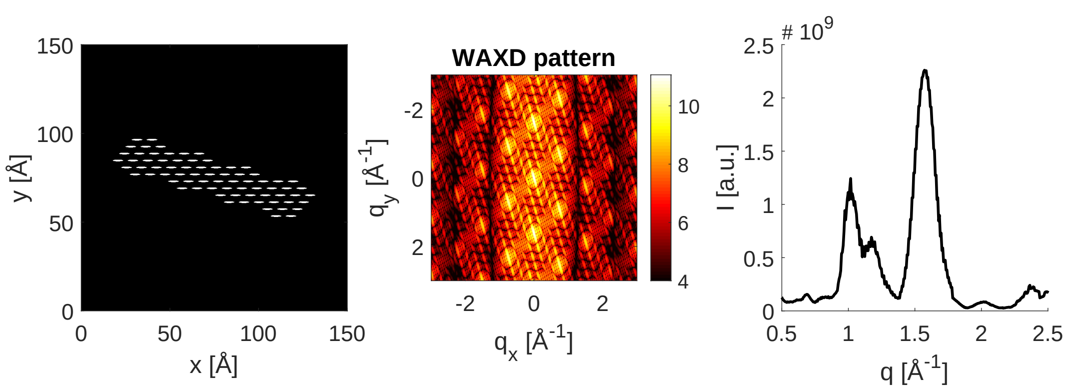
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

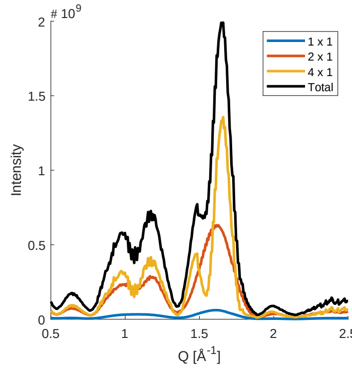






Model: H1-

Aggregation direction: (110)

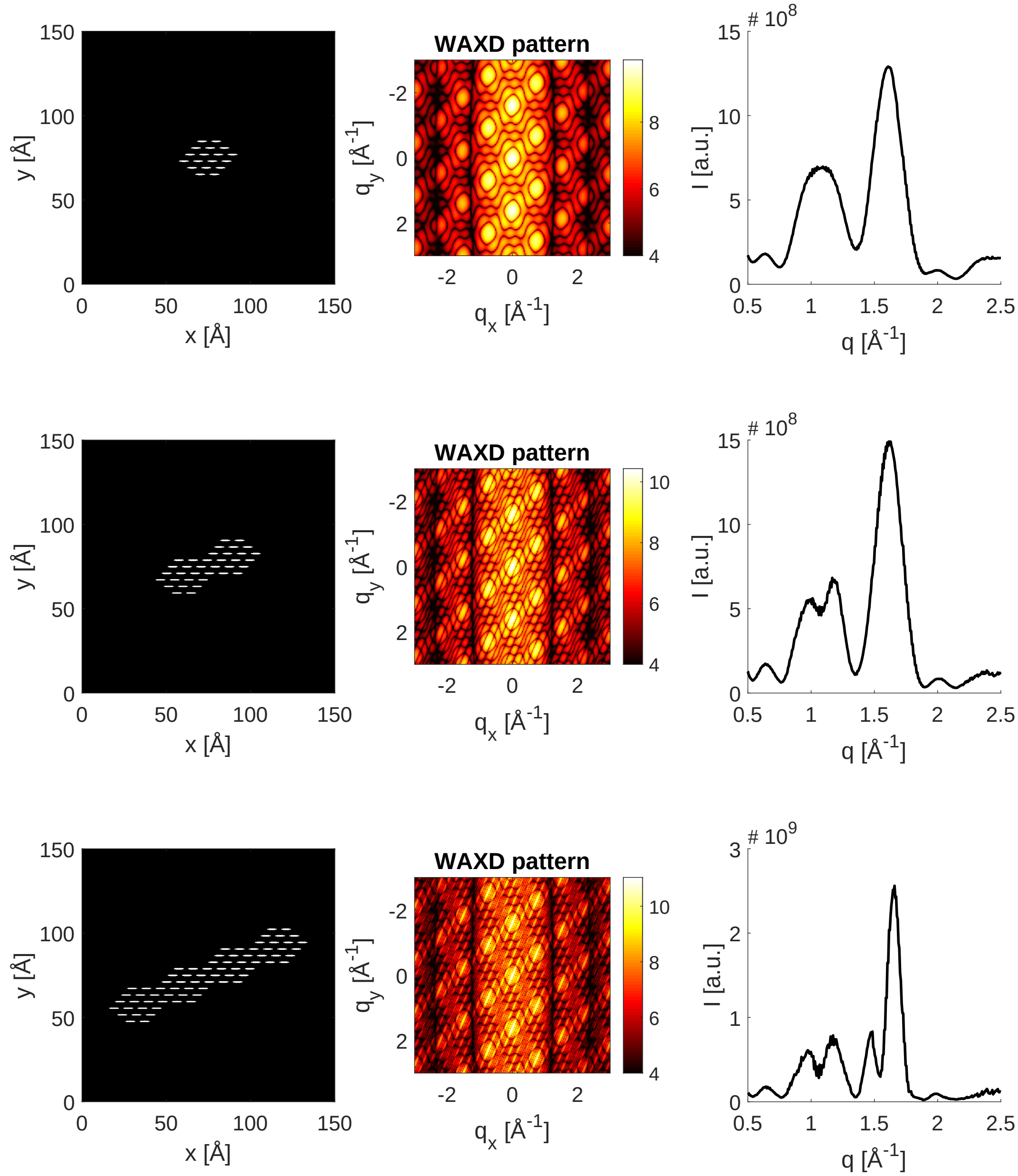


Sample #1

Vol% 1x1: 4.7

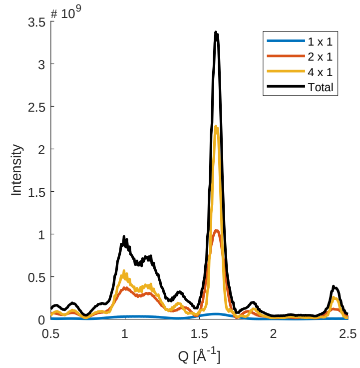
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: H1-

Aggregation direction: (200)

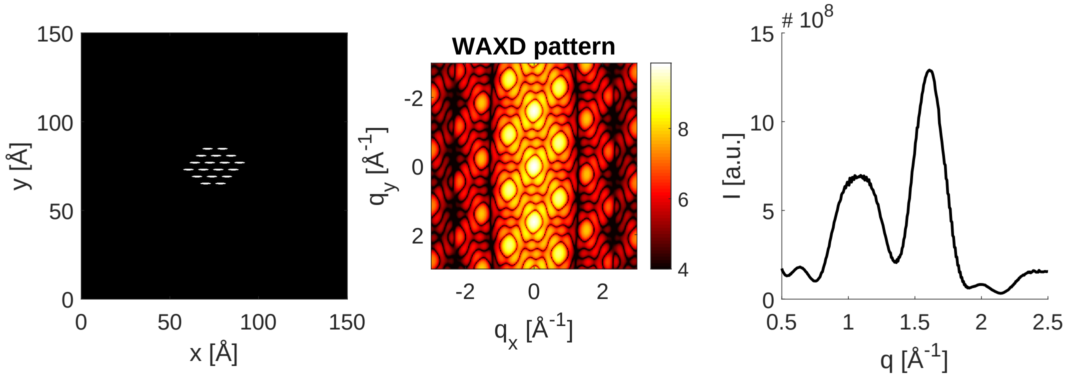


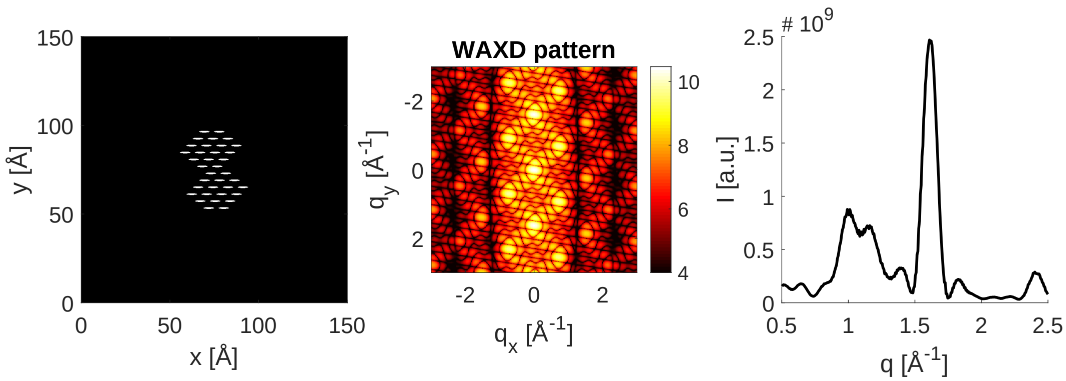
Sample #1

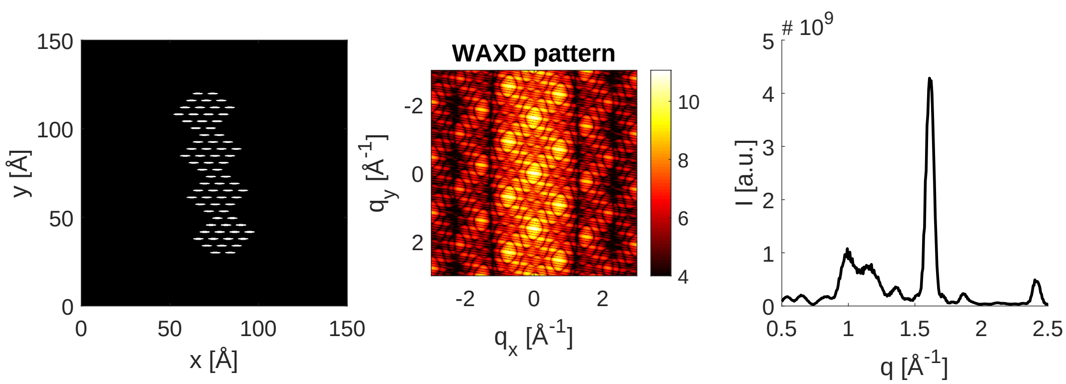
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

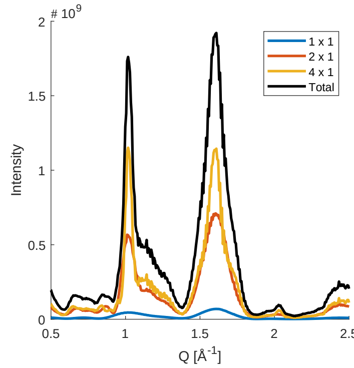






Model: H2+

Aggregation direction: (1-10)

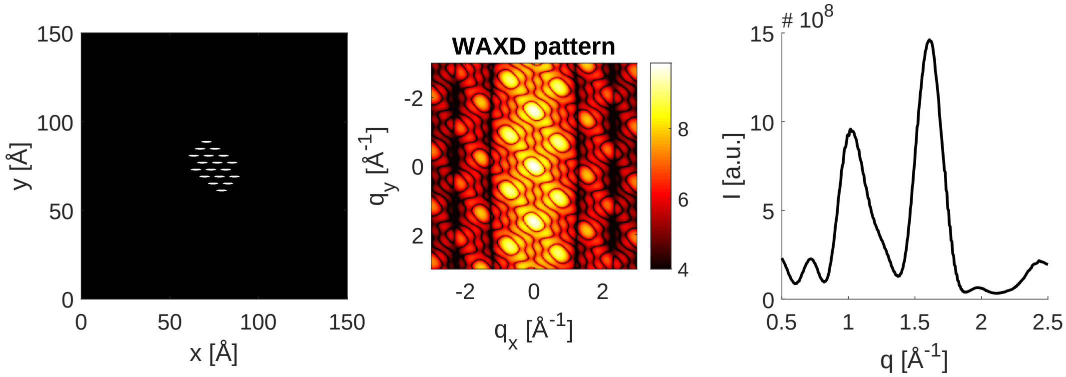


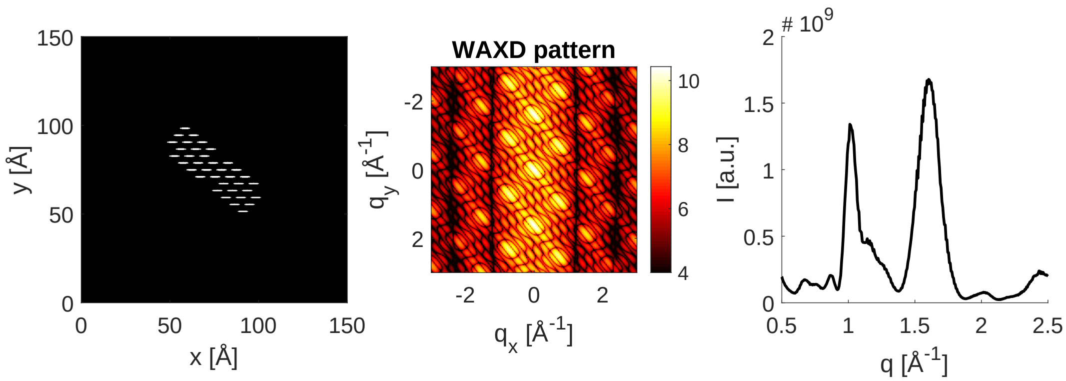
Sample #1

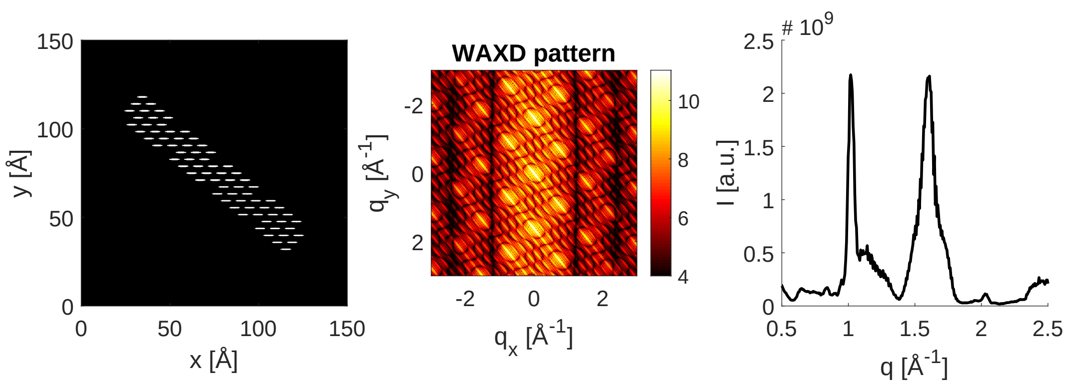
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

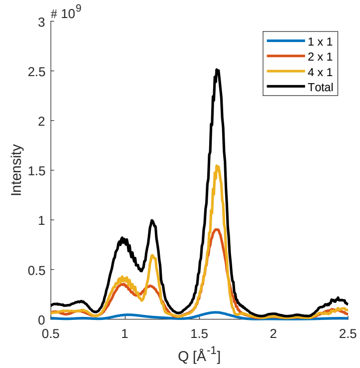






Model: H2+

Aggregation direction: (110)

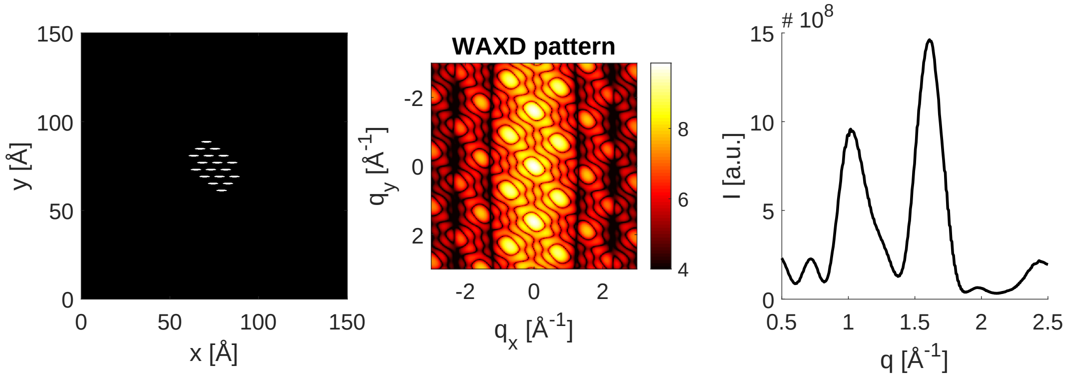


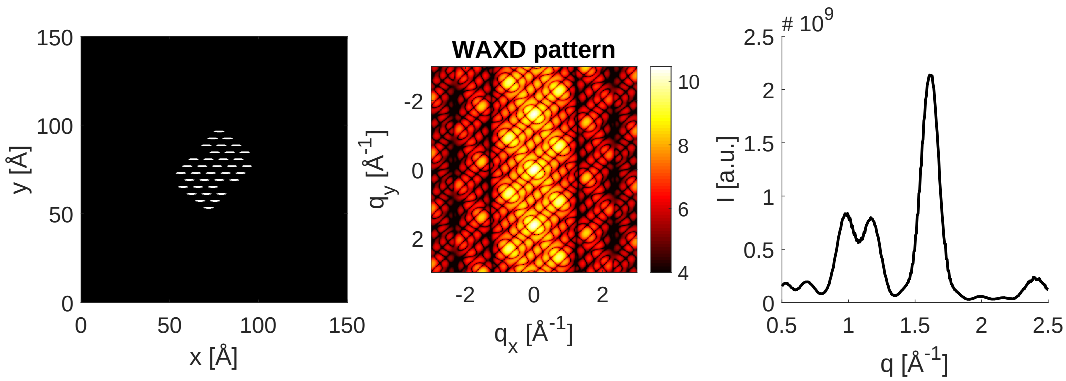
Sample #1

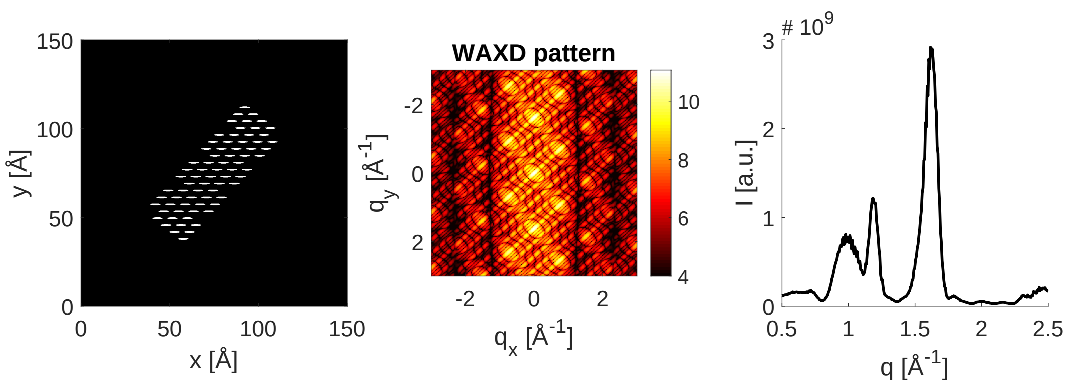
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

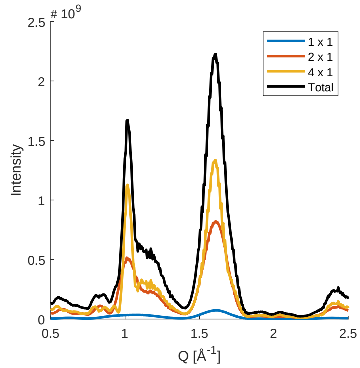






Model: H2-

Aggregation direction: (1-10)

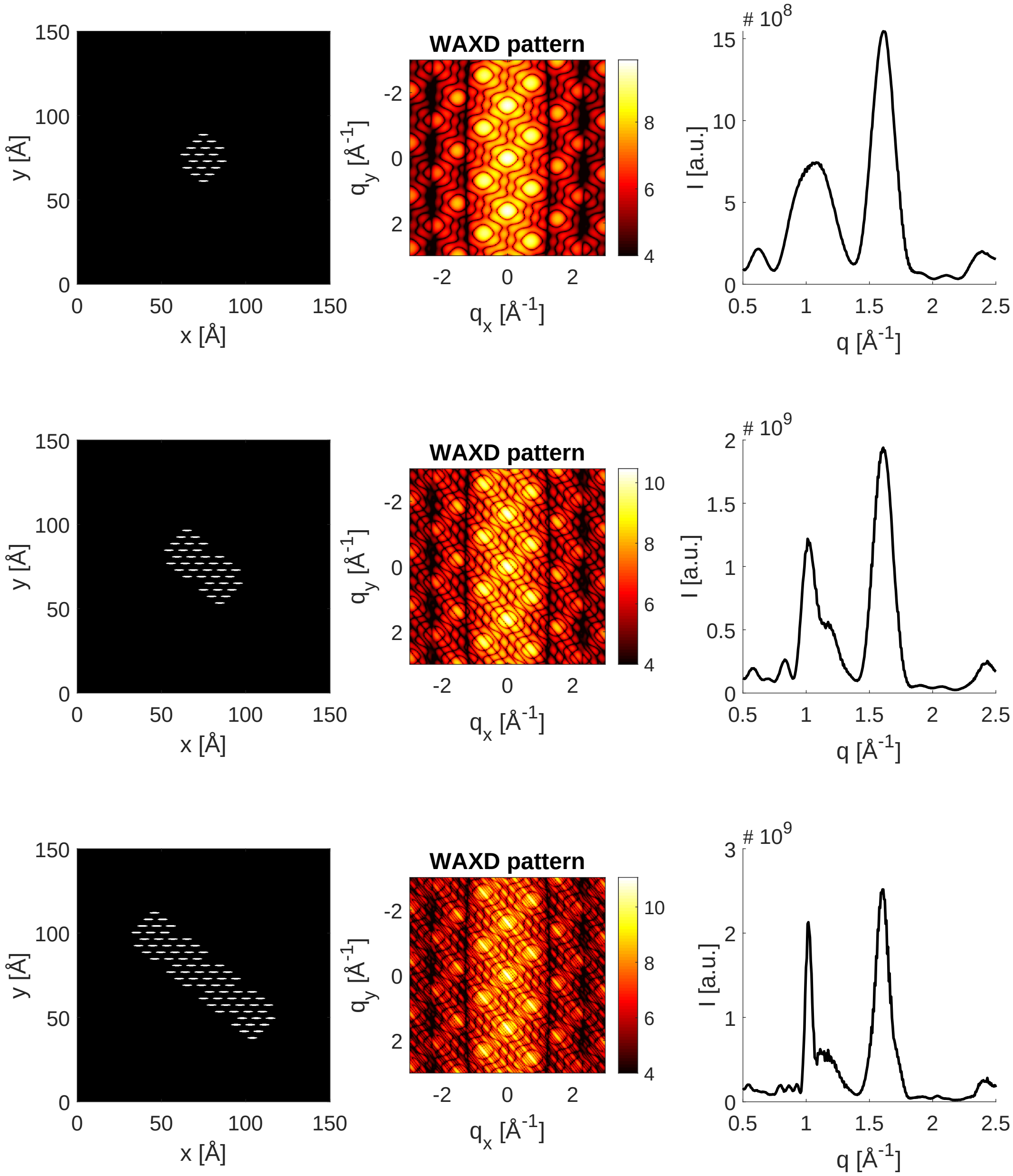


Sample #1

Vol% 1x1: 4.7

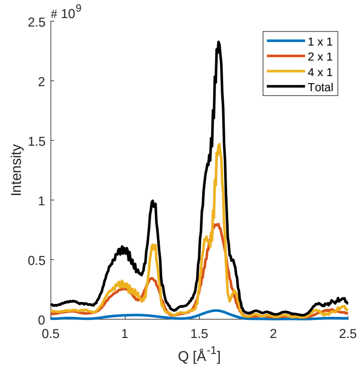
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: H2-

Aggregation direction: (110)

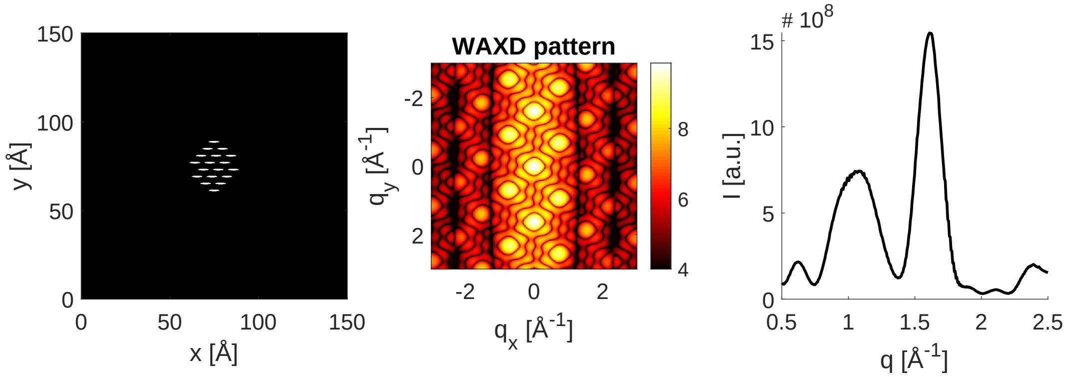


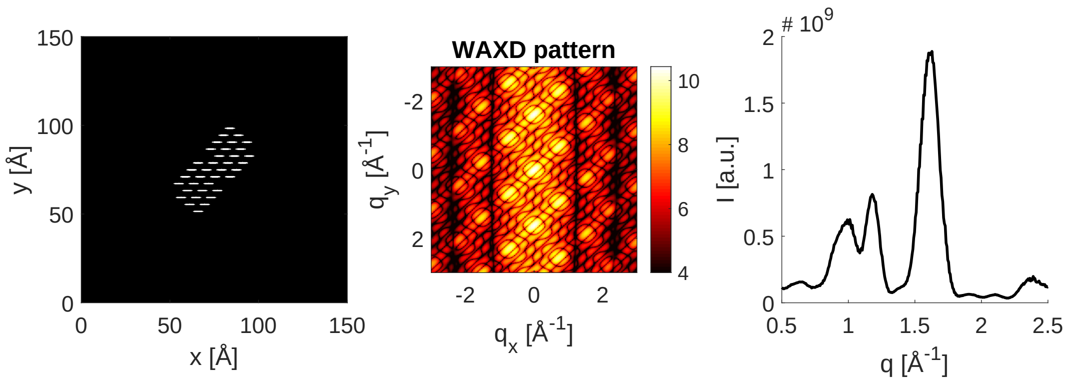
Sample #1

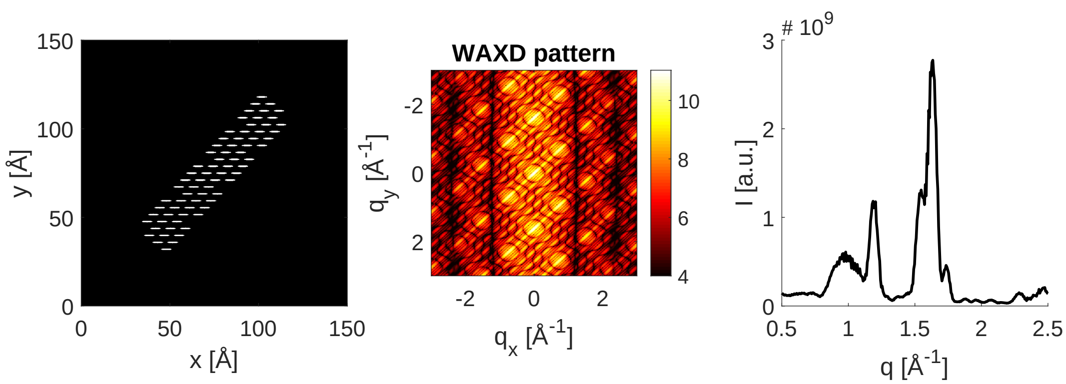
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

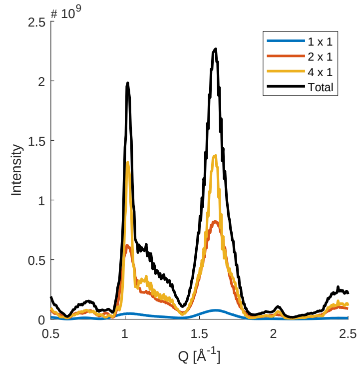






Model: R1+

Aggregation direction: (1-10)

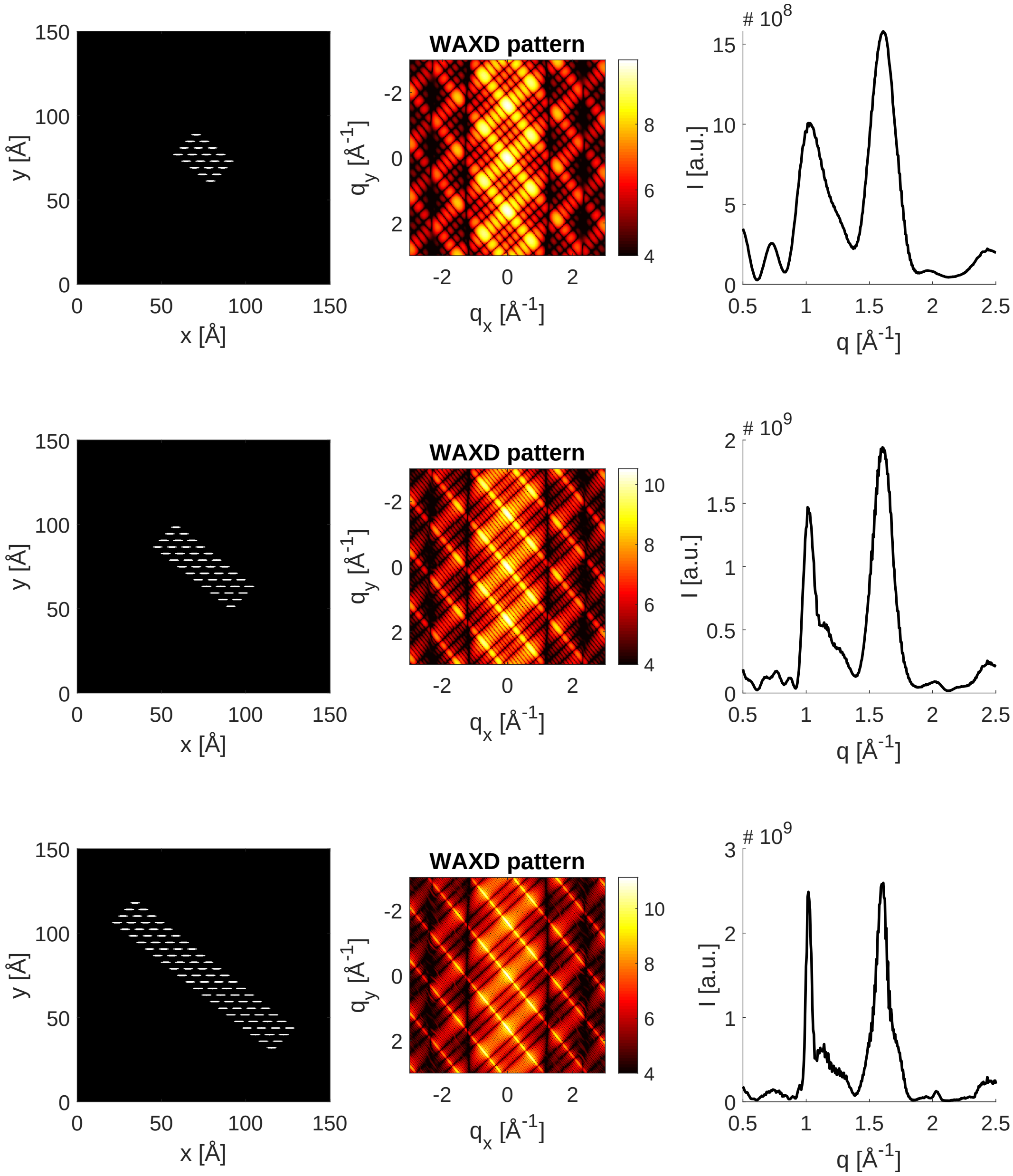


Sample #1

Vol% 1x1: 4.7

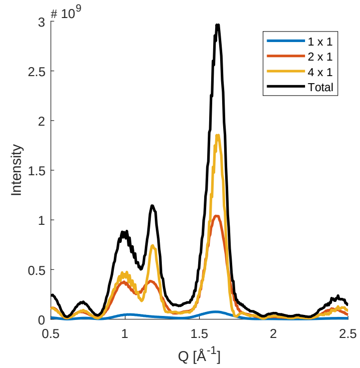
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: R1+

Aggregation direction: (110)

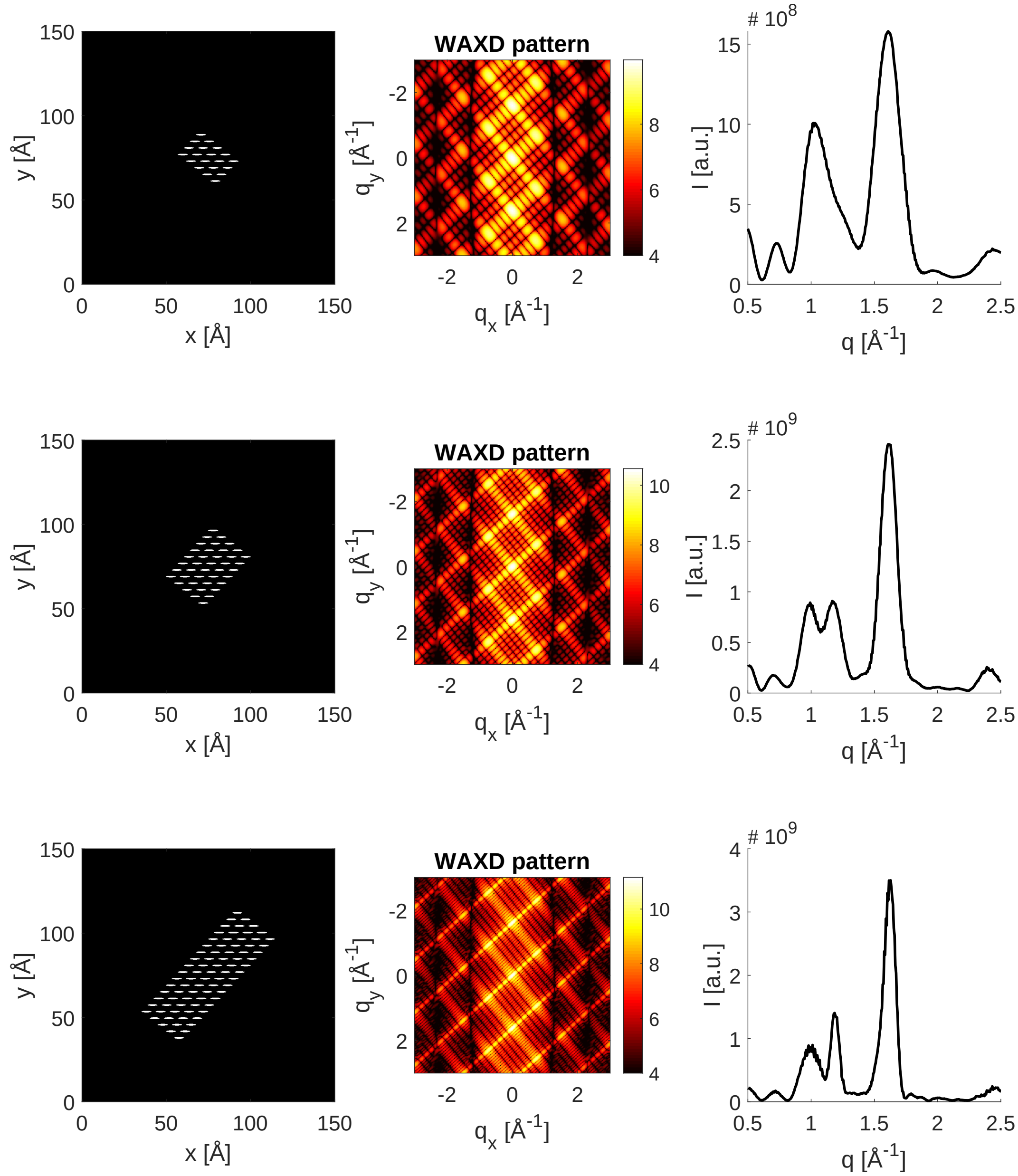


Sample #1

Vol% 1x1: 4.7

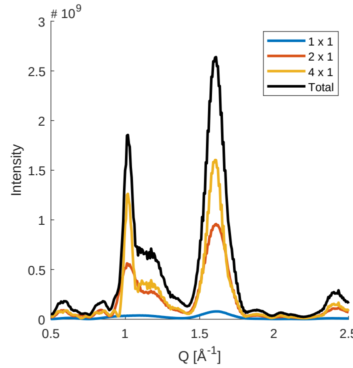
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: R1-

Aggregation direction: (1-10)

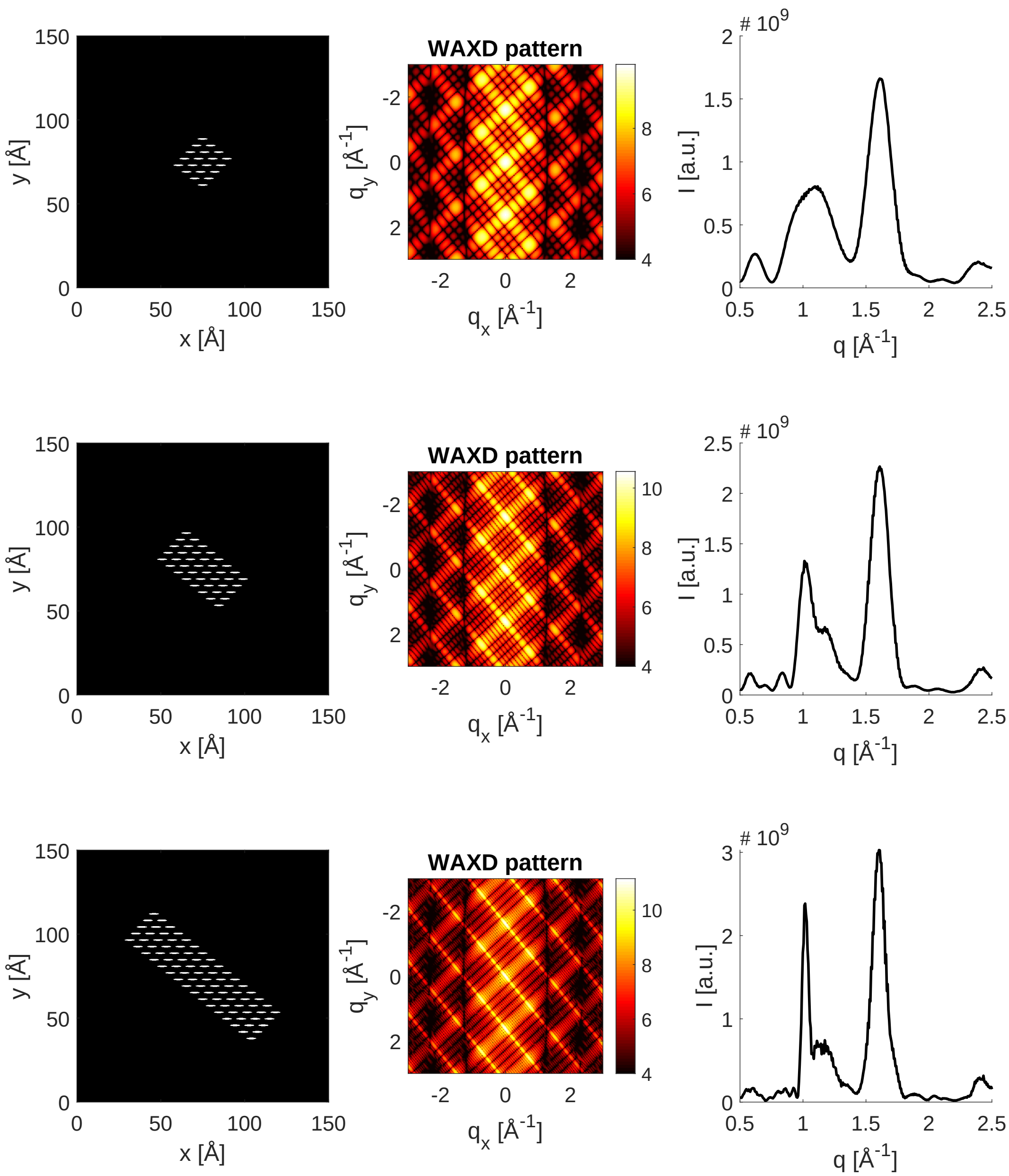


Sample #1

Vol% 1x1: 4.7

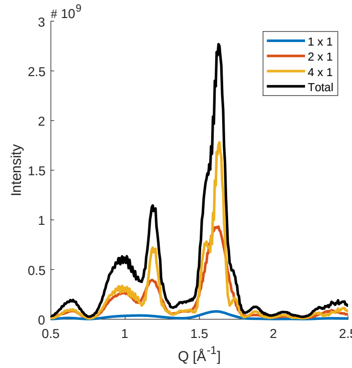
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: R1-

Aggregation direction: (110)

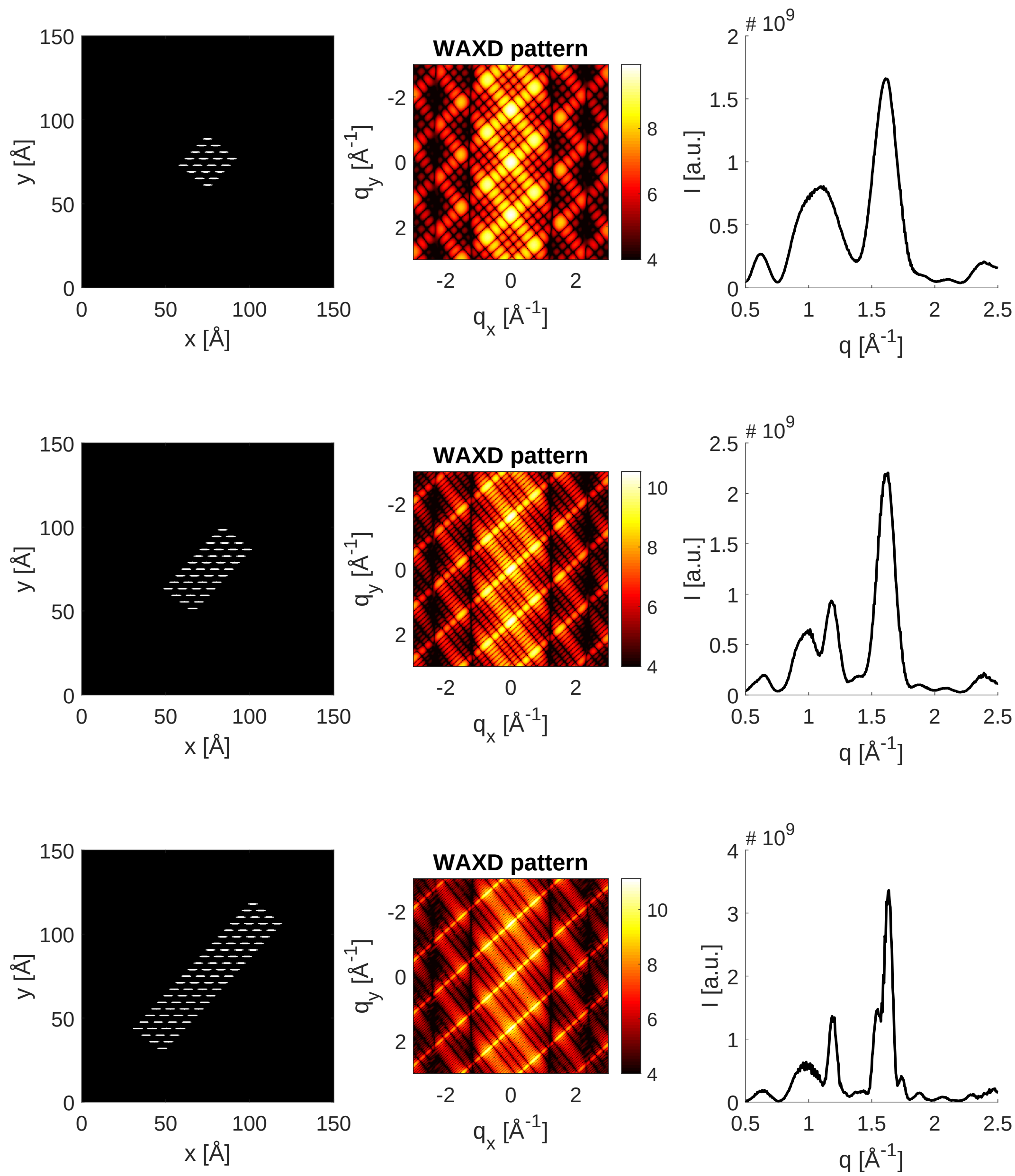


Sample #1

Vol% 1x1: 4.7

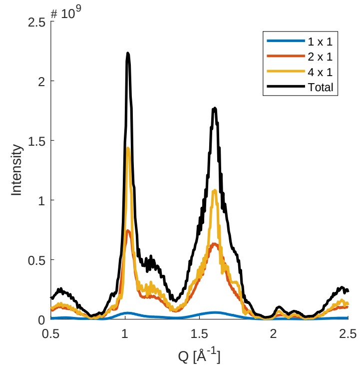
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: R2+

Aggregation direction: (1-10)

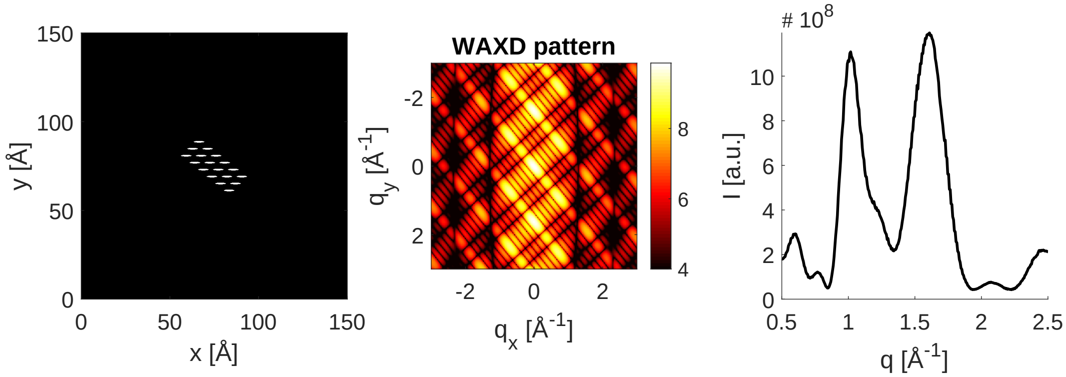


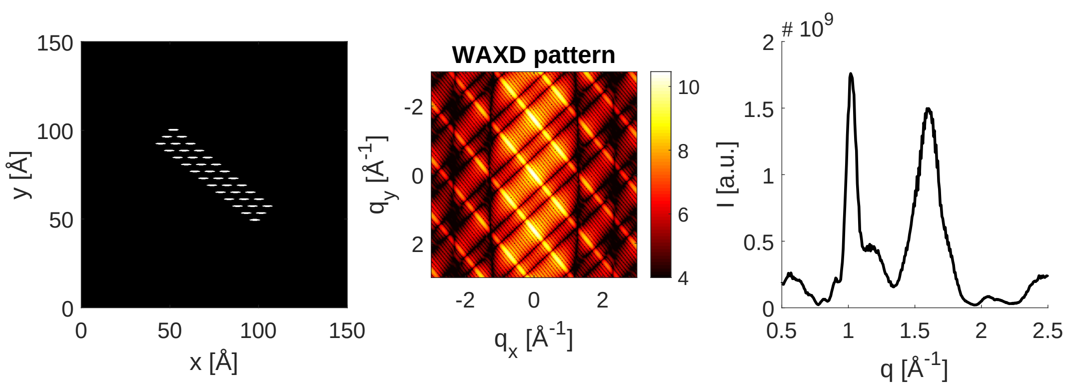
Sample #1

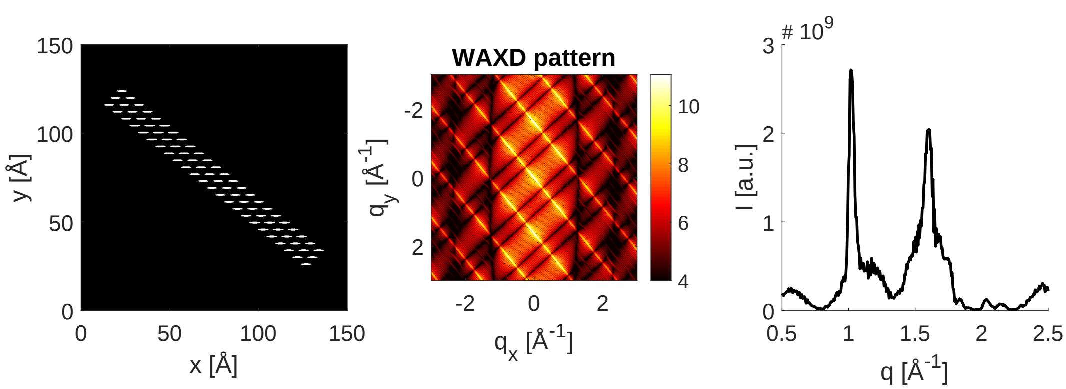
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

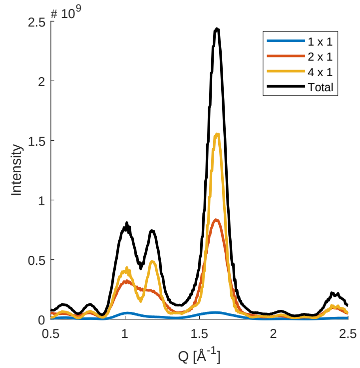






Model: R2+

Aggregation direction: (110)

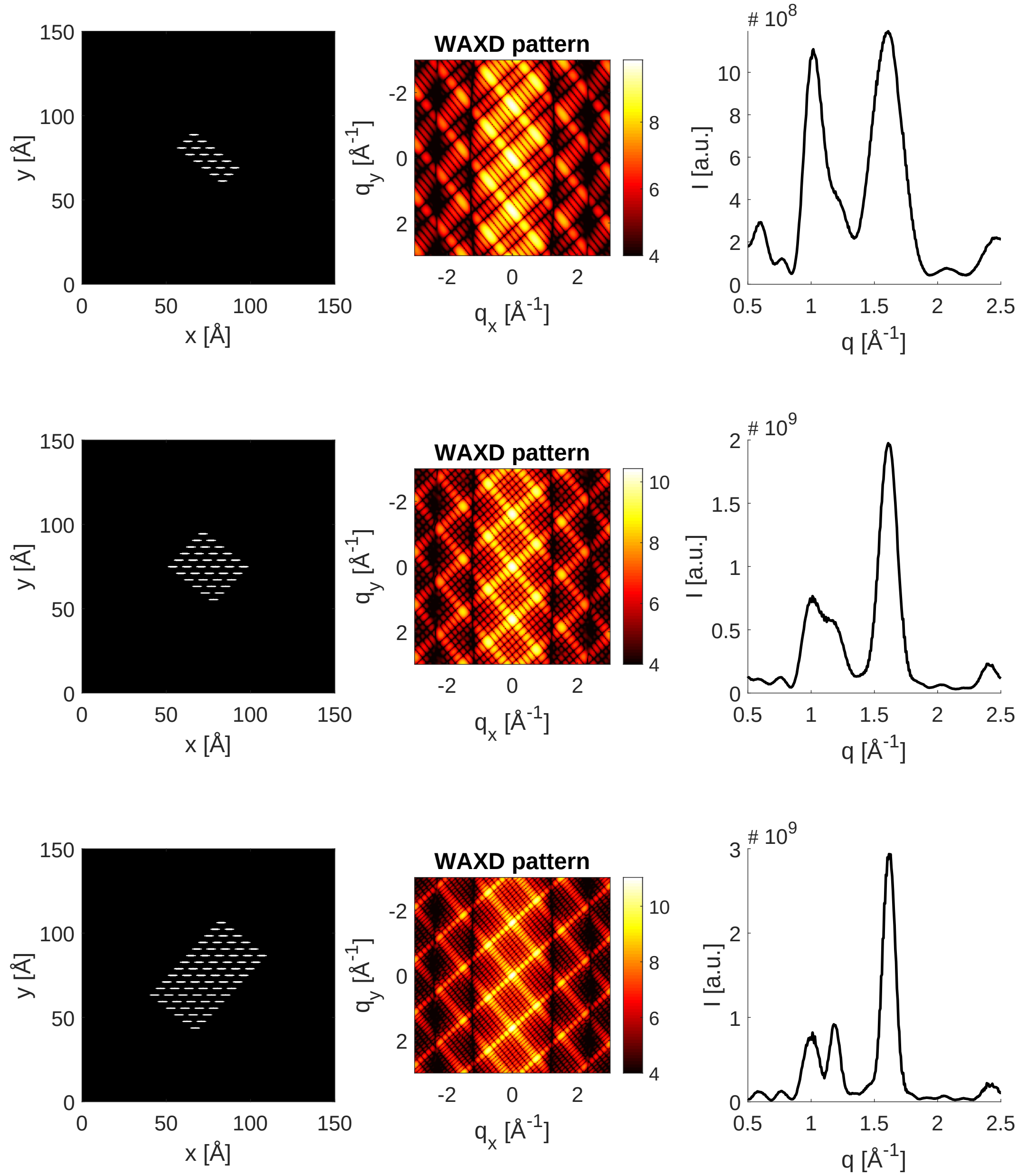


Sample #1

Vol% 1x1: 4.7

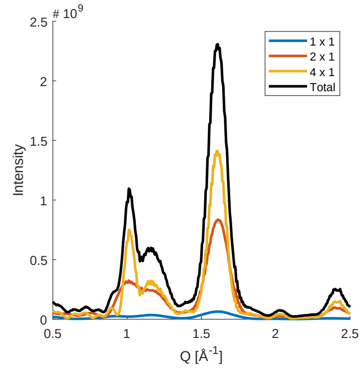
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: R2-

Aggregation direction: (1-10)

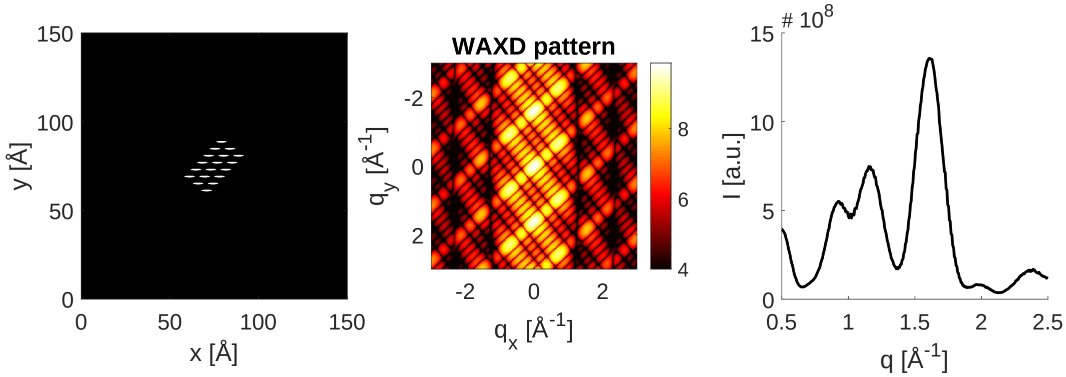


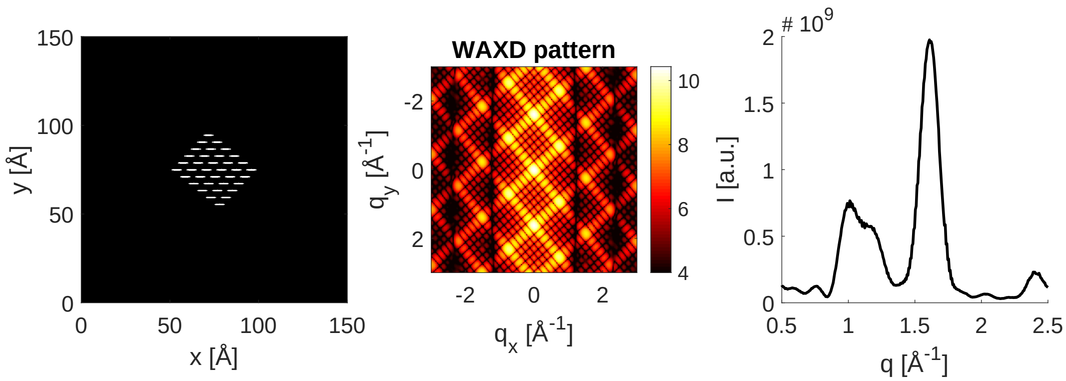
Sample #1

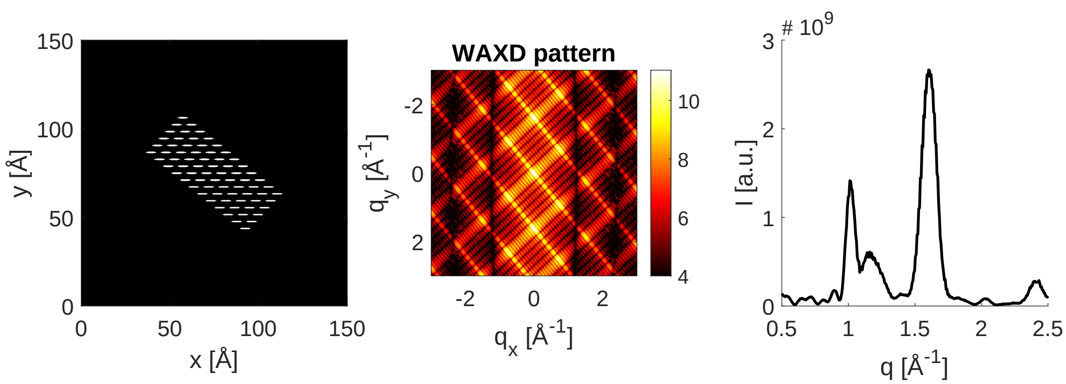
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

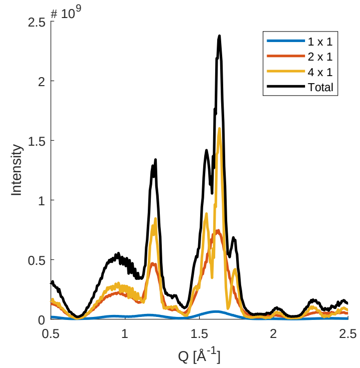






Model: R2-

Aggregation direction: (110)

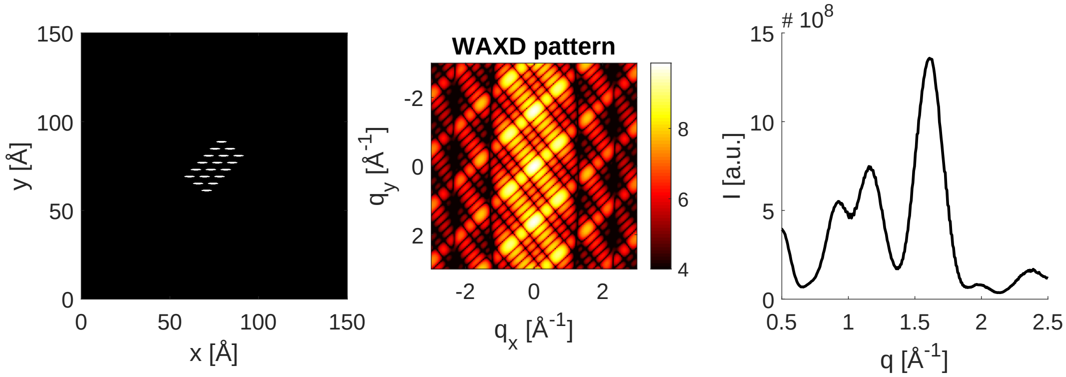


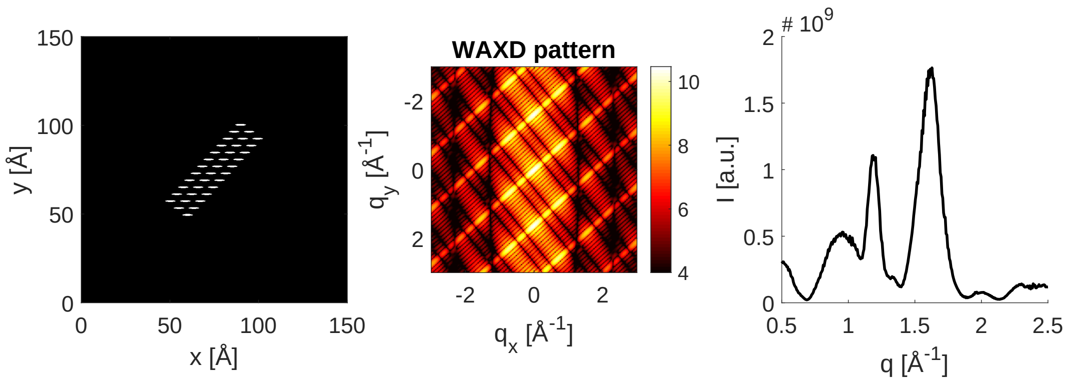
Sample #1

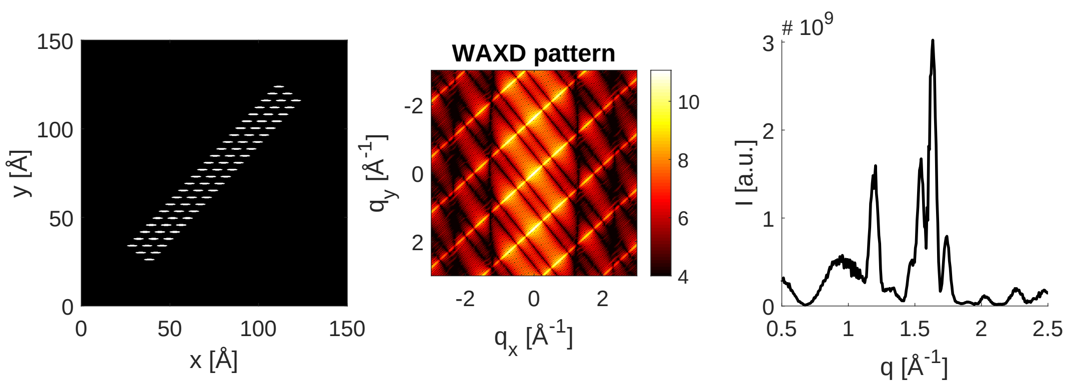
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

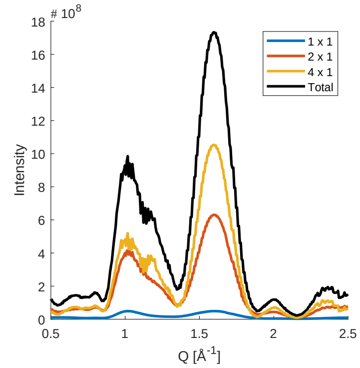






Model: Rh1+

Aggregation direction: (110)

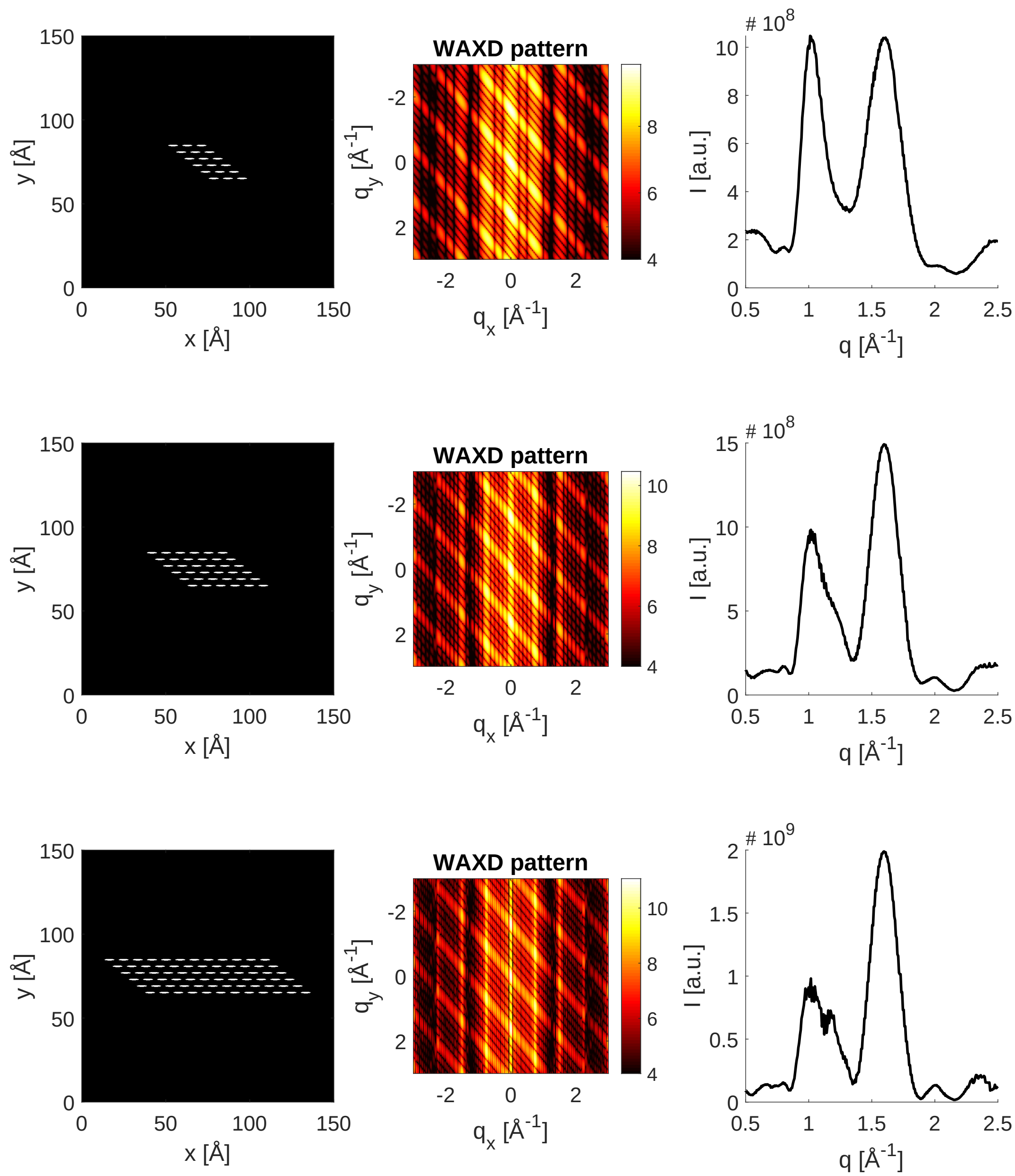


Sample #1

Vol% 1x1: 4.7

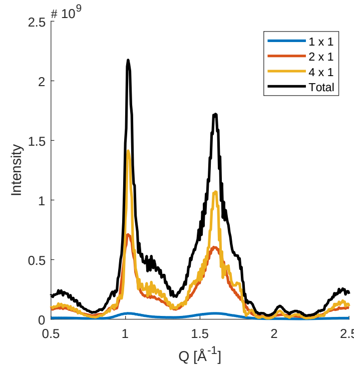
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: Rh1+

Aggregation direction: (200)

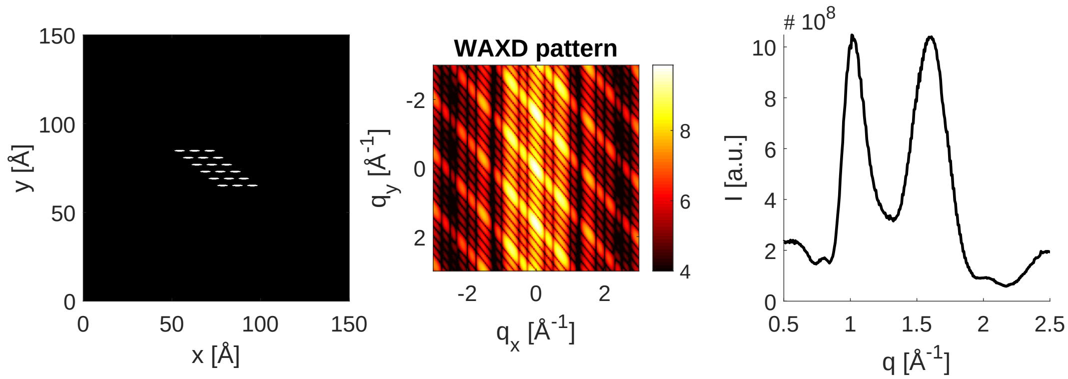


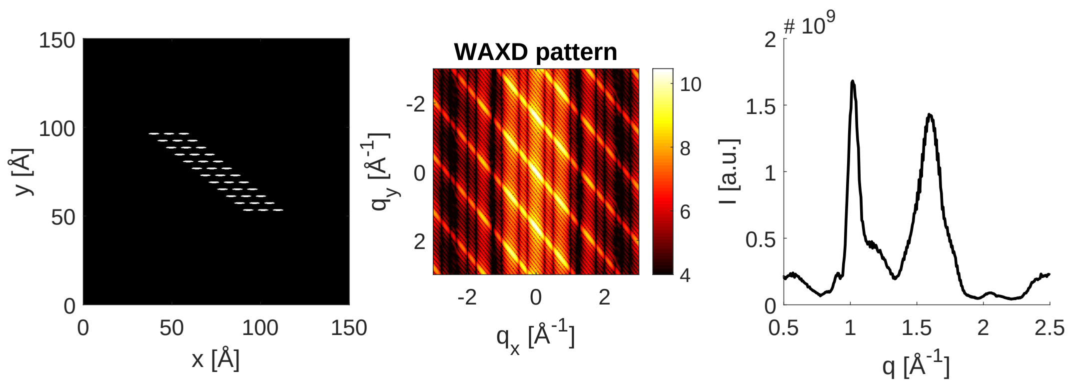
Sample #1

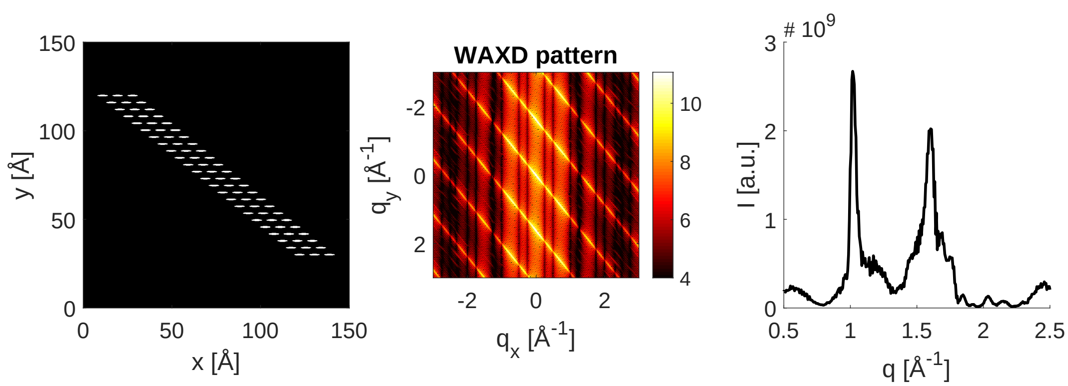
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

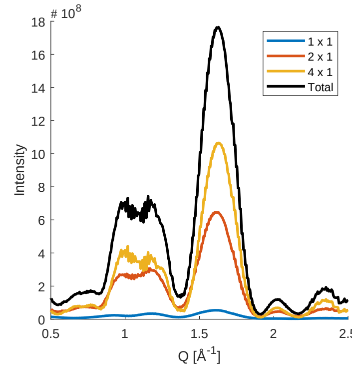






Model: Rh1-

Aggregation direction: (1-10)

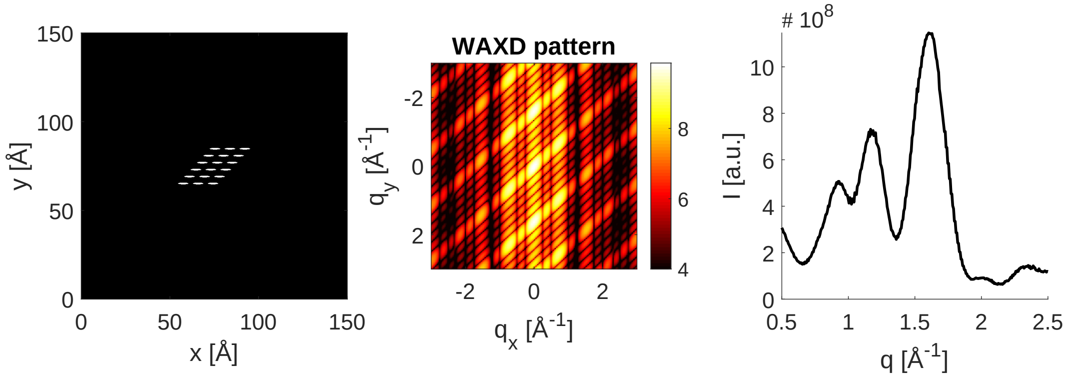


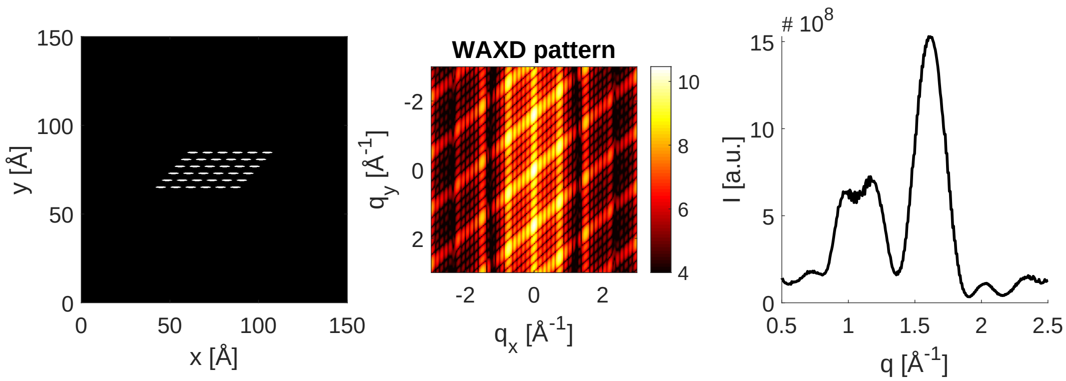
Sample #1

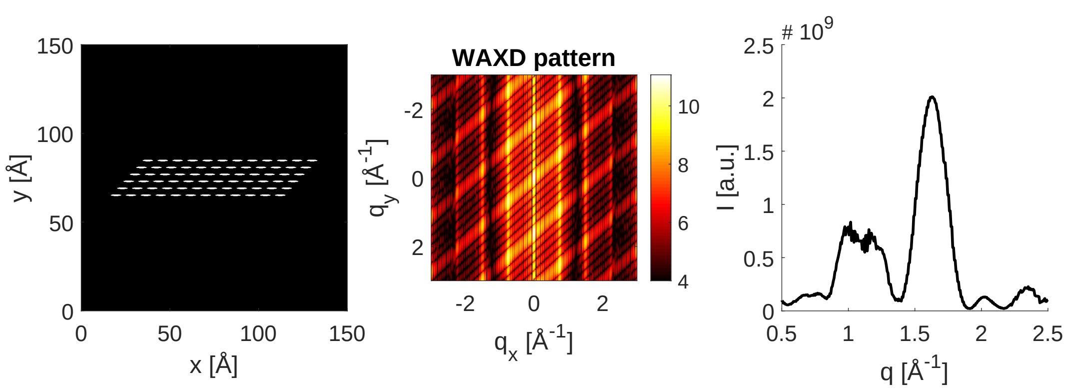
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

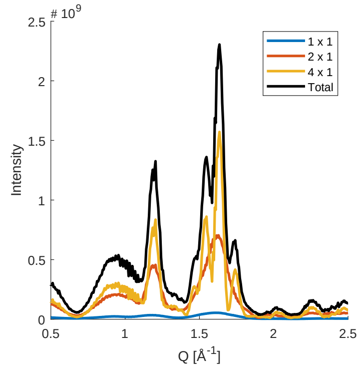






Model: Rh1-

Aggregation direction: (200)

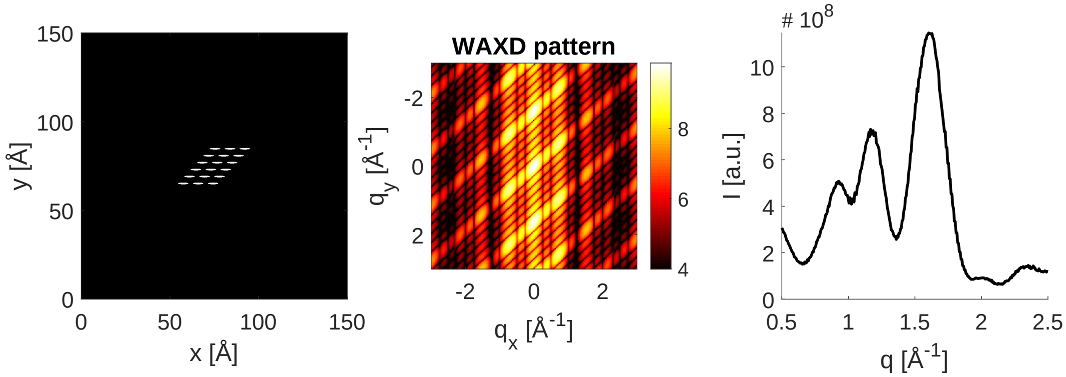


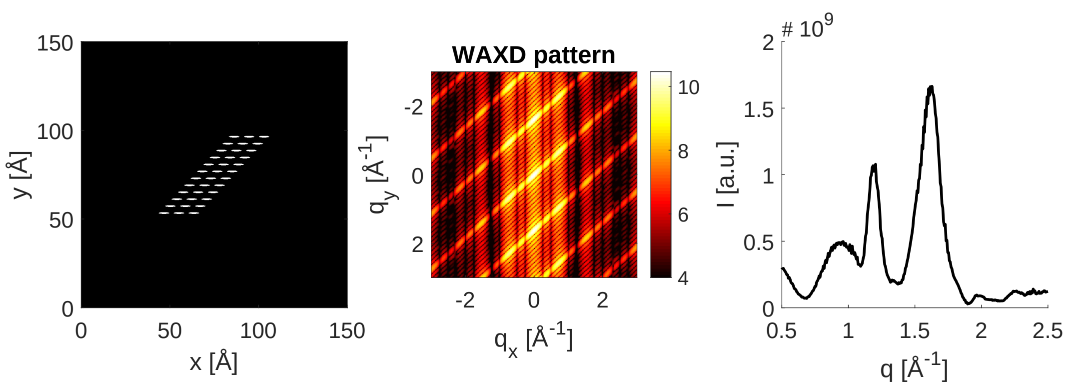
Sample #1

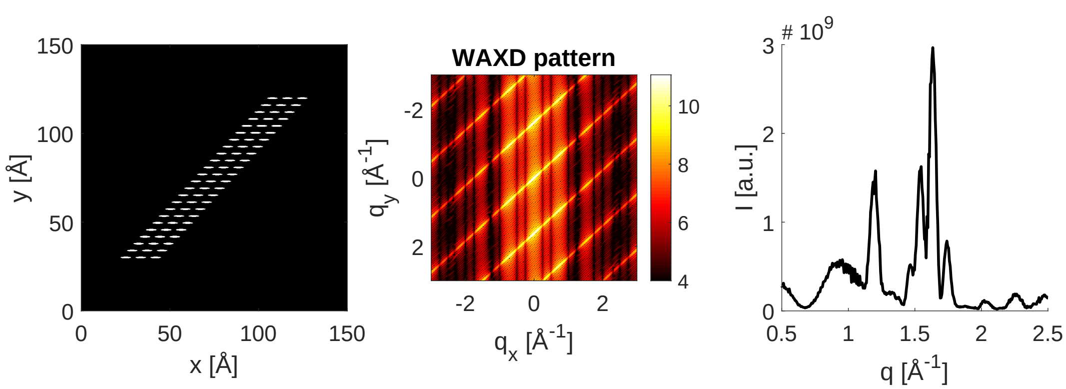
Vol% 1x1: 4.7

Vol% 2x1: 42.3

Vol% 4x1: 53.0

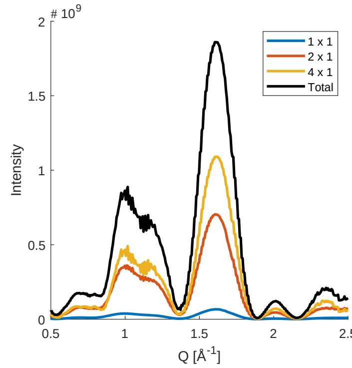






Model: Rh2

Aggregation direction: (010)

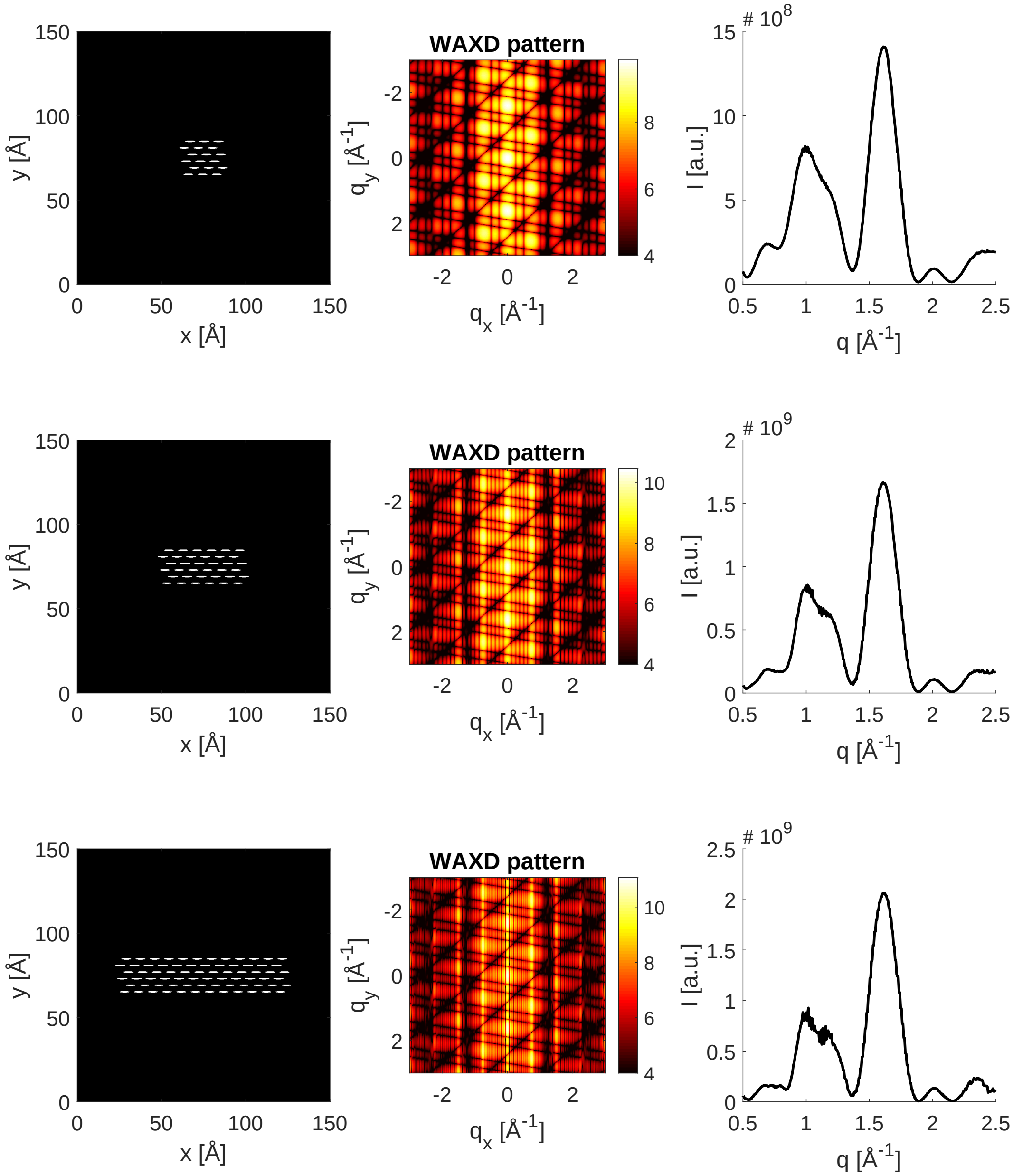


Sample #1

Vol% 1x1: 4.7

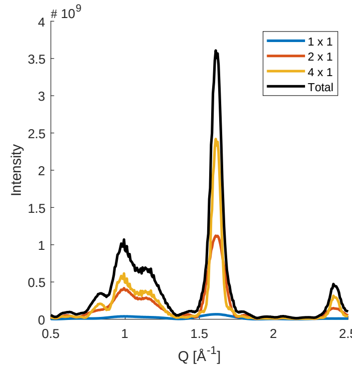
Vol% 2x1: 42.3

Vol% 4x1: 53.0



Model: Rh2

Aggregation direction: (200)

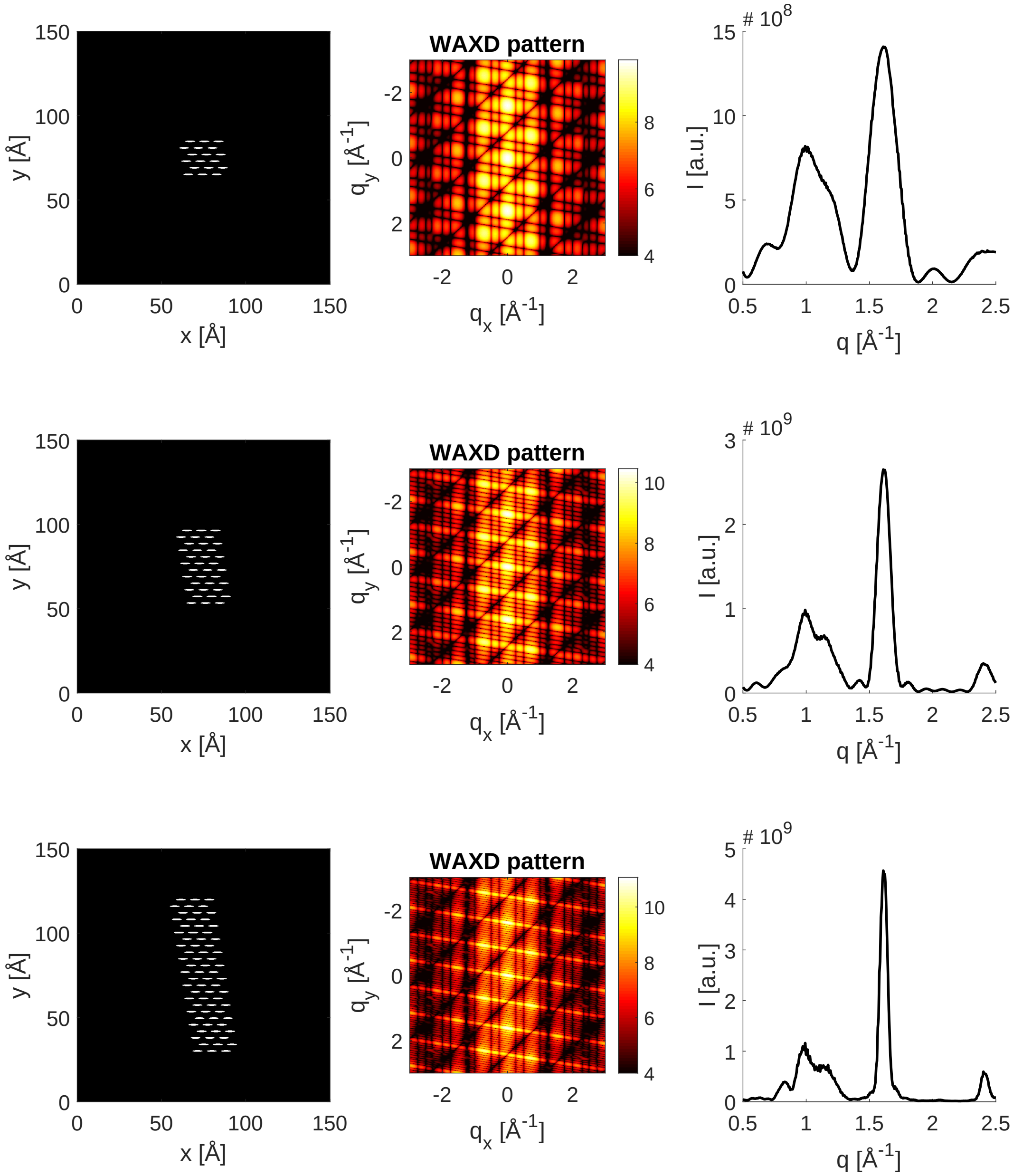


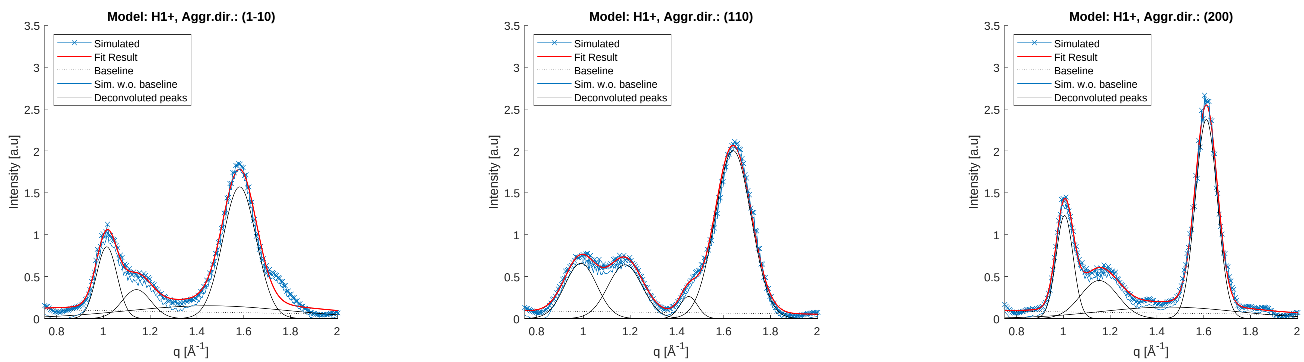
Sample #1

Vol% 1x1: 4.7

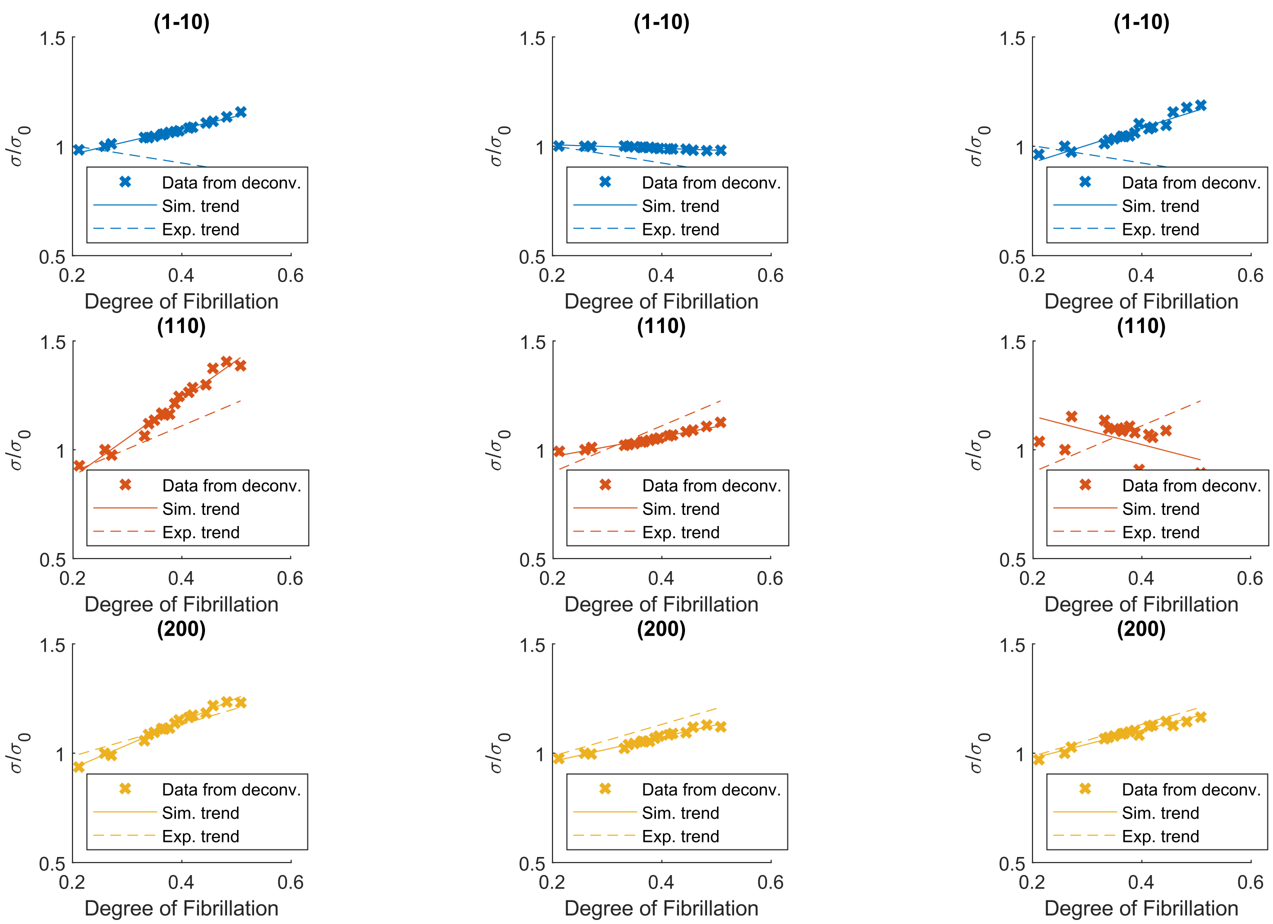
Vol% 2x1: 42.3

Vol% 4x1: 53.0

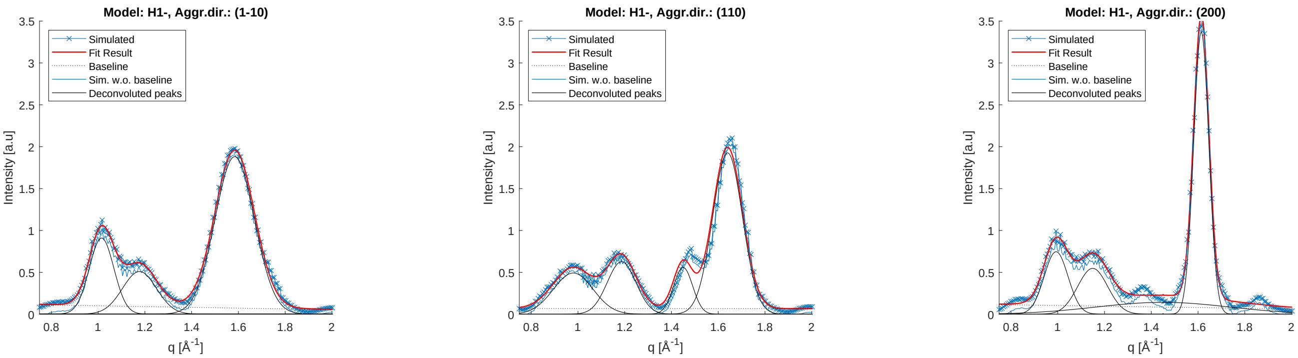


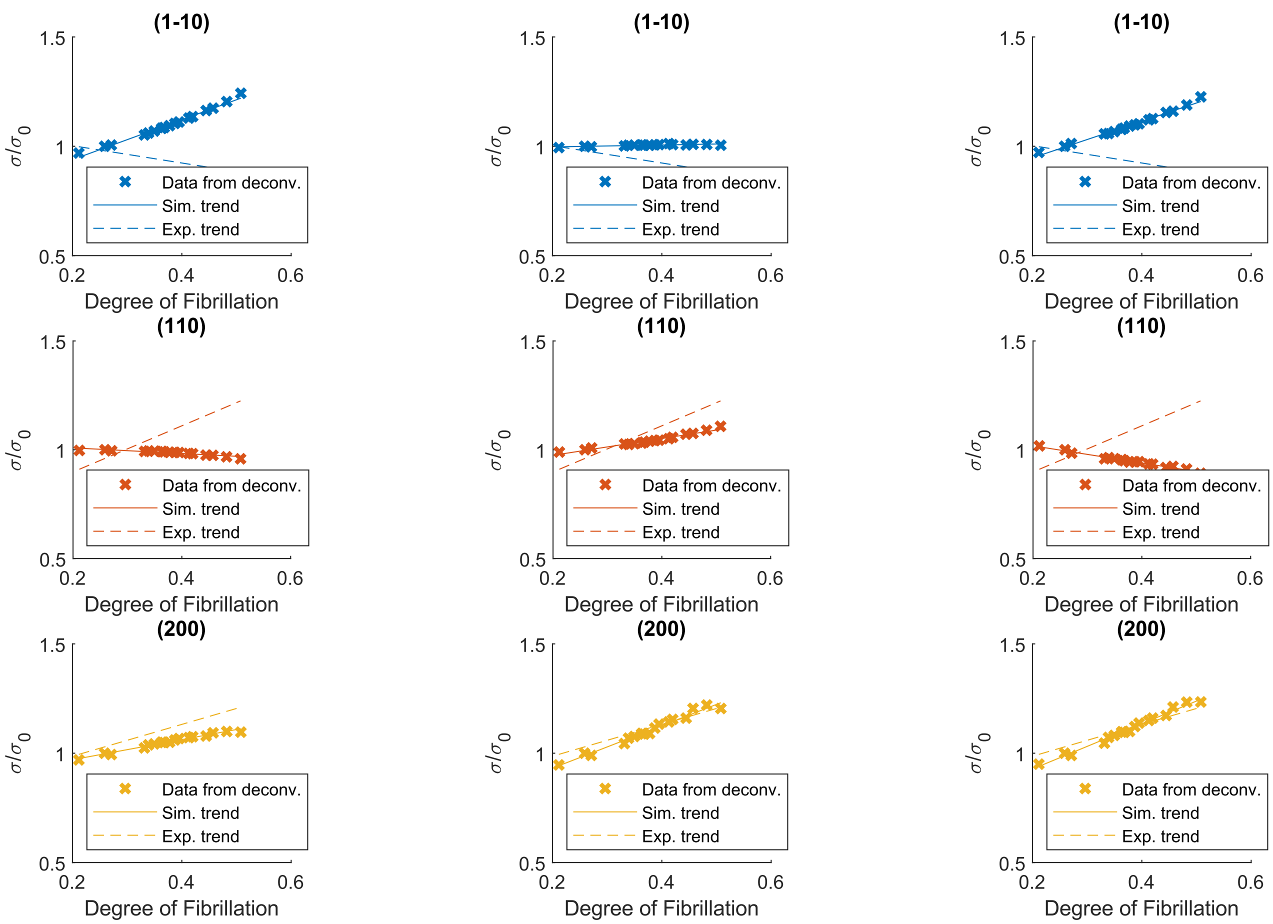


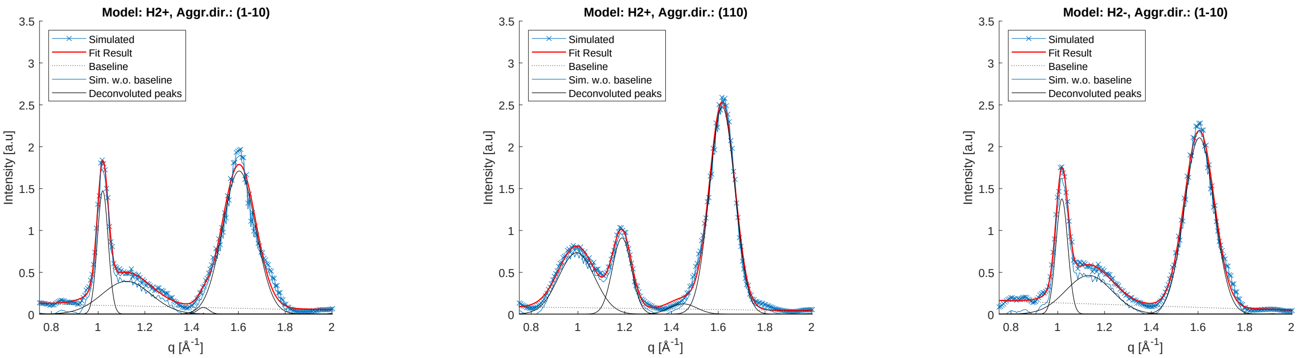
Model: H1+, Aggr.dir.: (1-10)
Model: H1+, Aggr.dir.: (110)
Model: H1+, Aggr.dir.: (200)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^-1]

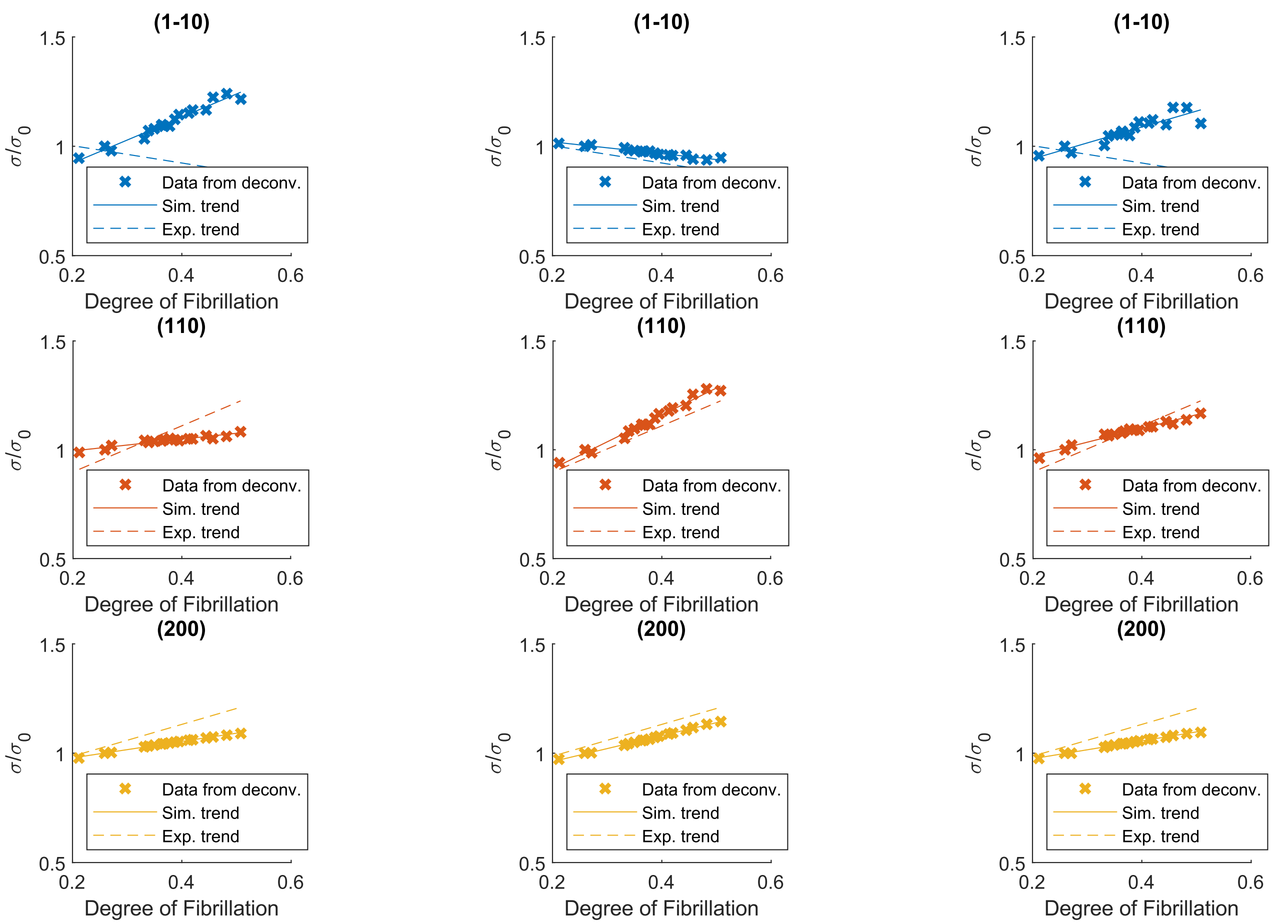


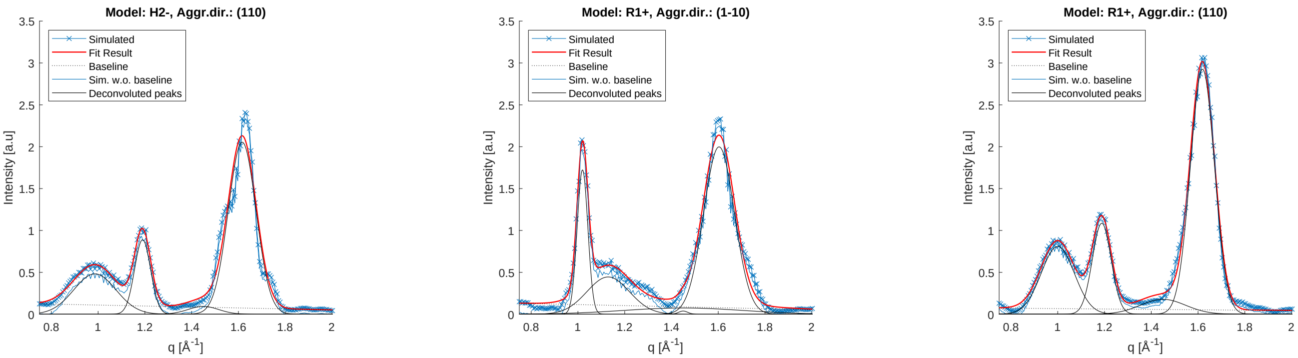
(1-10)
(110)
(200)
σ/σ0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation


Model: H1-, Aggr.dir.: (1-10)
Model: H1-, Aggr.dir.: (110)
Model: H1-, Aggr.dir.: (200)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å⁻¹]

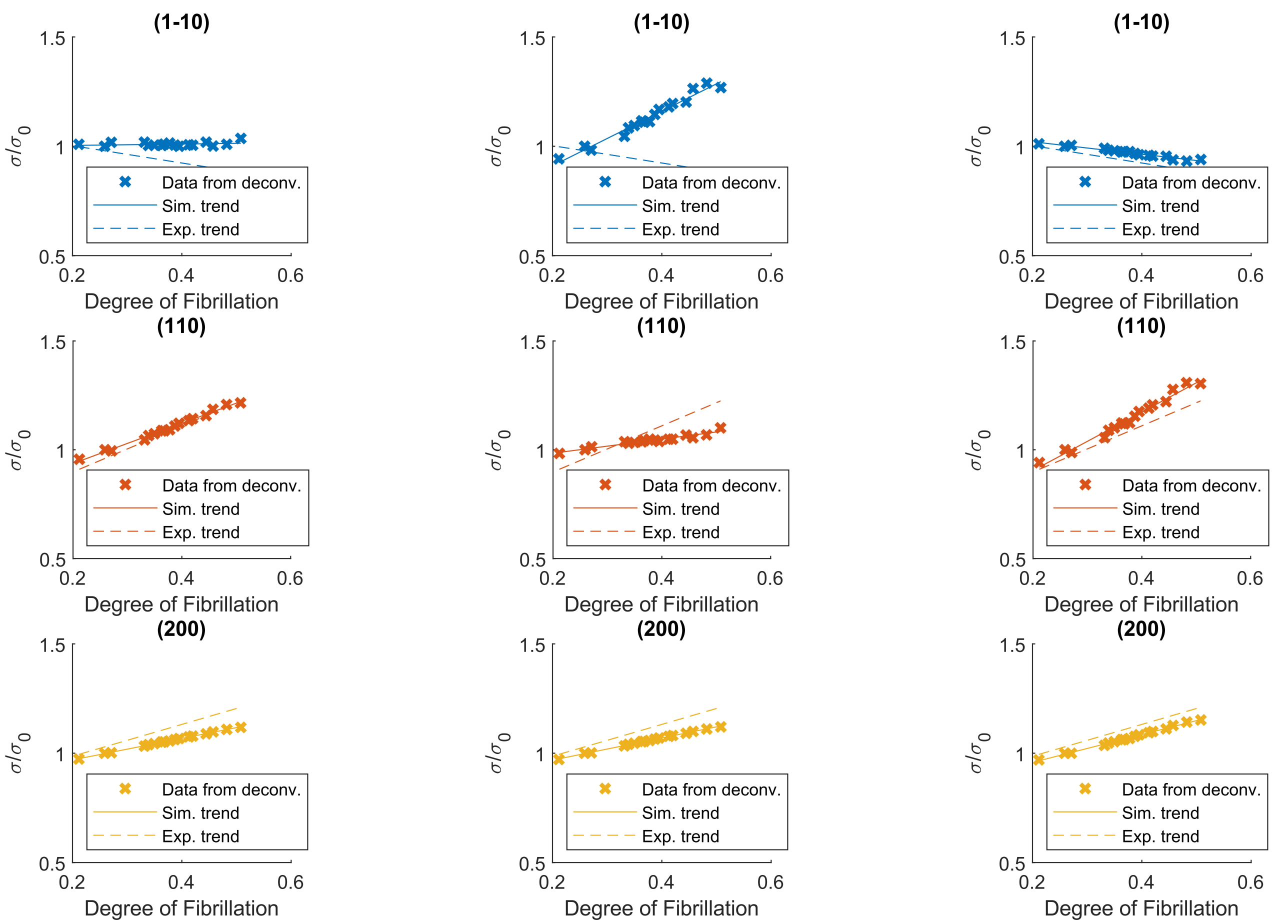

(1-10)
(110)
(200)
Data from deconv.
Sim. trend
Exp. trend
σ/σ0
Degree of Fibrillation


Model: H2+, Aggr.dir.: (1-10)
Model: H2+, Aggr.dir.: (110)
Model: H2-, Aggr.dir.: (1-10)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^-1]

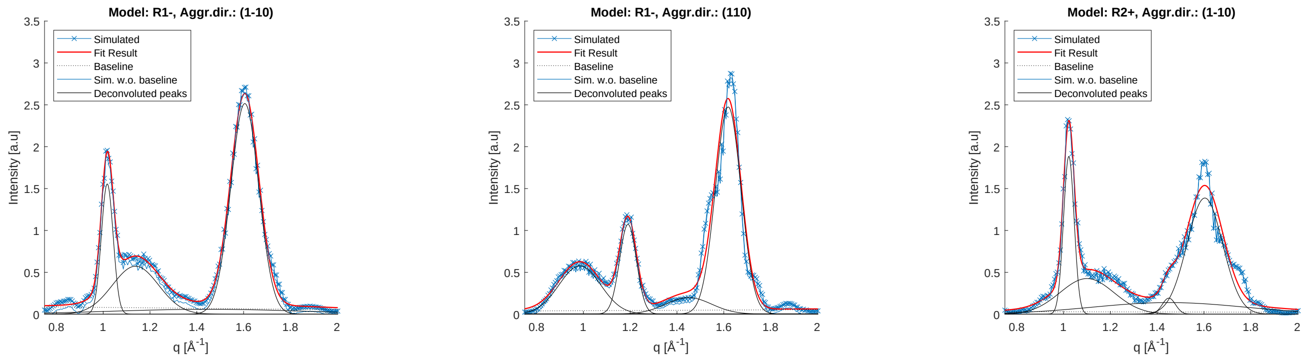

(1-10)
(110)
(200)
σ/σ0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation

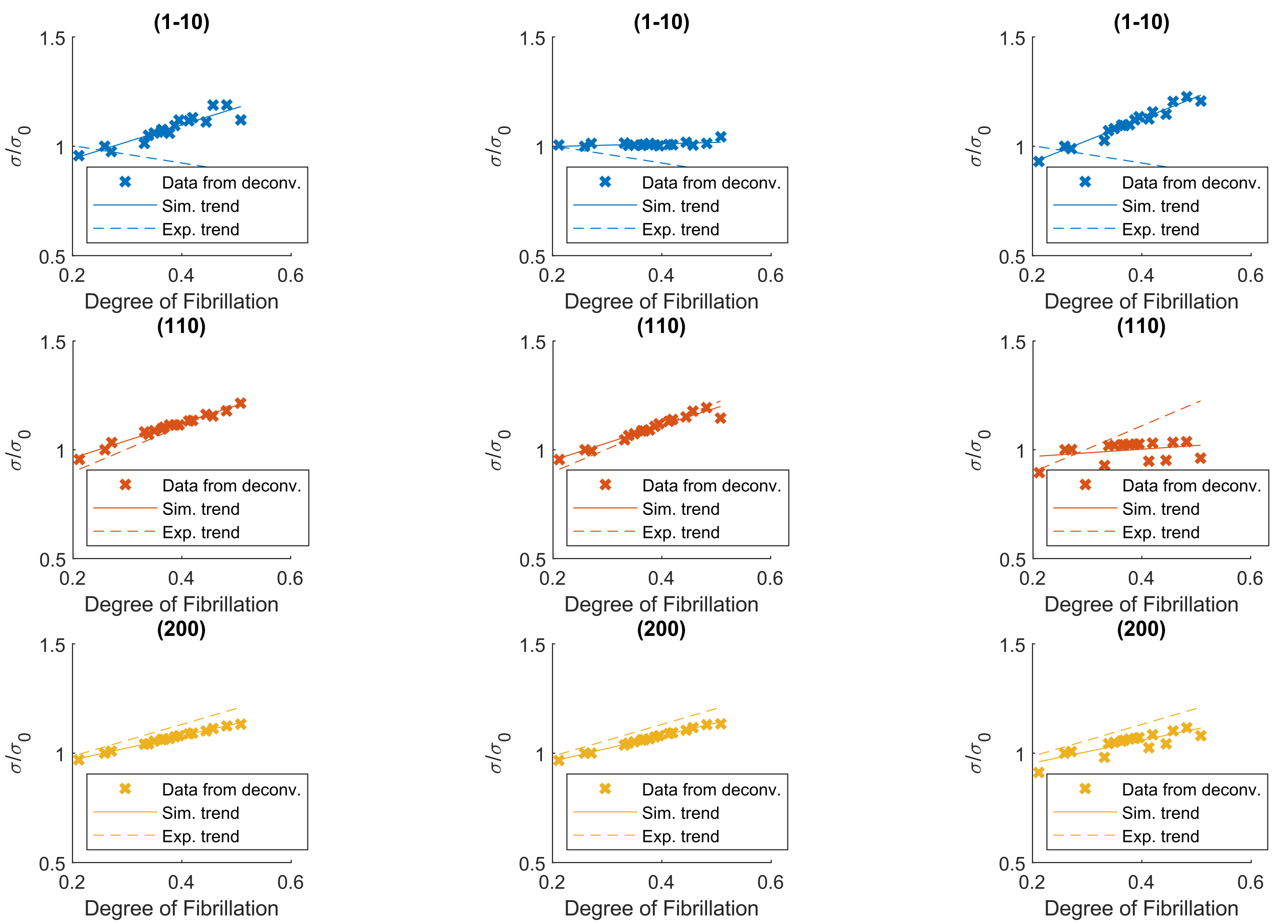


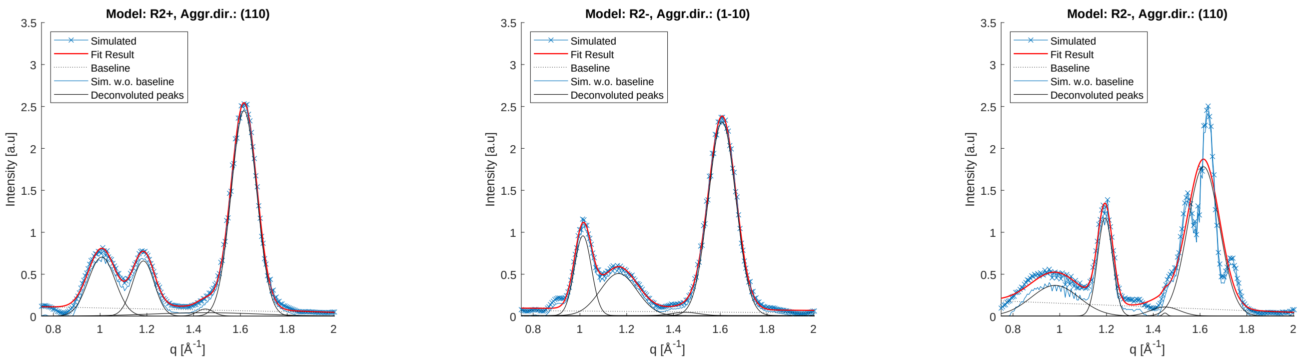
Model: H2-, Aggr.dir.: (110)
Model: R1+, Aggr.dir.: (1-10)
Model: R1+, Aggr.dir.: (110)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^{-1}]

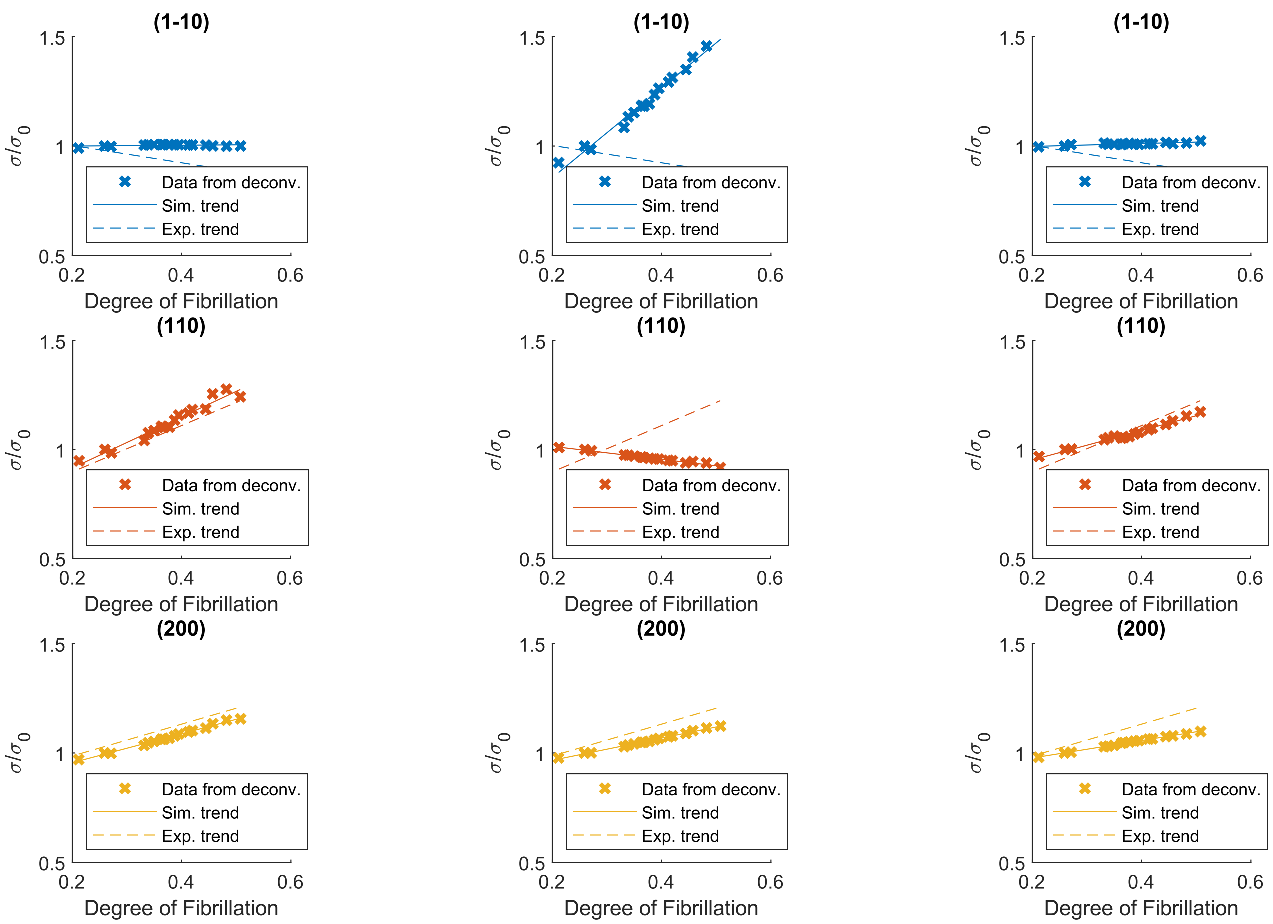


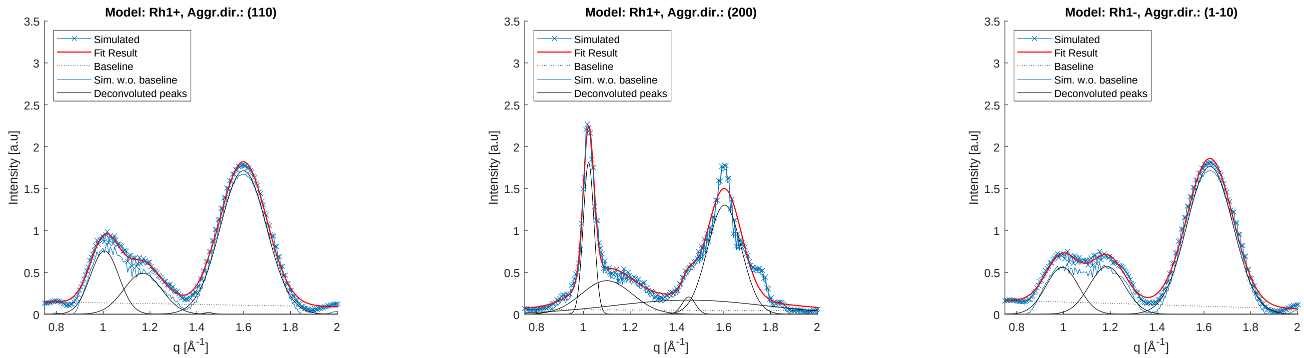
(1-10)
(110)
(200)
σ/σ_0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation

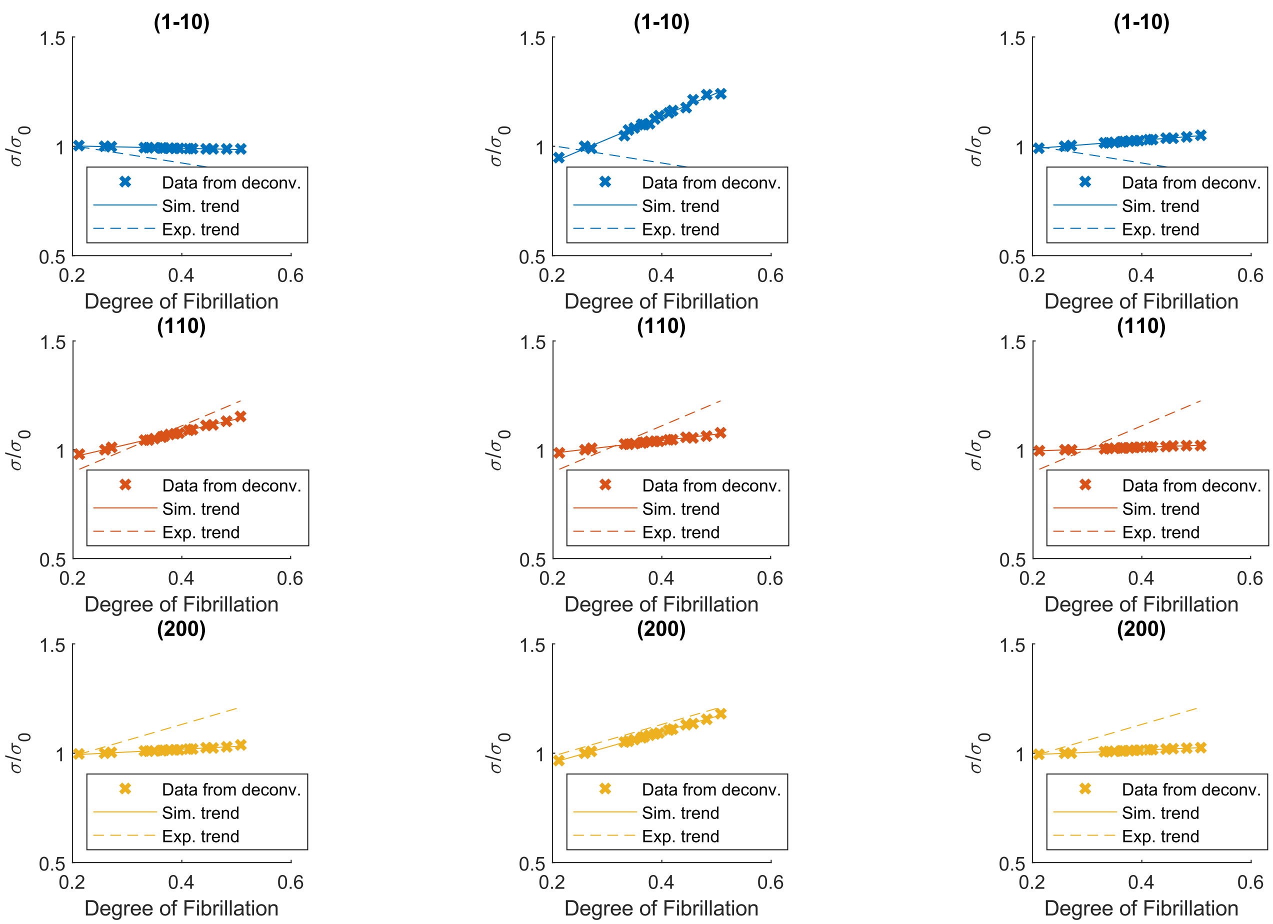

Model: R1-, Aggr.dir.: (1-10)
Model: R1-, Aggr.dir.: (110)
Model: R2+, Aggr.dir.: (1-10)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^{-1}]

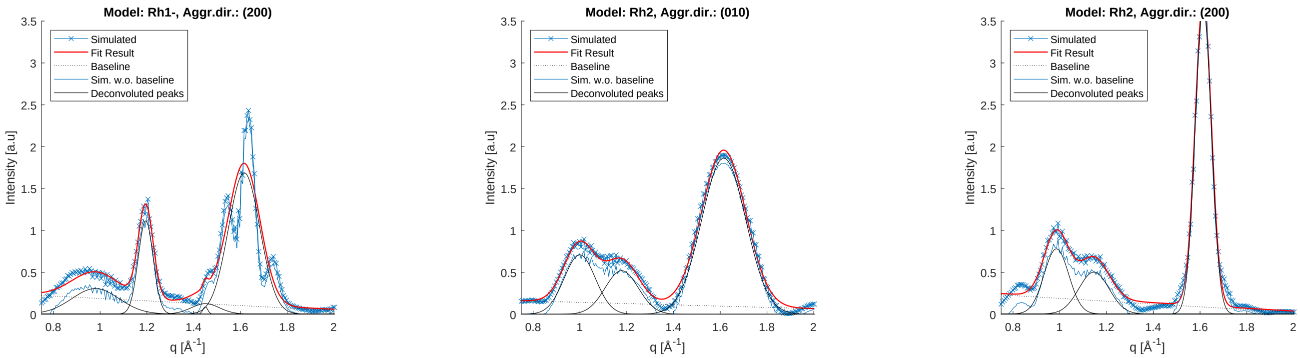

(1-10)
(110)
(200)
σ/σ_0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation

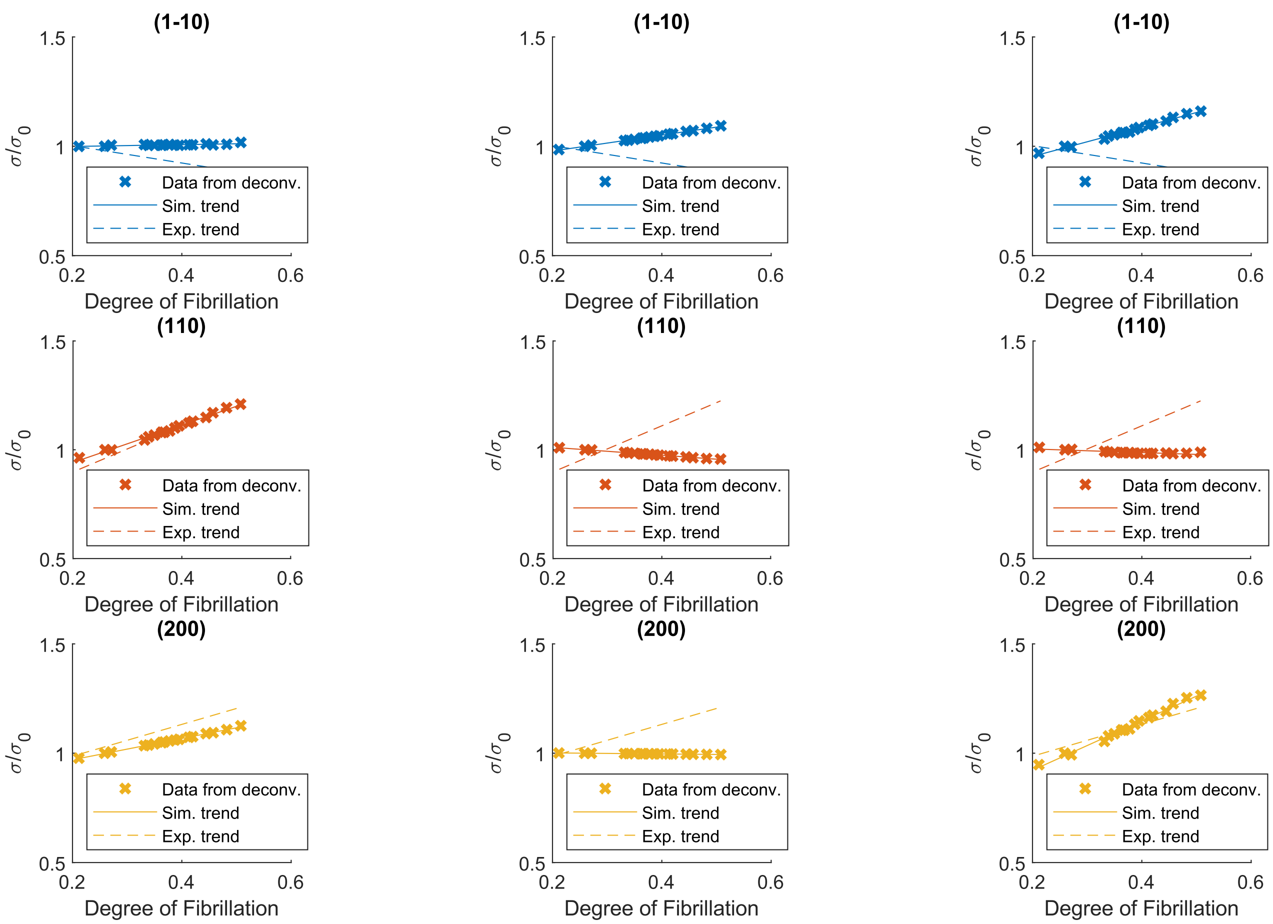

Model: R2+, Aggr.dir.: (110)
Model: R2-, Aggr.dir.: (1-10)
Model: R2-, Aggr.dir.: (110)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^{-1}]


(1-10)
(110)
(200)
σ/σ_0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation


Model: Rh1+, Aggr.dir.: (110)
Model: Rh1+, Aggr.dir.: (200)
Model: Rh1-, Aggr.dir.: (1-10)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^-1]


(1-10)
(110)
(200)
σ/σ0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation


Model: Rh1-, Aggr.dir.: (200)
Model: Rh2, Aggr.dir.: (010)
Model: Rh2, Aggr.dir.: (200)
Simulated
Fit Result
Baseline
Sim. w.o. baseline
Deconvoluted peaks
Intensity [a.u]
q [Å^-1]


(1-10)
(110)
(200)
σ/σ0
Data from deconv.
Sim. trend
Exp. trend
Degree of Fibrillation