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Supporting information for article:

Simulation of neutron dark-field data for grating-based interferometers

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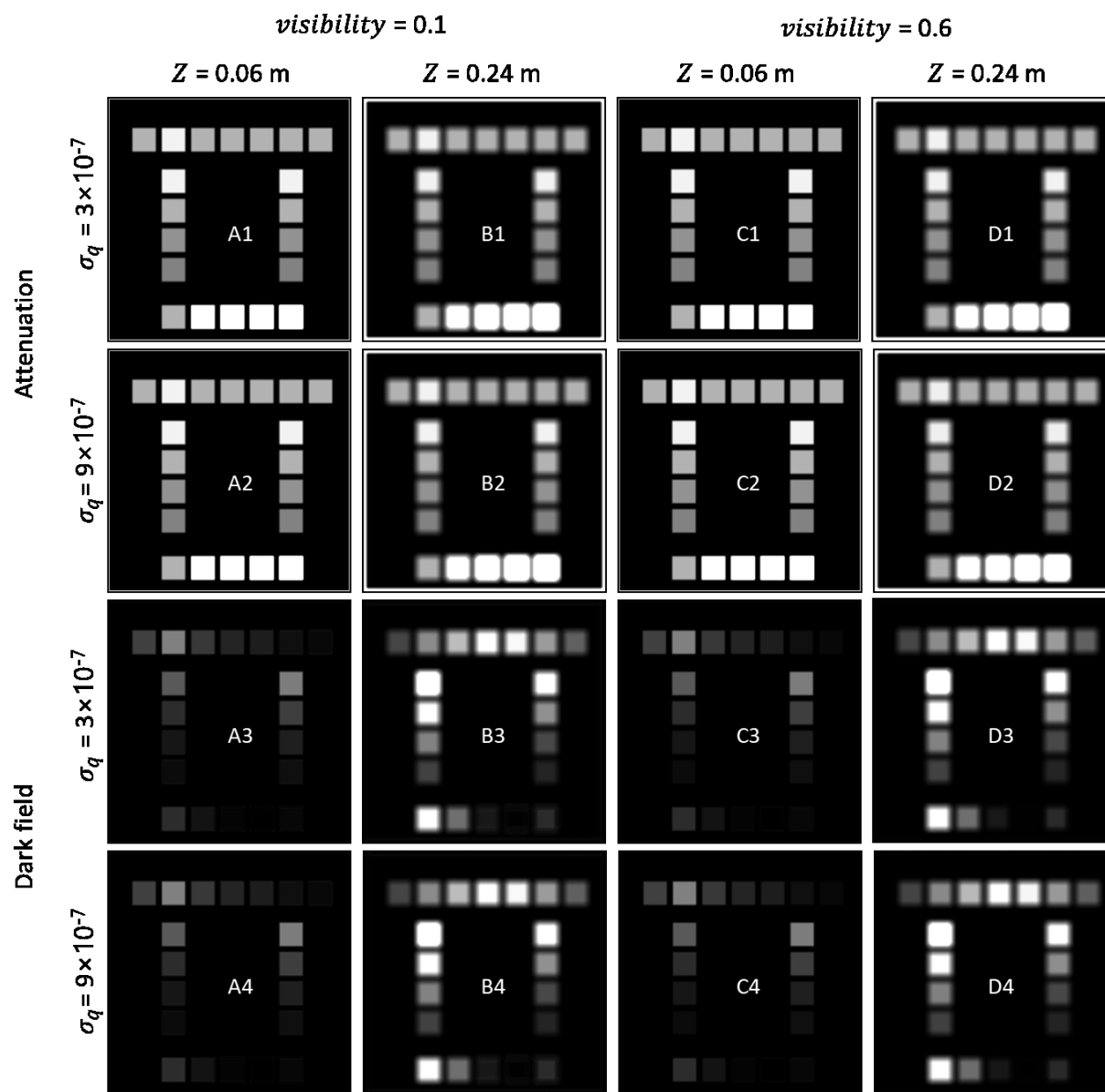
Figure S1. Example of attenuation contrast and dark field contrast image results of simulation with various experiment scenes. Other parameters are the period of Moiré pattern of 1 mm; the mean intensity of moiré pattern of 1e4; the wavelength of 3 Å; the distance from aperture to detector of 6 m; the aperture size of 10 cm; 6 phase steps. Distances from sample to detector of 60 mm and 240 mm correspond to autocorrelation length of 18 nm and 72 nm, respectively.

Model Parameters for Simulated Small-Angle Neutron Scattering and Neutron Dark Field Spectra

The following section includes all relevant model details for simulations of small-angle neutron scattering and neutron dark field data. The *correlogram-tools* package makes use of the existing library of small-angle scattering models available in SasView (Doucet et al., 2022), and so all definitions of specified form factors, structure factors, and model parameters are provided in the SasView documentation (*SasView Documentation*, n.d.). The only exceptions are the neutron wavelength and sample pathlength model parameters which are used by *correlogram-tools* to simulate the neutron dark field imaging data and are defined in Equation 4 of the main manuscript.

Table S1. Model parameters for simulated data in Figure 4 of the main manuscript.

Model Parameters	Value
Form Factor	sphere
Structure Factor	hardsphere
Scale	1
SLD (10^{-6} Å^{-2})	1.41
Solvent SLD (10^{-6} Å^{-2})	6.34
Radius (Å)	2500
Radius Polydispersity	0.1
Effective Radius (Å)	2500
Volume Fraction	0.1
Neutron Wavelength (Å)	(2, 3, 4, 5, 6)
Sample Pathlength (mm)	1

Table S2. Model parameters for simulated data in Figure 5(a-d) of the main manuscript.

Model Parameters	Subplots	
	(a, b)	(c, d)
Form Factor	sphere	sphere
Structure Factor	hardsphere	hardsphere
Scale	1	1
SLD (10^{-6} Å^{-2})	1.41	1.41
Solvent SLD (10^{-6} Å^{-2})	6.34	6.34
Radius (Å)	1000	(125, 250, 500, 1000, 2500, 5000)
Radius Polydispersity	0.1	0.1
Effective Radius (Å)	1000	(125, 250, 500, 1000, 2500, 5000)
Volume Fraction	(0.01, 0.05, 0.1, 0.2)	0.1
Neutron Wavelength (Å)	3	3
Sample Pathlength (mm)	1	1

Table S3. Model parameters for simulated data in Figure 5(e, f) of the main manuscript.

Model Parameters	Form Factor			
	Sphere	Rectangular Prism	Ellipsoid	Cylinder
Scale	0.1	0.1	0.1	0.1
SLD (10^{-6} Å^{-2})	1.41	1.41	1.41	1.41
Solvent SLD (10^{-6} Å^{-2})	6.34	6.34	6.34	6.34
Radius (Å)	1000			1000
Radius Polydispersity	0.1			0.1
Length (Å)		1000		10000
Length Polydispersity		0.1		0.1
Length B:A		1		
Length C:A		1		
Equatorial Radius (Å)			1000	
Equatorial Radius Polydispersity			0.1	
Polar Radius (Å)			5000	
Polar Radius Polydispersity			0.1	
Neutron Wavelength (Å)	3	3	3	3
Sample Pathlength (mm)	2	2	2	2

Table S4. Model parameters for simulated data in Figure 6(a-c) of the main manuscript.

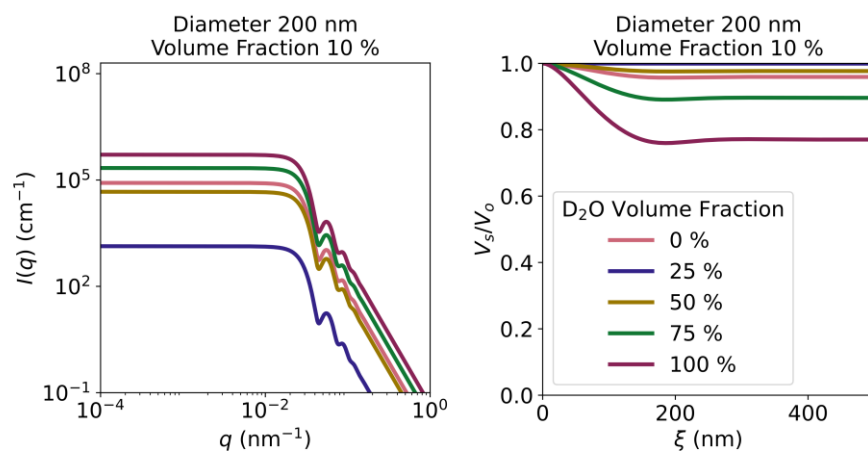| Model Parameters	Subplots		
	(a)	**(b)**	**(c)**
Form Factor	sphere	sphere	sphere
Structure Factor	hardsphere	hardsphere	hardsphere
Scale	1	1	1
SLD (10^{-6} Å^{-2})	3.87	3.87	1.4
Solvent SLD (10^{-6} Å^{-2})	6.34	-0.56	6.34
Radius (Å)	250	250	250
Radius Polydispersity	0.1	0.1	0.1
Effective Radius (Å)	250	250	250
Volume Fraction	0.1	0.1	0.1
Neutron Wavelength (Å)	3	3	3
Sample Pathlength (mm)	(1, 2, 5, 10, 20)	(1, 2, 5, 10, 20)	(1, 2, 5, 10, 20)

Figure S2. Simulated small-angle neutron scattering and loss in visibility data for 200 nm polystyrene nanoparticle dispersions in water at a volume fraction of 10 %. Contrast level was modulated by varying the light to heavy water ratio. The amount of heavy water in the solvent phase is shown in the legend of the right plot which is valid for both plots shown. All other relevant model parameters are shown in Table S5.

Table S5. Model parameters for simulations in Figure S2 of the supplementary information.

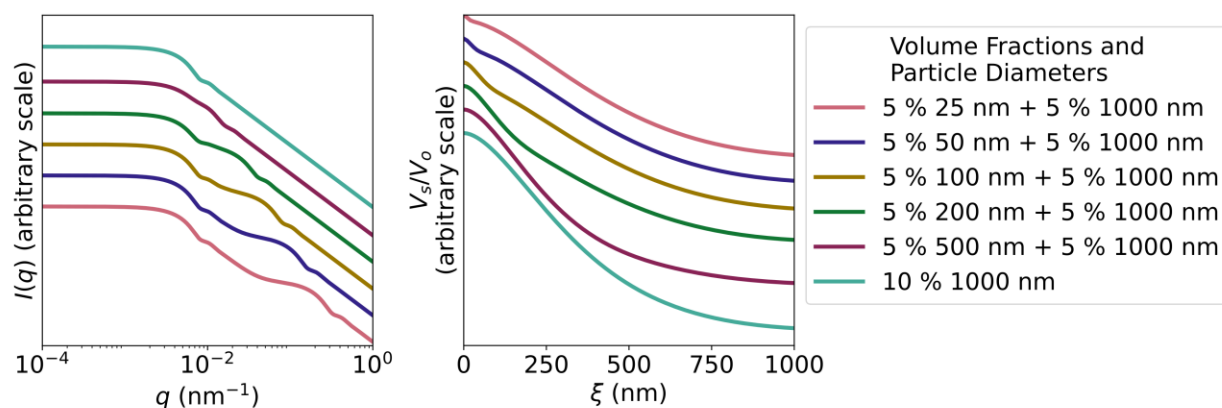| Model Parameters	Subplots
	(e,f)
Form Factor	sphere
Structure Factor	hardsphere
Scale	1
SLD (10^{-6} Å^{-2})	1.41
Solvent SLD (10^{-6} Å^{-2})	(-0.56, 1.16, 2.89, 4.61, 6.34)
Radius (Å)	1000
Radius Polydispersity	0.1
Effective Radius (Å)	1000
Volume Fraction	0.1
Neutron Wavelength (Å)	3
Sample Pathlength (mm)	1

Figure S3. Simulated small-angle neutron scattering and loss in visibility data for bimodal polystyrene nanoparticle dispersions in water. Total volume fraction of particles was 10 %. A unimodal distribution at 1000 nm is provided for comparison. All other relevant model parameters are shown in Table S6.

Table S6. Model parameters for simulated data in Figure S3 of the supplementary information.

Model Parameters	Sphere A + Sphere B
Form Factor	sphere+sphere
Scale	0.05
A Scale	1
A SLD (10^{-6} Å^{-2})	1.41
A Solvent SLD (10^{-6} Å^{-2})	6.34
A Radius (Å)	(125, 250, 500, 1000, 2500, 5000)
A Radius Polydispersity	0.2
B Scale	1
B SLD (10^{-6} Å^{-2})	1.41
B Solvent SLD (10^{-6} Å^{-2})	6.34
B Radius (Å)	5000
B Radius Polydispersity	0.2
Neutron Wavelength (Å)	3
Sample Pathlength (mm)	1

References

Doucet, M., Cho, J. H., Alina, G., Attala, Z., Bakker, J., Bouwman, W., Bourne, R., Butler, P., Cadwallader-Jones, I., Campbell, K., Cooper-Benun, T., Durniak, C., Forster, L., Gilbert, P., Gonzalez, M., Heenan, R., Jackson, A., King, S., Kienzle, P., … Wolf, C. (2022). *SasView version 5.0.5*. https://doi.org/10.5281/ZENODO.6331344

SasView Documentation. (n.d.). Retrieved October 5, 2023, from https://www.sasview.org/docs/