Complex samples 1

Mesocrystals, large particles and superlattices

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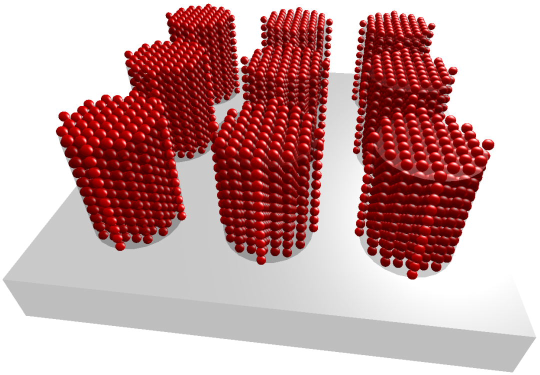
Overview

1. Mesocrystals
2. Large particles
3. Superlattices

Mesocrystals

- Mesocrystals consist of nanoparticles, ordered in a three dimensional lattice.
- A mesocrystal also has an outer shape.



Mesocrystal form factor

- The shape function of the mesocrystal is the product of its outer shape function with a 3d arrangement of nanoparticles:

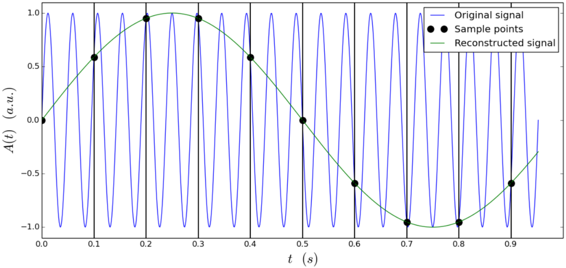
$$S_{meso}(\mathbf{r}) = S_{outer}(\mathbf{r}) \cdot \sum_{\mathbf{R_i} \in \Lambda} S_{nano}\left(\mathbf{r} - \mathbf{R_i}\right)$$

- The form factor then becomes a convolution:

$$F_{meso}(\mathbf{q}) = F_{outer}(\mathbf{q}) \otimes \sum_{\mathbf{Q_i} \in \Lambda^*} F_{nano}(\mathbf{Q_i})\delta\left(\mathbf{q} - \mathbf{Q_i}\right)$$

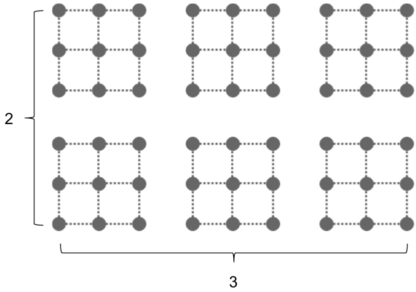
Large particles

- For very large particles, the fluctuations of the scattering cross section in each detector pixel cause aliasing when a single sample is used.
- BornAgain includes the possibility of using Monte Carlo integration over the pixel.



Superlattices

A superlattice consists of a finite lattice, embedded in another finite lattice:



Superlattice interference function

The interference function can be deduced as follows:

$$S(\mathbf{q}) = \left| \sum_{m=1}^{M} \sum_{n=1}^{N} e^{iq(ma+nb)} \right|^2$$

$$= \left| \sum_{m=1}^{M} e^{iqma} \sum_{n=1}^{N} e^{iqnb} \right|^2$$

$$= \left(\frac{\sin(qMa/2)\sin(qNb/2)}{\sin(qa/2)\sin(qb/2)} \right)^2$$