Advanced simulations

Walter Van Herck[1]

[1] Jülich Centre for Neutron Science at MLZ

BornAgain School and User Meeting, 2018

Overview

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.