

Supplementary Information

Structure of Casein Micelles in Milk Protein Concentrate Powders via Small Angle X-ray Scattering

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Combined Power law + Polydisperse Core-Shell Hard Sphere Model:

An alternative approach to fit the entire scattering profile is considered here. It is assumed that the colloidal calcium phosphate (CCP) core is surrounded by protein and hence forms core-shell structures. These core-shell structures are further suspended in a protein matrix (essentially similar to that of the shell protein), however it is anticipated that shell protein is more densely packed relative to the matrix (see figure 1s). These core-shell structures are closely packed within the casein micelles and a significant interaction between these structures is expected. Fitting of the SAXS data on an absolute scale (excluding packing density effects) by this combined model of a power law and polydisperse core-shell hard sphere for interfacial and internal structure respectively is shown in figure 1s. The resultant fitting parameters are shown in Table 1s.

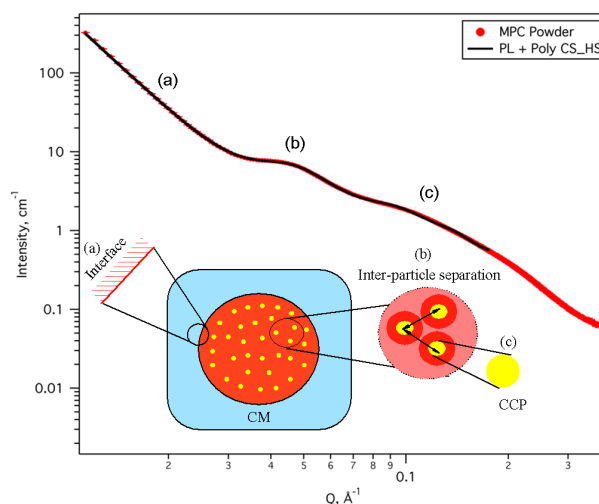


Fig. 1s - SAXS data from MPC powder. Cartoon illustrates different length-scales and associated scattering based on the power law + polydisperse core-shell hard sphere model (CM = Casein Micelles).

Table 1s Fitting parameters (Figure 1s) based on power law + polydisperse core-shell hard sphere model.

Parameters	Fitting value
Power Law	
PL Coefficient	4.64×10^{-6}
(-)Power	4.03
Poly Core-Shell HS	
Volume fraction	0.21
Avg core radius (Å)	21.0
Core polydispersity	0.1
Shell thickness (Å)	42.7
SLD core (Å ⁻²)	2.20×10^{-5}
SLD shell (Å ⁻²)	1.09×10^{-5}
SLD matrix (Å ⁻²)	1.07×10^{-5}
Bkg (cm ⁻¹)	0.481

In the fitting process, the scattering length density (SLD) values for core, shell and matrix were constrained, allowing the size of CCP core and shell to independently vary. SLD values were subsequently refined to generate best fits. However, such a model is unable to fit high Q data, namely a feature previously attributed to ellipsoidal micelles.