The Concentration Dependence of the Size and Symmetry of a Bottlebrush Polymer in a Good Solvent

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Supplemental Information

The general Guiner-Porod (GGP) model is described by Equations 1-3.[1] This model describes the scattering by using Guinier regions interconnected by power law regimes. Crossover points (Q_1, Q_2) and scaling factors (G_1,G_2) are calculated to ensure self-consistency in the transition between different regions. The model uses shape factors (s_1,s_2) to describe the approximate shape of the scattering features, where 0 represents a sphere, 1 represents a cylinder or rod, and 2 represents lamellae. A background and intensity scaling term were also included in the model. The implementation of the general Guinier-Porod model in Sasview is available in the Sasview marketplace (http://marketplace.sasview.org/), with the model name "2 Layer General Guinier Porod". The hard sphere structure factor was used where appropriate and its implementation is described in the sasview documentation.

$$I(Q) = \frac{G_2}{Q^{s_2}} \exp\left(-\frac{Q^2 R_{g,2}^2}{3-s_2}\right) \quad for\ Q \le Q_2 \tag{1}$$

$$I(Q) = \frac{G_1}{Q^{s_1}} \exp\left(-\frac{Q^2 R_{g,1}^2}{3-s_1}\right) \quad for\ Q_2 \le Q \le Q_1 \tag{2}$$

$$I(Q) = \frac{D}{Q^d} \quad for\ Q \ge Q_1 \tag{3}$$

Table 1: Fit Results to GGP model (Figures 3 and 4). Uncertainties represent 95% confidence intervals as evaluated by the Monte-Carlo Markov Chain analysis performed by the Dream algorithm in Sasview.

Volume Fraction	$R_{g,2}$ (Å)	$R_{g,1}$ (Å)	R_g	s_1	s_2	l_p (Å)
0.0870	39.8 ± 0.1	27.3 ± 0.1	35.0 ± 0.9	0.74 ± 0.13	0	7.9 ± 0.1
0.0792	39.0 ± 0.2	28.6 ± 0.1	35.5 ± 0.9	0.68 ± 0.15	0	7.7 ± 0.1
0.0739	38.3 ± 0.1	29.4 ± 0.1	35.8 ± 1.0	0.98 ± 0.18	0	7.4 ± 0.1
0.0578	40.5 ± 0.1	29.2 ± 0.1	36.6 ± 1.1	0.82 ± 0.12	0	8.2 ± 0.1
0.0504	41.7 ± 0.1	30.7 ± 0.1	38.0 ± 1.0	0.73 ± 0.15	0	8.8 ± 0.1
0.0424	41.6 ± 0.2	29.5 ± 0.1	37.2 ± 0.7	0.88 ± 0.16	0	8.7 ± 0.1
0.0350	45.8 ± 0.1	32.2 ± 0.1	40.8 ± 1.4	0.9 ± 0.18	0	10.7 ± 0.1
0.0287	47.5 ± 0.2	30.0 ± 0.1	40.3 ± 1.7	0.8 ± 0.33	0	11.5 ± 0.1
0.0232	53.2 ± 0.4	35.5 ± 0.1	46.3 ± 0.2	0.64 ± 0.08	0	14.7 ± 0.1
0.0196	60.3 ± 0.3	36.4 ± 0.1	50.1 ± 0.2	0.61 ± 0.05	0	19.3 ± 0.1
0.0165	66.4 ± 0.1	29.5 ± 0.1	49.6 ± 0.2	1.01 ± 0.08	0	23.9 ± 0.1
0.0124	77.2 ± 0.3	28.6 ± 0.1	55.2 ± 0.2	1.1 ± 0.09	0	33.8 ± 0.2
0.0085	82.9 ± 0.8	26.0 ± 0.1	57.3 ± 0.4	1.25 ± 0.10	0.1 ± 0.01	40 ± 0.4
0.0074	84.1 ± 1.5	25.9 ± 0.1	58.0 ± 0.9	1.24 ± 0.11	0.2 ± 0.02	41.6 ± 0.8
0.0043	89.0 ± 1.2	25.8 ± 0.1	60.8 ± 0.6	1.3 ± 0.03	0.1 ± 0.01	47.9 ± 0.7
0.0021	96.2 ± 1.4	22.5 ± 0.1	64.1 ± 0.7	1.47 ± 0.04	0.1 ± 0.02	58.5 ± 0.8
0.0010	99.5 ± 4.0	22.5 ± 0.1	66.0 ± 2	1.37 ± 0.06	0.1 ± 0.05	65.7 ± 2.7

References

(1) Hammouda, B. A New Guinier–Porod Model. *J. Appl. Crystallogr.* **2010**, *43* (4), 716–719. https://doi.org/10.1107/S0021889810015773.