Appendix C

ParallelPiped FormFactor-Details

C.1 Homogeneous ParallelPiped FormFactor(FF)

Imagine a parallelpiped with edges $C > B > A$ aligned roughly with C(length) along z, B(width) along y and A(thickness) along x directions. Scattering vector Q vector is in some arbitrary direction at angle α from z-axis and β from y axis. Then it can be written in terms of unit vectors as

$$\vec{Q} = |Q|(\sin\beta\sin\alpha\hat{x} + \cos\beta\sin\alpha\hat{y} + \cos\alpha\hat{z}) \tag{C.1}$$

The phase factor $e^{i\vec{Q}\cdot\vec{r}}$ will be given as

$$i\vec{Q}\cdot\vec{r} = iQ(\sin\beta\sin\alpha x + \cos\beta\sin\alpha y + \cos\alpha z) \tag{C.2}$$

This gives the scattering term as

$$\int_V e^{i\vec{Q}\cdot\vec{r}} = \int_{-C/2}^{C/2}\int_{-B/2}^{B/2}\int_{-A/2}^{A/2} e^{iQ(\sin\beta\sin\alpha x+\cos\beta\sin\alpha y+\cos\alpha z)}\,dx\,dy\,dz \tag{C.3}$$

$$= I(A,B,C) \qquad \text{where} \tag{C.4}$$

$$I(A,B,C) = \frac{\sin(QA/2\sin\alpha\sin\beta)}{QA/2\sin\alpha\sin\beta}\frac{\sin(QB/2\sin\alpha\cos\beta)}{QB/2\sin\alpha\cos\beta}\frac{\sin(QC/2\cos\alpha)}{QC/2\cos\alpha} \times ABC \tag{C.5}$$

To obtain the Form factor of parallelpiped, two orientational averages have to be done over the angles α and β. Above term is written in terms of the reduced lengths given by

$$a \equiv \frac{A}{B}; \qquad b \equiv \frac{B}{B} = 1; \qquad c \equiv \frac{C}{B};$$

$$\begin{aligned} F_{(A,B,C)}(Q) & \\ = & \int_0^{\pi/2}\int_0^{\pi/2} \left(I_{(A,B,C)}(Q)\right)^2 \sin\alpha\, d\alpha\, d\beta \\ = & \int_0^{\pi/2}\int_0^{\pi/2} \left(\frac{\sin(QA/2\sin\alpha\sin\beta)}{QA/2\sin\alpha\cos\beta}\frac{\sin(QB/2\sin\alpha\cos\beta)}{QB/2\sin\alpha\cos\beta}\right)^2 \left[\frac{\sin(QC/2\cos\alpha)}{QC/2\cos\alpha}\right]^2 \\ \times & \sin\alpha\, d\alpha\, d\beta \end{aligned} \tag{C.6}$$

This is written in terms of variables $\mu = QB$, $\cos\alpha = \sigma$ and $\beta = (\pi/2)u$ and the function $S(x) = \sin x/x$ as

$$F_{a,b,c}(Q) = \int_0^1\int_0^1 \left\{S[\mu a/2\sqrt{1-\sigma^2}\sin(\pi/2u)]S[\mu b/2\sqrt{1-\sigma^2}\cos(\pi/2u)]\right\}^2 du\,[S(\mu c\sigma/2)]^2\, d\sigma \tag{C.7}$$

Notes:

1. The integrals need to be done only from (0,$\pi/2$) due to rectangular symmetry (check if factor of 2 off or not for inner integral..unlike cylinder FF, where integral over d$\phi \equiv \beta = 2\pi$, we DO NOT have the cylindrical symmetry here, and need a double integral over dβ).

To obtain the FF on an absolute scale, the above equation is multiplied by

$$(\pi/2) \times (Scale/Volume) \times (\delta\rho)^2 10^8$$

where $\delta\rho = \rho_p - \rho_0$ is the contrast term between the parallelpiped and solvent of SLDs ρ_p and ρ_0 respectively.

2. Eqn.(3) is equivalent to the expression given in SANS Analysis package when the integrals are written in terms of $\sigma \equiv \cos\alpha$; $\mu = QB$ and u

3. The factor $(\pi/2)$ factor is needed to get correct limits of the PP formfactor with that of sherical/ellipsoidal shapes.

C.2 CoreShell-ParallelPiped FF

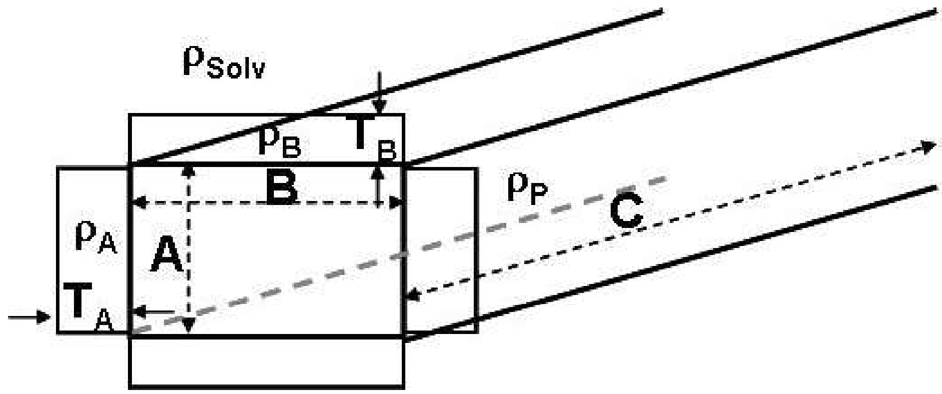


Figure C.1: A schematic of the coreshell PPiped model, showing the rims on sides A and B of thickness T_A and T_B respectively.

For a core-shell structure Parallelpiped, of edge lengths $(A+2T_A, B+2T_B, C+2T_C)$ (the rims of lengths T_A, T_B and T_C extend out on each face), and of SLDs (ρ_a, ρ_b, ρ_c) and ρ_p in the core, the phase factor becomes

$$
\begin{aligned}
\int_V e^{i\vec{Q}\cdot\vec{r}} &= \int_{-(C/2+T_C)}^{C/2+T_C}\int_{-(B/2+T_B)}^{B/2+T_B}\int_{-(A/2+T_A)}^{A/2+T_A} e^{iQ\cdot r}\,dx\,dy\,dz \\
&= I(A,B,C) \\
&+ \left(\int_{-(A/2+T_A)}^{-A/2} + \int_{A/2}^{(A/2+T_A)}\right)\int_{-B/2}^{B}\int_{-C/2}^{C} \\
&+ \int_{-A/2}^{A/2}\left(\int_{-(B/2+T_B)}^{-B/2} + \int_{(B/2)}^{B/2+T_B}\right)\int_{-C/2}^{C} \\
&+ \int_{-A/2}^{A/2}\int_{-B/2}^{B/2}\left(\int_{-(C/2+T_C)}^{-C/2} + \int_{(C/2)}^{C/2+T_C}\right)
\end{aligned}
$$

For each edge, this gives an extra term besides the core term as

$I(A+2T_A,B,C) =$

$$
\left(\frac{\sin(Q(A+2T_A)/2\sin\alpha\sin\beta)}{Q(A+2T_A)/2\sin\alpha\sin\beta} - \frac{\sin(QA/2\sin\alpha\sin\beta)}{QA/2\sin\alpha\sin\beta}\right)\frac{\sin(QB/2\sin\alpha\cos\beta)}{QB/2\sin\alpha\cos\beta}\frac{\sin(QC/2\cos\alpha)}{QC/2\cos\alpha} \\
\times(\rho_a-\rho_0)(V1\equiv 2T_ABC)
$$

$I(A,B+2T_B,C) =$

$$
\frac{\sin(QA/2\sin\alpha\sin\beta)}{QA/2\sin\alpha\sin\beta}\left(\frac{\sin(Q(B+2T_B)/2\sin\alpha\cos\beta)}{Q(B+2T_B)\sin\alpha\cos\beta} - \frac{\sin(QB/2\sin\alpha\cos\beta)}{QB/2\sin\alpha\cos\beta}\right)\frac{\sin(QC/2\cos\alpha)}{QC/2\cos\alpha} \\
\times(\rho_b-\rho_0)(V2\equiv A2T_BC)
$$

$I(A,B,C+2T_C)$ is similarly

$$
\frac{\sin(QA/2\sin\alpha\sin\beta)}{QA/2\sin\alpha\sin\beta}\frac{\sin(QB/2\sin\alpha\cos\beta)}{QB/2\sin\alpha\cos\beta}\left(\frac{\sin(Q(C+2T_C)/2\cos\alpha)}{Q(C+2T_C)/2\cos\alpha} - \frac{\sin(QC/2\cos\alpha)}{QC/2\cos\alpha}\right) \\
\times(\rho_c-\rho_0)(V3\equiv AB2T_C)
$$

which can be written in terms of reduced lengths

$$a + t_a \equiv \frac{A + 2T_A}{B};$$
$$b + t_b \equiv \frac{B + 2T_B}{B};$$
$$c + t_c \equiv \frac{C + 2T_B}{B}$$

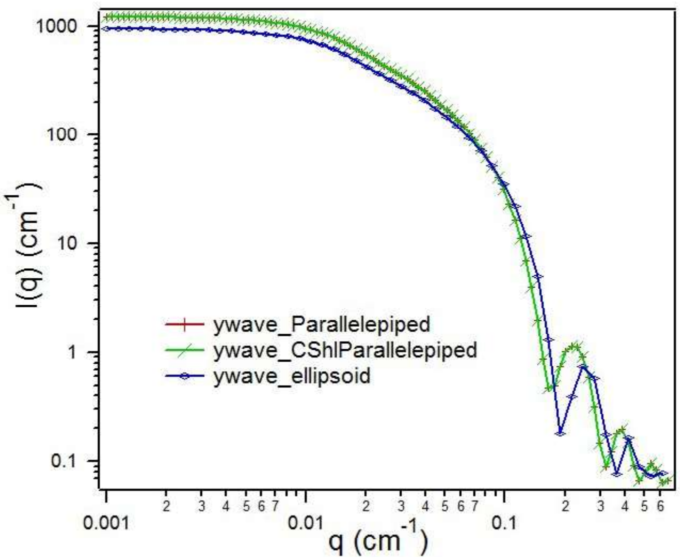
This gives the form factor as the sum of inner core term plus extra terms for each edge with the correct SLD term variation and volumes as

$$\begin{aligned} F_{(a+t_a,b+t_b,c+t_c)}(Q) &= \frac{1}{V_{ot}} \int_0^{\pi/2} \int_0^{\pi/2} \{(\rho_p - \rho_0) I(a,b,c) ABC \\ &+ (\rho_a - \rho_0)[I(a+t_a,b,c) - I(a,b,c)] 2T_A BC \\ &+ (\rho_b - \rho_0)[I(a,b+t_b,c) - I(a,b,c)] A2T_B C \\ &+ (\rho_c - \rho_0)[I(a,b,c+t_c) - I(a,b,c)] AB2T_C\}^2 \sin\alpha \, d\alpha \, d\beta \end{aligned} \tag{C.8}$$

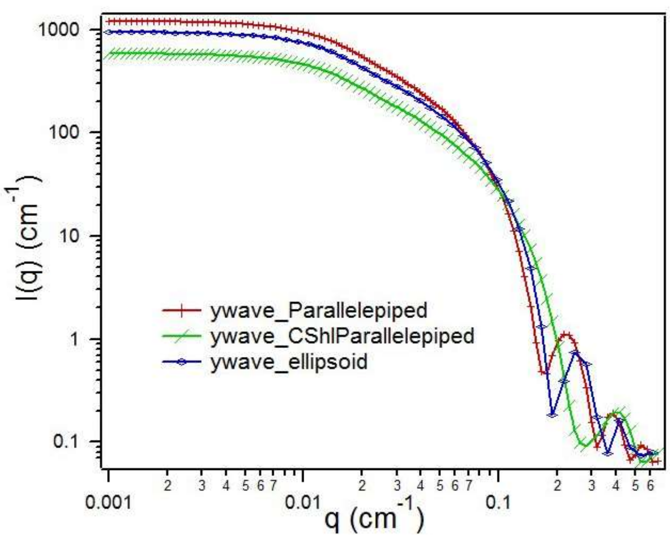
where V_{ot} is the total volume of the parallelpiped, and is equal to

$$V_{ot} = ABC + 2T_A BC + A2T_B C + AB2T_C$$

The CshlPP formfactor is written in Igor to go with the SANS Analysis Package.



(a)



(b)

Figure C.2: (a)The coreshellPPiped model compared with the regular PP and a cylinder with ellispoidal cross-section. Rims of core-shellPPiped model have been made equal to zero. Dimensions of PP edges A, B and C are 40, 40 and 300Årespectively, chosen to compare with cylinder of radius 20Åand length 300Å. (b) Effect of rims: In core-shellPPiped model, rims A and B are 5Åeach and edges A and B are 35Åeach.