**Igor NIST macro vs SASView 4.0.1 vs SASView 4.1**

Problem: different results with different software / version. Igor-Macro provides the best fits; also global fit possible (but only with “simple global fit” function). If coefficients from Igor macro are entered in SASview, different function results (without fitting; figure 4). Modell should theoretically be the same, when no distribution of the shell fitted it SASview

SASview 4.0.1 had a bug in calculating the correlation length, which was supposed to be fixed in version 4.1. Nothing about bugs in Igor Macro known.

Table 1. SLD of NP components. All components hydrated (known from other methods, but hydration degree unknown)

|  |  |
| --- | --- |
| PLGA (shell) | 2.11 e-6 |
| PFCE (core) | 3.87e-6 |
| PVA (could be in the shell) | 9.4e-7 (cannot be calculated exactly, as exact hydrolysis degree unknown) |

Table 2. Fitting coefficients OK105 D2O.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **Igor Macro**  **(no PD shell)** | **Sasview 4.0.1**  **(no PD shell)** | **Sasview 4.0.1** | **Sasview 4.1**  **(no PD shell)** | **Sasview 4.1** |
| vol. fraction | 0.007 | 0.007 | 0.007 | 0.007 | 0.007 |
| block radius /Å | 88 | 105 | 115 | 82 | 83 |
| shell thickness / Å | 41 | 31 | 18 | 24 | 19 |
| corr. length ξ/ Å | 447 | 416 | 398 | 330 | 312 |
| fractal dimension | 3.1 | 3.3 | 3.4 | 3.8 | 3.8 |
| SLD core\*10-6 | 5.91 | 5.82 | 5.71 | 4.74 | 4.86 |
| SLD shell\*10-6 | 3.17 | 3.18 | 2.15 | 2.02 | 1.8  (lowest limit) |
| SLD solvent\*10-6 | 6.36 | 6.36 | 6.36 | 6.36 | 6.36 |
| Distribution of radius | 0.6 | 0.5 | 0.4 | 0.999 | 0.82 |
| Distribution of thickness |  |  | 0.7 |  | 0.079 |
| background | 0.005 | 0.004 | 0.004 | 0.004 | 0.0034 |
| Chi2/Npts | 1.2 | 13 | 10 | 7.3 | 19 |



Figure 1. OK105 D2O; FraPolyCore from NIST Igor Macro

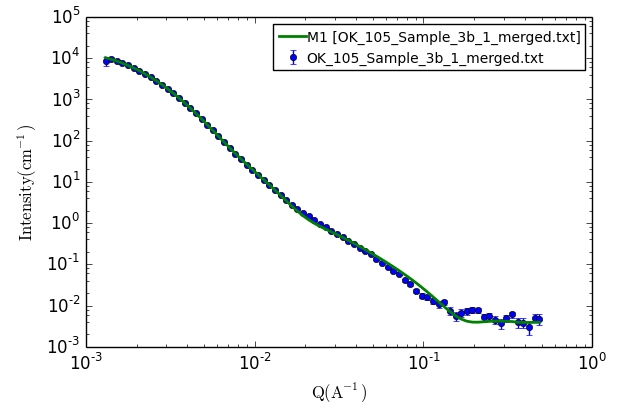


Figure 2. OK105 D2O; SASview 4.0.1; only distribution of core fitted

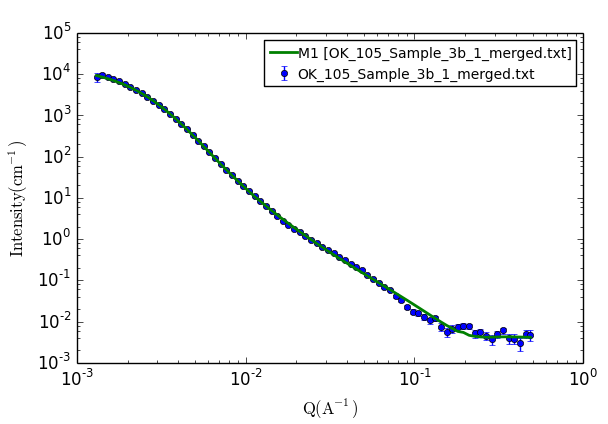


Figure 3 OK105 D2O SASview 4.1; only distribution of core fitted

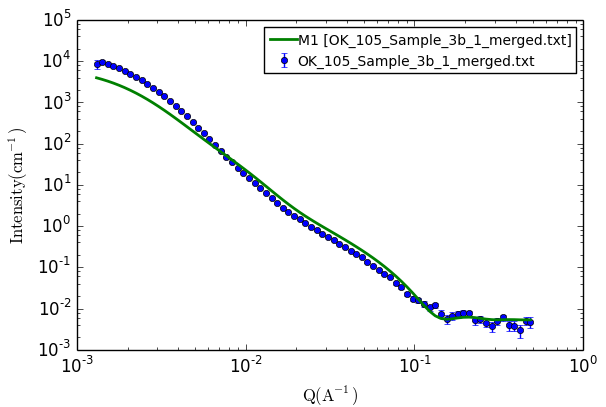


Figure 4. OK105 D2O. SASView 4.1 with coefficients from Igor macro.