

Vikki Bird thesis: guide to the electronic supplementary data

The data associated with this DOI corresponds to the electronic supplementary information associated with V. Bird's 2016 PhD thesis.¹

The Origin files² provided contain quasielastic neutron scattering $I(Q,t)$ vs. t curves for PS/SWCNT nanocomposites fitted with the KWW function (Equation 1) for various values of β .

$$\text{KWW}(t; \tau_{\text{KWW}}, \beta) = \exp \left[- \left(\frac{t}{\tau_{\text{KWW}}} \right)^\beta \right]$$

Equation 1

The data are organised as follows:

1. The percentage in the file name corresponds to the weight percent nanotubes in the nanocomposite
2. Data from chain-deuterated polystyrene is labelled either d3 or h5 PS
3. Data from ring-deuterated polystyrene is labelled either d5 or h3 PS
4. The first tab in each file contains the $I(Q,t)$ vs. t data for each detector grouping at the temperature contained in the tab label, *e.g.* 177C data corresponds to data recorded at 177 °C. The detector groupings correspond to the Q values outlined in Table 1
5. Fittings were conducted with various constraints put on the selection of the parameter β .

The data corresponding to each type of β used have three associated tabs:

- a. $b = x$, where $x = \text{variable}$, 0.61, 0.44 or straight line: this tab contains all data associated with the fitting of the data using b to vary between 0 and 1; $\beta = 0.61$, $\beta = 0.44$ and β varying as a straight line function of Q , respectively. This tab features plots of the fitted $I(Q,t)$ curves; the x -axes correspond to time in ns, and the y -axes correspond to $I(Q,t)$, which has no units.
- b. $b = x$ curve: this tab contains the individual data points corresponding to the curves and their fits, and the data points for the residuals
- c. $b = x$ results: this tab contains the parameters extracted from the KWW fits. The values of Q corresponding to the detector groupings are listed in Table 1. Fittings conducted with $\beta = 0.44$ were conducted on detector groups 10–17.

Table 1: Q-values according to detector grouping

Detector grouping	Q value/\AA^{-1}
1	0.4836
2	0.6079
3	0.7291
4	0.8470
5	0.9609
6	1.070
7	1.175
8	1.273
9	1.366
10	1.452
11	1.532
12	1.604
13	1.668
14	1.725
15	1.773
16	1.814
17	1.845

References

1. V. Bird, PhD, Durham University, 2016.
2. Origin 8 SR4, v. 8.0951, OriginLab Corporation, MA, USA, 2008.