Datreat theory: ring

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theory id-name: ring
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 Dynamic scattering function for a polymer ring melt as developed in the PRL of S. Goossen
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Parameters(15):
  1: ampli     >      prefactor
  2: diff      > ABS :limiting diffusion (NMR value) in [A**2/ns]
  3: r02       > ABS :reference mean squared displacement at transition point to D0 in [A**2]
  4: alpha     > ABS :sub-diffussion  exponent of short time diffusion
  5: a_cross   > ABS :transition exponent between short and long time diffusion (sharper kink for
larger a)
  6: nring     > INT :number of segments in one ring (cannot be fitted INT!)
  7: lseg      > ABS :effective segment length
  8: nu        > ABS :chain statistics exponent (nu=0.5 => random walk, Gaussian)
  9: wl4       > ABS :Rouse rate in [A**4/ns]
 10: pmin      > ABS :transition mode number between simple ring-Rouse and large p modification
 11: pwidth    > ABS :sharpness of transition
 12: f0        > ABS :prefactor f(p) limit for large p > pmin values (default 1)
 13: finf      > ABS :prefactor f(p) limit for small p < pmin values (default F=0.9??) transitin
width is pwidth
 14: tauinf    > ABS :small p tau(p) = tauinf/p**pexinf
 15: pexinf    >     :small p tau(p) = tauinf/p**pexinf
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INPUT: Parameters that are extracted from the actual considered data records:
..there may be default assumptions, but better make sure that these parameters are set properly!
  1: q         > q
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OUTPUT: Parameters that are computed and added to the records parameters as information:
  1: Rg        > predicted ring radius of gyration
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cite:  S. Goossen et al., PRL 2014, 113, 168302 !
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Modified polymer ring structure factor with sublinear diffusion.

Diffusion factor:

$$\exp\left(-\langle r^2(t)\rangle\, q^2/6\right)$$

with

$$\langle r^2(t)\rangle = \left[\left(\exp\{-\log[r_0^2/D/6]\,\alpha\}\, r_0^2\, t\, \alpha\right)^a + \left(6Dt\right)^a\right]^{1/a}$$

describing sublinear-linear center-of-mass diffusion with a normal long time diffusion constant D and a sublinear diffusion with exponent α combined such that the transition from sublinear to linear diffusion happens at distance r_0. The sharpness of the transition is controlled by a, the larger the value the sharper is the transition.

Ring structure factor (without diffusion):

$$S(q,t) = \frac{1}{N}\sum_{i,j}^{N} \exp\left[\frac{(ql)^2}{6}\left(|i-j|\{N-|i-j|\}/N\right)^{2\nu} - B_{i,j}(t)\right]$$

with

$$B_{i,j}(t) = A\sum_{p,even}\frac{F(p)}{p^2}\cos(p\pi[i-j]/N)\,[1-\exp(-t\Gamma(p))]$$

with the mode p dependent amplitude $F(p)$ and rate $\Gamma(p)$ parameters.

Here

$A = 2N^{2\nu}(lq)^2/(3\pi^2)$

and

$F(p) = F_0[1 - T_f(p)] + F_\infty T_f(p)$

and

$\Gamma(p) = [1 - T_f(p)]p^2/\tau_R + T_f(p)p^\mu/\tau_\infty$

the transition function is

$T_f(p) = \{1 + \exp([p - p_{min}]/p_{width})\}^{-1}$

the Rouse time is computed as

$\tau_R = N^2/(W\pi^2)$ with $W = Wl^4/l^4$

Parameter correspondences

Observe units, if not other specified: Angstroems and nanao-seconds

diff $\rightarrow D$
r02 $\rightarrow r_0^2$
alpha $\rightarrow \alpha$
a_cross $\rightarrow a$
nring $\rightarrow N$
lseg $\rightarrow l$
nu $\rightarrow \nu$
wl4 $\rightarrow Wl^4$
pmin $\rightarrow p_{min}$
pwidth $\rightarrow p_{width}$
f0 $\rightarrow F_0$
finf $\rightarrow F_\infty$
tauinf $\rightarrow \tau_\infty$
pexinf $\rightarrow \mu$