A1: Transient self-assembled networks: Restructuring & mechanical behavior

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Supervisors: C. Friedrich, J. P. Wittmer

Presentations

- 9 oral IRTG
- 13 posters IRTG
- 5 oral other
- 3 posters other

Publications

[1] **P. Polińska**, **C. Gillig**, J.P. Wittmer, J. Baschnagel, EPJE (2014)

[2] J.P. Wittmer, H. Xu, **P. Polińska**, **C. Gillig**, J. Helfferich, F. Weysser, J. Baschnagel, EPJE 36, 11 (2013)

[3] G. Bauer, C. Friedrich, **C. Gillig**, F. Vollrath, T. Speck, C. Holland, J. R. Soc. Interface 11, 20130847, 30 (2013)

[4] J.P. Wittmer, H. Xu, **P. Polińska**, F. Weysser, J. Baschnagel, JCP 138, 19 (2013)

[5] J.P. Wittmer, H. Xu, **P. Polińska**, F. Weysser, J. Baschnagel, JCP 138, 12 (2013)

[6] H. Xu, J.P. Wittmer, **P. Polińska**, J. Baschnagel, PRE 84, 4 (2012)

[7] N. Schulmann, H. Xu, H. Meyer, **P. Polińska**, J. Baschnagel, J.P. Wittmer, EPJE 35, 9 (2012)

[8] J.P. Wittmer, N. Schulmann, **P. Polińska**, J. Baschnagel, JCP 135, 18 (2011)

[9] J.P. Wittmer, A. Cavallo, H. Xu, J.E. Zabel, **P. Polińska**, N. Schulmann, H. Meyer, J. Farago, A. Johner, S.P. Obukhov, J. Baschnagel, J. Stat. Phys. 145, 4 (2011)

[10] J.P. Wittmer, **P. Polińska**, H. Meyer, J. Farago, A. Johner, J. Baschnagel, A. Cavallo, JCP 134, 23 (2011)

Other activities

Organization of a training camp "Experimental and theoretical methods for investigating polymer dynamics", Schauinsland, Germany
C. Gillig, P. Polińska

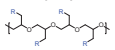
Organization of an international conference "Workshop on Dendrimers and Hyperbrached polymer chains", Strasbourg, France
M. Dolgushev, P. Polińska, J. Wittmer,

Participation in Master Class
C. Gillig, P. Polińska

Topology and interactions

0 — Degree of branching — 1

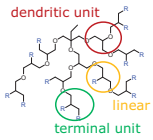
linear polymers



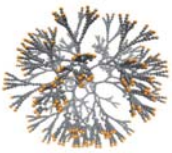
Polyglycerol (PG)

-R: -OH
-OMe
-OTMS
M = 600-200 000 kg/mol
DB ≈ 60%

Hyperbranched (hb) polymers

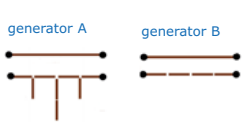


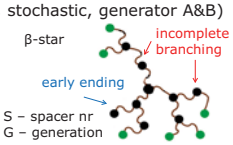
Dendrimers



Simulated molecules

regular dendrimers, α-stars ($M_g \sim g^{\alpha-1}$), β-stars (self-similar, generator A), γ-stars (self-similar, stochastic, generator A&B)





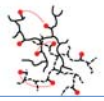
Structure-property relation

linear non-associating polymers

hyperbranched non- associating polymers

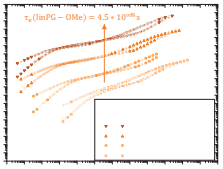
linear associating polymers

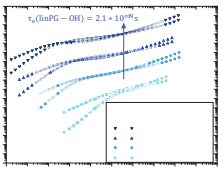
hyperbranched associating polymers

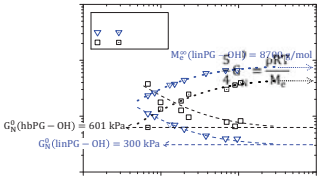


Viscoelastic response

Rheological experiments [3]

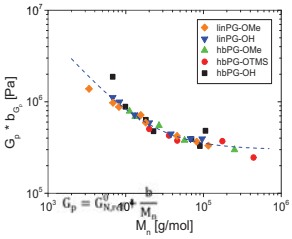






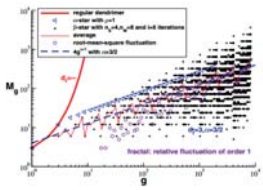
HbPG shows entanglement relaxation phenomena even though $M_e < M_x$

All plateau moduli can be shifted to one ‚mastercurve' - independant of functionality and topology



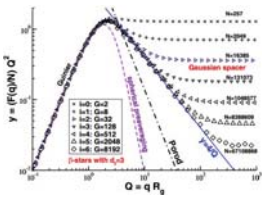
Structural properties

Classification of molecules [1]



Depending on imposed topology molecules with different generations may have same mass.

Fractal molecules show strong fluctuations but on average they resemble other molecular types.



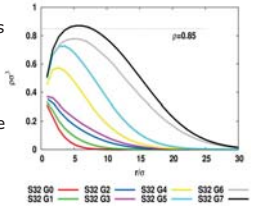
Kratky plot for β-stars with d_f=3.

These self-similar objects decay with a power law Q^{2-d_f} in the intermediate wave vector regime. Molecules gets more compact with growing mass.

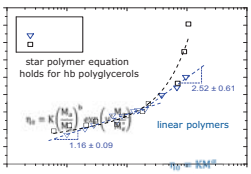
Unexpected result:
Nonmonotoneus density profile

Mass density profiles for dendrimers with S=32 chain length and different generations.

The curves show nonmonotonous behavior with a depletion zone close to the center for high generation numbers.
Such conformation enables the encapsulation of other molecules.



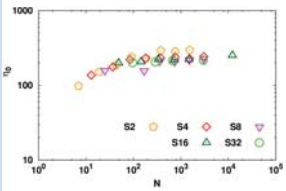
Linear vs. hyperbranched polymers



Shear experiments using oscillatory shear measurements

- due to entanglements the viscosity of hbPG is higher than for linPG at high M
- η_0-M relation of hbPG can be described by star polymer equation

Dendrimers



Shear experiments using non-equilibrium simulation methods

- zero shear viscosity η_0 increases up to certain molecular weight, after which it actually reaches the plateau
- since the intrinsic viscosity is expressed in volume per mass, the interplay between both is visible in the viscosity η_0 curves

Conclusions & outlook

Linear vs. hyperbranched polymers

- hb polymers with $M_e < M_x$ entangle for high M ($M >> M_e^{lin}$)
- viscosity and T_g can be tuned in wide ranges by M and DB
- η_0-M relation of hbPG can be described by star polymer equation
- τ_e is the same for linPG and hbPGs, but H-bonds decelerate the relaxation time

Structure

- molecules condensation with growing generation
- increasing asymetry of non-fractal molecules with Mw
- no entanglements
- a depletion zone in the density profile for high generation numbers