Soft Matter exercise, Chapter 5: Polymers

1. Polyethylene

For a linear polyethylene molecule with a molar mass of 128242 g/mol calculate

a. the contour length
b. the root mean square end-to-end distance.

Assume an angle between the C-C groups of 109° and a C-C length of 0.155 nm.

2. Poly(ethylene glycol)

Calculate the radius of gyration of poly(ethylene glycol) (PEG) with a molecular weight of 6000 g/mol if dispersed in

a. a good solvent
b. a poor solvent.
c. What is the coil overlap concentration if PEG is dispersed in a good solvent?
d. What would be the PEG concentration in mol/l where $c = c_m^*$?

Assume an angle between the C-C bonds and C-O bonds of 109°, a C-C length of 0.155 nm and a C-O length of 143 pm.

3. Polymers in solution

You are asked to design a poly(ethylene glycol)-poly(lactic acid) (PEG-PLA) block-copolymer that forms polymersomes. The PLA block is given; its molecular weight is 5 kDa and its cross-section area is 6 nm^2. You are told that the hydrophilic block should be composed of poly(ethylene glycol) (PEG) and is dissolved in a good solvent. What molecular weight would you choose? Assume the length of a C-C bond to be 0.154 nm, that of a C-O bond to be 0.143 nm, and the angle between the bonds to be 109°.

4. Polymer melts

You have a product composed of polyethylene chains, each one having 1000 repeat units for which you optimized the processing conditions. You now decide that the properties would be better if you increased the number of repeat units by a factor of 100.

a. What would change in your processing and why?
b. What could you do to compensate for these changes?

5. Viscosity of entangled melts

For an entangled melt of polybutadiene, the plateau value of the shear modulus at room temperature is 1.15 × 10^6 Pa. Assume the density of poly(butadiene) to be 900 kg/m^3 and the statistical step length is 0.65 nm. The molar mass of a monomer unit is 54 g/mol. The zero shear viscosity η_0 as a function of the degree of polymerization N and the temperature T may be written as

$$\eta_0 = 3.86 \times 10^{-3} \exp\left(\frac{1404}{T-128}\right) N^{3.4} Pas$$

a. Calculate the relative molecular mass between entanglements, M_x, using $G = \frac{\rho RT}{M_x}$
b. Estimate the diffusion coefficient of poly(butadiene) with a relative molecular mass of 100 000 g/mol at 298 K.
c. Based on the result obtained in (b) judge if this diffusion is fast. If yes, why? If not, why not?

6. Poly(styrene)

a. Measurements of the plateau modulus of poly(styrene) reveal $G = 2 \times 10^5$ Pa at $T = 160$ °C. Using a density of 1.05 g/cm³, determine the molar mass between two entanglements using $G = \frac{\rho RT}{M_x}$.

7. Crosslink density of an elastomer

The data shown in Table 1 gives the experimental relation between stress and strain for a piece of rubber at 20°C.

a. Use the data of table 1 at small strains to calculate the density of cross-links
b. Plot the data over the full range of strains, together with the prediction of rubber elasticity, assuming the density of crosslinks you calculated and discuss possible discrepancies.

Table 1: Stress as a function of strain.

strain	σ (MPa)
0	0
0.162	0.152
0.27	0.246
0.433	0.327
0.678	0.42
0.95	0.489
1.358	0.605
1.657	0.697
2.338	0.882
2.964	1.067
3.48	1.253
4.35	1.613
4.973	1.986
5.461	2.313
6.19	3.05
6.403	3.448
6.699	3.811
6.914	4.151
7.019	1.503
7.151	4.878
7.256	5.242
7.361	5.605
7.489	6.321

8. Thermosets

a. How are thermosets typically processed?
b. Name an example of a thermoset. Where is this thermoset used?