HW5

Monday, March 8, 2021 7:02 PM

510.316 Biomaterials I **Spring 2021**

Problem Set #6

Due date: March 12, 2021

1. How does polybutadiene-g-polystyrene (PB-*g*-PSt) graft copolymer differ from homopolymers PSt and PB, in terms of their mechanical property (strength, modulus, toughness)? Sketch out the stress-strain curves for the three polymers.

2. Briefly explain why copolymerizing a small fraction (2-5%) of acrylic acid moieties in UHMWPE will further increase the mechanical property? What need to be added in order to achieve the maximum mechanical strength?

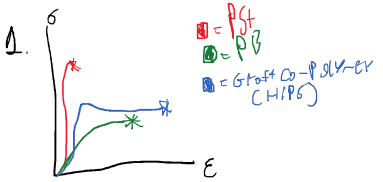
3. Given a linear polyethylene (PE) chain (no branches) with a degree of polymerization of 10,000, and a C–C bond length of 0.154 nm.

   a. Calculate the end-to-end distance for a fully stretched PE chain of this polymer, while maintaining all C–C–C bond angle of 109.5° (not freely jointed, hinged chain).
   b. Calculate the root-mean-square end-to-end distance, assuming that these PE chains are freely jointed and hinged.
   c. Calculate the root-mean-square end-to-end distance, assuming that the PE chains maintain fixed C–C–C bond angle of 109.5°, but fully rotatable for each C–C bond segment, i.e. assuming that these PE chains are freely rotating chains.

4. Consider a polymer solution dissolved in a good solvent. Discuss the relationship between the chain dimensions (*e.g.* root mean square end-to-end distance), Kuhn's length, and chain rigidity. How would introduction of same type of charges (either positive or negative charges) influence the chain rigidity and Kuhn's length?

20-30?

1.



As we can see from the diagram PST is a very brittle material which can take a lot of stress while PB is a very rubbery/flexible material that can take a lot of strain, but by making a graft copolymer which is referred to as HIPS you essentially get a combo of this properties as the PS graft provide Tolerance to stress and the poly butadiene backbone provide some flexibility and thereby a larger strain tolerance thereby overall providing a high toughness high impact resistant copolymer

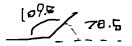
2. Comparatively to PE, acrylic acid has the added hydrogen bonds to its intermolecular force which provides even more of a barrier to keep the material together further increasing its strength and toughness. You can even further/guarantee strengthening by addition of a cation like zinc which will act like collection point for all these carbonyl groups further strengthening the co-polymer.

3. a)

$$\text{end to end} = (10{,}000-1)\cdot 0.154\,\text{nm}\cdot \sin\left(\frac{109.5}{2}\right)$$
$$= 1257.50\,\text{nm}$$

b) $\langle R^2 \rangle = nL^2$

$$= 10{,}000 \cdot 0.154^2 = 237.16\,\text{nm} \rightarrow \sqrt{\langle R^2 \rangle} = 15.4\,\text{nm}$$

c) $\langle R^2 \rangle = nL^2\left(\frac{1+\cos(\theta)}{1-\cos(\theta)}\right)$ 

$$= 237.16\left(\frac{1+\cos(70.5)}{1-\cos(70.5)}\right)$$
$$= 474.826\,\text{nm} \rightarrow \sqrt{\langle R^2 \rangle} = 21.7904\,\text{nm}$$

4. So having a good solvent means that our polymer is more spread out and is more opened up. Because of this we will have a larger end to end chain length and we will be able to define much larger Kuhn segments as there will be les changes in direction as the expanding out provides more linear segments. This also means there is less chain rigidity as there is less chain-chain interaction in exchange for chain-solvent forces. The addition of a charged particle can have some substantial effects such as if the polymer like the polymer form question 2 has sites for columbic interaction it will cause there to be some clumping of chains although not as windy as compared to a bad solvent, this might not cause a huge change to the Kuhn's length or end to end distance but it would massively increase chain rigidity which is actually what we saw in question 2