Homework 4

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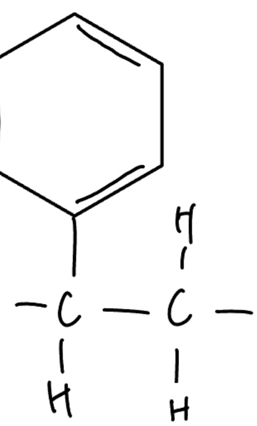
October 5, 2024

1 Polymer Structure

a. polystyrene

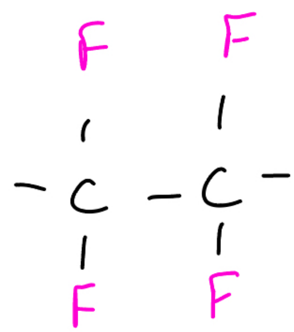
(i) Polystyrene is a thermoplastic polymer.
(ii) A common object made from polystyrene is a styrofoam cup.
(iii) The repeat unit for polystyrene is shown below.



(iv) The repeat unit molecular weight is 104.15 g/mol.

b. polytetrafluoroethylene

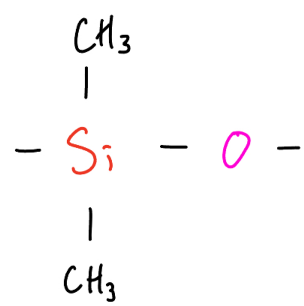
(i) Polytetrafluoroethylene is a thermoplastic polymer.
(ii) A common object made from polytetrafluoroethylene is teflon tape and non-stick cookware.
(iii) The repeat unit for polytetrafluoroethylene is shown below.



(iv) The repeat unit molecular weight is 100.02 g/mol.

c. polydimethylsiloxane

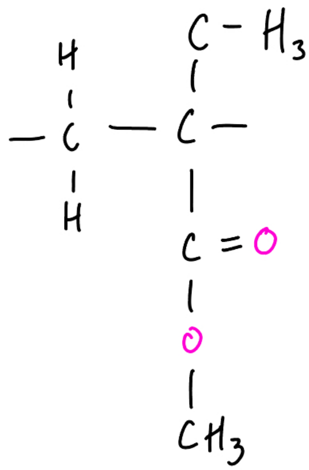
(i) Polydimethylsiloxane is a thermoplastic polymer.
(ii) A common object made from polydimethylsiloxane is silicone rubber.
(iii) The repeat unit for polydimethylsiloxane is shown below.



(iv) The repeat unit molecular weight is 74.15 g/mol.

d. poly(methyl methacrylate)

(i) Poly(methyl methacrylate) is a thermoplastic polymer.
(ii) A common object made from poly(methyl methacrylate) is plexiglass.
(iii) The repeat unit for poly(methyl methacrylate) is shown below.



(iv) The repeat unit molecular weight is 100.12 g/mol.

2 Polymer Molecular Weight

For this question I could have used excel but I did it all in a jupter notebook (python) and then copied the code here. I hope this is okay since Prof. Hewlett did not explicitly say that this was okay, but he did say Excel is okay. The code is shown below

```
import numpy as np
import matplotlib.pyplot as plt

amounts = np.ones(4)
molecular_weights = np.array([1e3,1e4,1e5,1e6])
repeat_unit_weight = 104.15

num_molecules =  amounts / molecular_weights

mole_fractions = num_molecules / np.sum(num_molecules)
number_average = np.sum(molecular_weights * mole_fractions)
print(f'number average molecular weight: {number_average:.1f}')

weight_fractions = amounts / np.sum(amounts)
weight_average = np.sum(weight_fractions * molecular_weights)
print(f'weight average molecular weight: {weight_average}')

ndegree_of_polymerization = number_average / repeat_unit_weight
print(f'number average degree of polymerization: {ndegree_of_polymerization:.1f}')

wdegree_of_polymerization = weight_average / repeat_unit_weight
print(f'weight average degree of polymerization: {wdegree_of_polymerization:.1f}')

pdi = weight_average / number_average
print(f'polydispersity index: {pdi:.1f}')
```

Property	**Value**
Number average molecular weight	3600.4
Weight average molecular weight	277750.0
Number average degree of polymerization	34.6
Weight average degree of polymerization	2666.8
Polydispersity index	77.1

3 co-polymers

I'll assume 100g as a basis for calculations to make my life easier

$$30\text{g Acrylonitrile} \times \frac{1\text{mol}}{53.06\text{g}} = 0.5654\text{mol}$$

$$70\text{g Styrene (repeat units)} \times \frac{1\text{mol}}{104.15\text{g}} = 0.6721\text{mol}$$

Now for the repeat unit aka mole fractions, denoted as χ

$$\chi_{\text{acrylonitrile}} = \frac{0.5654}{0.5654 + 0.6721} = \boxed{0.4569}$$

$$\chi_{\text{styrene}} = \frac{0.6721}{0.5654 + 0.6721} = \boxed{0.5431}$$

4 Crystallinity in Polymers

Setting up the two equations

$$0.74 = \frac{\rho_c \left(1.41\text{g/cm}^3 - \rho_a\right)}{1.41\text{g/cm}^3 \left(\rho_c - \rho_a\right)}$$

$$0.31 = \frac{\rho_c \left(1.34\text{g/cm}^3 - \rho_a\right)}{1.34\text{g/cm}^3 \left(\rho_c - \rho_a\right)}$$

Which is a silly little system of equations. I'll isolate ρ_c in the top equation

$$\rho_c = \frac{\left(0.74 \cdot 1.41\text{g/cm}^3\right) \cdot \rho_a}{\left(0.74 \cdot 1.41\text{g/cm}^3 - 1.41\text{g/cm}^3\right) + \rho_a} = \frac{1.043\rho_a}{\rho_a - 0.367}$$

Now taking that and plugging it back into the second equation

$$0.31 = \frac{\rho_c \left(1.34\text{g/cm}^3 - \rho_a\right)}{1.34\text{g/cm}^3 \left(\rho_c - \rho_a\right)} = \frac{\frac{1.043\rho_a}{\rho_a - 0.367} \left(1.34\text{g/cm}^3 - \rho_a\right)}{1.34\text{g/cm}^3 \left(\frac{1.043\rho_a}{\rho_a - 0.367} - \rho_a\right)}$$

In theory this could be solved by hand, but... I just plugged it into wolfram alpha and got this solution

$$\rho_a = \boxed{1.29\text{g/cm}^3}$$

and then since I have ρ_a I can plug it back into the equation for ρ_c

$$\rho_c = \frac{1.043 \cdot 1.29}{1.29 - 0.367} = \boxed{1.46\text{g/cm}^3}$$

b.

Bringing back the original formula for the degree of Crystallinity

$$\chi_s = \frac{\rho_c \left(\rho_s - \rho_a\right)}{\rho_s \left(\rho_c - \rho_a\right)}$$

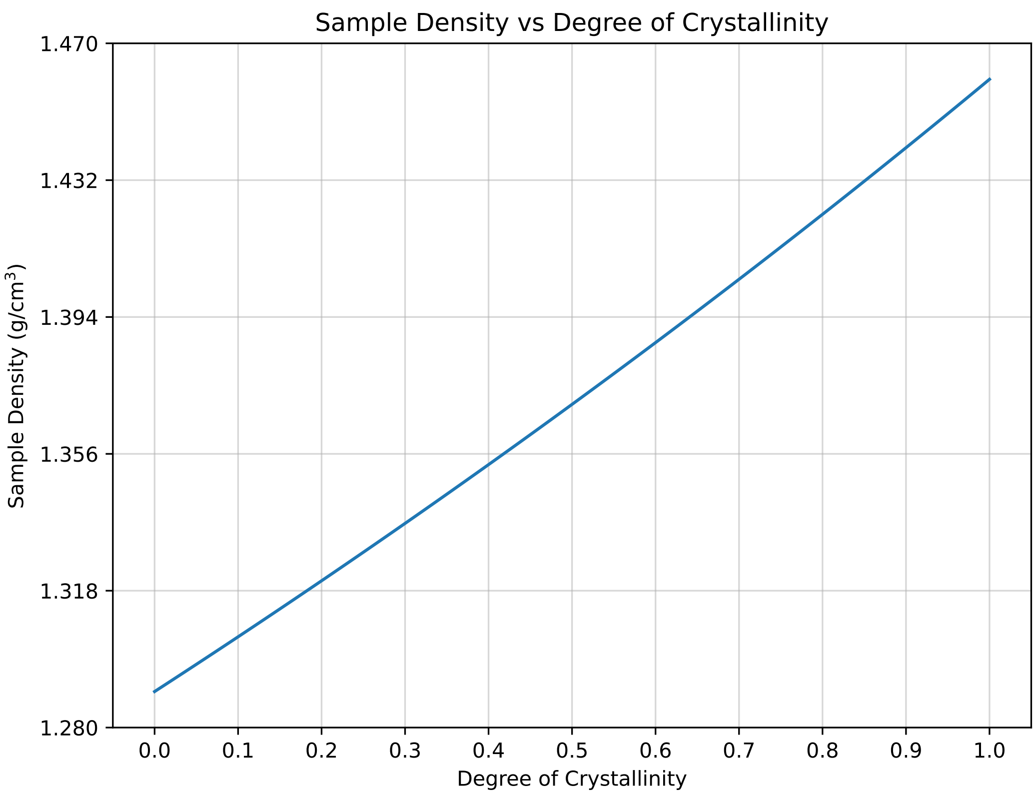
Now just plugging in the known densities and the new 1.38 sample density

$$\chi_s = \frac{1.46 \cdot (1.38 - 1.29)}{1.38 \cdot (1.46 - 1.29)} = \boxed{0.56}$$

As an interesting side note I wanted to plot the volume of a sample as a function fo the degree of crystallinity. I used the following formula

$$\rho_s = \frac{\rho_c \rho_a}{\rho_c + \chi_s \rho_a - \chi_s \rho_c}$$

Which looks like



This is actually quite an interesting trend. As the degree of crystallinity increases the density of the sample increases, but not linearly. Very cool.