Homework Questions for Unit 2

1. Give the correct term for the following definitions.
   a) A portion of a polymer chain that leaves the crystal lamellae and then returns into the organized crystal structure.
   b) The length of polymer that goes (one time) through the crystal lamellae.
   c) A polymer chain that starts in one lamellae, leaves that lamellae, and enters another crystal lamellae.

2. A chain is composed of 150 repeating links and each of the repeating links is the same length. Calculate the following parameters (to 3 significant figures) for the following scenarios.
   a) In poly(3-hexylthiophene) (P3HT) the scattering vector for the (010) plane is at ~16.5 nm⁻¹. Calculate the spacing between the crystal planes in this crystal direction to two significant figures.
   b) Which of the following does the (010) distance represent in P3HT?
      a. The alkyl-alkyl spacing distance.
      b. The distance along the polymer chain
      c. The distance from the sulfur in one thiophene repeat unit to the sulfur in the next thiophene repeat unit
      d. The π-π stacking distance
      e. None of the above

3. Based upon the data in the following plot answer, the following questions.

   ![Heat Flow vs Temperature Diagram]

   a) What is the melting temperature of P3HT?
      a. 190 °C
      b. 200 °C
      c. 210 °C
      d. 230 °C
      e. 250 °C
b) In the melting curve for P3EHT there are two peaks between 60 °C and 100 °C. What is a possible explanation for these two peaks?

a. There is poor instrument response for this particular sample.
b. The polymer melts, recrystallizes, and then melts again.
c. The P3EHT sample has a large dispersity value that causes the higher molecular weight chains to melt at a different temperature than the lower molecular weight chains.
d. The sample has a number of impurities in it, which cause the crystal to have a depressed melting temperature in some parts of the sample.
e. There are two different crystal structures (polymorphs) present in the sample.

4. For semicrystalline poly(ethylene oxide) (PEO), change in the enthalpy of fusion is 8.7 kJ mol\(^{-1}\) and the change in the entropy of fusion is 25.1 J K\(^{-1}\) mol\(^{-1}\).

a. Predict the melting temperature of an infinite crystal of PEO to 2 significant figures.
b. Use the result from part (a) and the fact that for a particular PEO crystal the value of \(\frac{2\gamma}{\Delta H_0} = 14 \times 10^{-10} m\) to estimate the lamellae thickness (to 2 significant figures) for this PEO crystal that melts at 66 °C.

5. It can be shown that the following equation is a solid prediction for the dependence of the melting temperature on the molecular weight of a polymer material.

\[
\Delta T_m = \frac{RT_m}{\Delta H_f} \frac{T_m^\infty}{2M_0} \frac{2M_0}{M_n}
\]

For poly(ethylene oxide) (PEO), predict what the molecular weight would need to be in order to bring a 1 K decrease in the melting temperature of an initial PEO sample that had a number-average molecular weight of 12 kg mol\(^{-1}\), if all other factors stayed the same.

a) 2.5 kg mol\(^{-1}\)
b) 5.5 kg mol\(^{-1}\)
c) 6.7 kg mol\(^{-1}\)
d) 8.6 kg mol\(^{-1}\)
e) 10.3 kg mol\(^{-1}\)

6. For each of the following two schematic depictions of liquid crystalline materials, please match one of the following choices to the appropriate picture.

Options

a) Smectic A
b) Smectic B
c) Smectic C
d) Nematic
e) Isotropic