POLYMER STRUCTURE, PHYSICAL PROPERTIES, AND CHARACTERIZATION

ChBE/ME/MSE 6768

Instructor: Karl I. Jacob (MSE/ME)
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Please communicate through Canvas mail.

Class Time: 2:00 pm – 3:15 pm, TR Mason 5134
Office Hours: After class, or per request.

Areas covered/Learning Objectives:

The course covers structure and the resulting properties of polymers, which includes: (1) geometrical aspects of single polymer chain (2) behavior of single chains, (3) behavior of polymer assemblies primarily in the solid state. Specifically:
Conformational aspects of polymer molecules – single chain and chain assemblies
Phenomenological and molecular models for rubber elasticity and viscoelasticity
Phenomenological and molecular models of phase transitions in bulk polymers
Foundations of structure property relations

Books:
Richard Stein and Joseph Powers: Topics in Polymer Physics (required)
Rubinstein & Colby: (required)

Reference Books:
Ward & Hadley: An introduction to mechanical properties of polymers
Treloar: Physics of rubber elasticity
Ferry: Viscoelastic properties of polymers
Aklonis, et al., An introduction to viscoelasticity in polymers
Schultz: Polymer material science
Notes are also available, papers will be provided periodically if needed

TA

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One hours: One hour per week, exact time to be decided. Additional help on request.

Topical outline:

Review of structure and physical states of polymers
Foundations of thermodynamics (will not be covered in class in detail)
Basics in statistical mechanics (part of which will be covered)

Conformations and spatial configurations – single chains
Polymer chain assembly
Rubber elasticity
Viscoelasticty
Aspects relating process and morphology
Kinetics and thermodynamics of melting, nucleation, and crystal growth
Phase separations and transitions in solutions (briefly) and bulk polymers
Anisotropy in polymers
Structure/mechanical property relations
Diffusion (only if time permits)
Experimental characterization (only if time permits)
Special topics (current topics of interest – if time permits)

Detailed Topics

(1) Review of Thermodynamics (Only an in-class overview)
Fist and second law of thermodynamics, reversible process, quasi-static state, entropy
Energies: internal energy, enthalpy, Helmholtz & Gibbs free energy
Thermodynamic parameters from energy
Maxwell's relations, Gibbs-Duhem equation
Application of thermodynamics in polymers
(Ref. Video; and posted notes, many basic books)

(2) Elements of statistical mechanics – Partial review
Ensemble: micro-canonical, canonical and grand canonical ensemble
Partition function
Thermodynamic parameters from partition function
(Ref. Video; posted notes; Appendix 2A Page 73- Stein)

(3) Conformation of single polymer chain
Chain spanning in one dimension, two, and three dimensions
Probability density function for the end-to-end distance
1, 2, and 3 degrees of freedom for chains
(Chapter 1, Rubinstein; Chapter 2 Stein; notes)

(4) Characterization of polymer chains
Self-avoiding random walk
Dependence of force on the end-to-end distance using statistical mechanics and thermodynamics for one, two and three dimensional chains (from notes)
Kuhn segments and Persistence length
Porod-Kartky chain and Kuhn chain
Radius of gyration
Chains subjected to large deformation
Non-linear behavior of chains & Langevin function
Chains in a solvent - pervaded volume
Conformation and dimension of real chains
Excluded volume
Fractals in polymer chain
Concept of tension blob and its applications in scaling theories

(Chapter 3, 2 Rubinstein; Chapter 2, Stein; notes)

(5) Connected polymer chains
Rubber elasticity
Response to 1-D, 2-D and 3-D stresses and deformation
Entanglement slippage, molecular sliding, conformational changes
Molecular and continuum theories
(Chapter 7, Stein; Chapter 7, Rubinstein, notes)

(6) Viscoelasticity
Molecular and continuum approach
Relaxation/retardation time
Maxwell, Kelvin, and complex models
Behavior under cyclic and shock loading
Laplace transform, and applications
(notes)

(7) Polymer morphology
Amorphous and crystalline structures
Composite model of polymers
Free volume and its significance
T_g and T_m
Degree of crystallinity, orientation function, pair-correlation function, etc
Melting, nucleation and crystal growth
Kinetics of crystal growth, effect of undercooling
Instabilities at the interface, effect of impurities
Polymer aging
(notes, and reference books)

(8) Anisotropy in polymers
Anisotropic molecular orientation and nucleation rate
Anisotropy and mechanical properties
Birefringence
Rigid rod polymers
(notes, and reference books)

(9) Mechanical properties*
Time dependent properties
Temperature dependent properties
Frequency dependent properties
Time-temperature-frequency superposition
Structure-property relationship
Polymer fracture
(notes)

(10) Optical properties*
Refractive index and birefringence
Lorentz-Lorenz equation
Clausius-Mossotti relation
Non-linear optics
(Chapter 4, Stein)

(11) Diffusion*
Self and mutual diffusion
Dependence of temperature
Dependence of structure
Anomalous diffusion
(12) Introduction to conductive polymers*
(13) Overview of experimental characterization*
(14) Current topics**
(15) Applications and practical examples**

* Depends on whether we have enough time to cover them. I was able to cover them only four times in the past.

"Notes" mentioned in the "Detailed Topics" are from a past student.

Item (1) will not be covered in the class in detail, that is assumed to be background information. I will post some videos on that and you are expected to study them (this is covered in MSE 6411). Part of Item (2), on partition function, will be covered in class.

This course particularly focuses on the quantitative aspects, so there will be math associated with it.

Grading policy:

There will be three tests and a final, each with a maximum of 25 points. Final exam will be comprehensive. All tests are closed book, closed notes tests, approximately one hour or one and 30 minutes (1). You are allowed to bring one 4x5 index card with whatever you want to write on both sides.

Periodic homework will be given, but will not be collected or graded, they are simply for preparing for the exams. This is the policy used by other MSE core courses.

For each test, the highest score will be scaled to 100, and the class average will be scaled to 80 points if it is below 80, other scores will be scaled using a linear scaling based the scaling factors used for the highest score and the class average.

There will be 5 extra points from unannounced five mini-quizzes, each with one point, out of which ½ point will be given for taking the quiz, and the other ½ point is given for the correct answer. Up to two missed quizzes with prior authorized legitimate excuses will be replaced with the average of the remaining three or quizzes.

If you miss a test for an authorized excuse, it will be replaced by the final exam score.

Letter Grades:

Final letter grade is based on the sum of all three testes, the final exam, and the extra points.

Scores with 90 points and above A

80 – 89	B
70 – 79	C
60 – 69	D
< 60	F

Tentative Test Schedule (subject to change, if needed)

Test 1 Feb 15
Test 2 March 12 (1)
Test 3 April 11

(1) Test 2 could also be a 24 hour take-home test, due 5:00 PM March 13. I will make that decision March 1, based on Test 1. One main constrain is the drop date.

Drop Date: March 13 4:00 PM

Spring Break March 18 – March 22

Last day of classes: April 23

Final Exam: Thursday, Apr 25, 2:40 – 4:10 PM.

This part particularly applies to MS students, as many of them, especially the self-financed MS students, are taking a heavy course load with five or six courses to finish the degree quickly. MSE 6768, which was an elective course, was re-designed for Ph.D. students as an MSE core course, and MSE PhD students are generally taking either two or at the most three courses this semester and have more time. This course is also a blend of different topics since it about a material, and cannot be made as structured as thermodynamics or crystallography. Historically, most students who were taking more than two or three courses had noticeable difficulties in keeping up with this course because of the lack of time. Thus, in order to protect your GPA and to avoid a lot of frustration, I would encourage to take this course when you are taking fewer courses. I have seen comments such as “didn’t have time to study”, “there is too much material”, etc. in CIOS opinion; I cannot do much about the level of material, and it takes more time to gain insight into various concepts behind the behavior of polymers. However, I have seen a few MS students doing extremely well.

We used to grade homework in the past, but students last year overwhelmingly recommended not to grade homework for accuracy, as in the other MSE core courses. Final grades based only on tests and quizzes is consistent with other MSE core courses, thus no projects or other work is needed for grades.

Problems solved in the class will not be posted in Canvas. HW solutions will be posted.

Depending on the circumstances, policies may change with adequate notice.