POLYMER STRUCTURE, PHYSICAL PROPERTIES, AND CHARACTERIZATION

ChBE/ME/MSE 6768

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Please communicate through Canvas mail.

Class Time: 2:00 pm - 3:15 pm TR Mason 5134

Areas covered:

Conformational aspects of polymer molecules – single chain and chain assemblies
Polymer synthesis
Phenomenological and molecular models in rubber elasticity and viscoelasticity
Phenomenological and molecular models of phase transitions in bulk polymers
Foundations of structure property relations in anisotropic bulk polymers

Topical outline:
Polymer Synthesis
Review of structure and physical states of polymers
Foundations of thermodynamics
Basics in statistical mechanics
Conformations and spatial configurations – single chains
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
Experimental characterization (if time permits)
Special topics (current topics of interest – if time permits)

Detailed Topics

(1) Introduction to polymers
General nomenclature
Classifications
Overview of polymer synthesis

(2) Thermodynamics (Review, only briefly covered, but handout may be given)
- 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

(3) Elements of statistical mechanics - Review
- Ensemble: micro-canonical, canonical and grand canonical ensemble
- Partition function
- Thermodynamic parameters from partition function

(4) 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

(5) 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
- 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

(6) 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

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

(8) 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

(9) Anisotropy in polymers
Anisotropic molecular orientation and nucleation rate
Anisotropy and mechanical properties
Birefringence
Rigid rod polymers

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

(11) Optical properties
Refractive index and birefringence
Lorentz-Lorenz equation
Clausius-Mossotti relation
Non-linear optics

(12) Diffusion
Self and mutual diffusion
Dependence of temperature
Dependence of structure
Anomalous diffusion

(13) Introduction to conductive polymers
(14) Overview of experimental characterization
(15) Current topics
(16) Applications and practical examples

Time permitting, some videos of experimental components will be added, such as: (1) viscosity measurements, (2) radius of gyration measurements, (3) birefringence measurements. We may or may not be able to cover all the topics given here.

Grading policy:

Homework will be given almost every Monday evening, due the next Monday evening. No extensions will be given, as we have to post the answers. Please make a copy of the Homework for your records, graded HW may not be returned. HW grading will be based on effort also, rather than the accuracy of the answers alone.

Mini quizzes will be given periodically (most probably at least every two weeks) on Thursdays (from 7:00 PM – 11:59 PM), which will be take home, open book, open notes, but no consultations with others. It will take much less time to do a quiz than the allotted hours, the longer duration is given to make it convenient for all. Upcoming quiz on a Thursday will be announced on the Tuesday of that week or earlier. No makeup quiz will be given, but two quizzes with the lowest points will not be counted for grade. There is no assurance that all quizzes will be of the same difficulty, some may be easier than others depending on the topic. Thus, logistically it is impossible to allow any compensation in case you happen to miss a quiz that is simpler than the other ones. HW and quizzes should serve as practice to prepare for the tests, so trying to do HW and quizzes well should help with the grade.

There will be two tests and one Final Exam that will be comprehensive; those will be in-class, closed book, closed notes exams. Some more complex formulas will be given.

MS students who are taking four or five courses in a semester may have to find enough time to keep up with the work, since the primary group of Ph.D. students, for whom this course was designed as a core course, may not be taking that many courses in one semester. As a graduate core course for MSE, this course might take more time from some if they don't have some background, although it is fairly straight forward to build that background with some effort.

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

Grading formula:

Homework:	5 %
Quizzes:	20%
Two Tests:	25% each
Finals:	25%

Test Schedule (subject to change, if needed)

Test 1 Feb 26

Test 2 April 6

Withdraw Deadline: March 15

Spring Break March 20 – 24

Last day of classes: April 25

Finals: Tuesday, May 2 2:40 PM - 5:30 PM (This is fixed)

Office Hours: Before or after the class, or by appointment

Required (or Strongly Recommended) Books:

Richard Stein and Joseph Powers: Topics in Polymer Physics, Imperial College Press, ISBN 1-86094-411-6

M. Rubinstein & R. Colby: Polymer physics, Oxford University Press, ISBN 0 19 852059 X

Reference Books

L. H. Sperling, Introduction to Physical Polymer Science, Wiley, ISBN: 9780471706069

F. W. Billmeyer, Textbook of Polymer Science, Wiley, ISBN-13: 978-0471031963

J. R. Fried, Polymer Science and Technology, Prentice-Hall, ISBN-13: 978-0-13-703955-5, 10: 0-13-703955-7

P. J. Flory, Principles of Polymer Chemistry, Cornell University Press, ISBN: 9780801401343, 0801401348

Ward & Hadley: An introduction to mechanical properties of polymers, Wiley, ISBN:0471938874
L. R. G. Treloar: The physics of rubber elasticity, Oxford University Press, ISBN: 9780198570271
J. D. Ferry: Viscoelastic properties of polymers, Wiley, ISBN 0-471-04894-1
M. T. Shaw, J. T. Aklonis, W. J. MacKnight, Introduction to polymer viscoelasticity, Wiley, ISBN 10: 0471018600 / ISBN 13: 9780471018605
J. M. Schultz: Polymer materials science, Prentice-Hall, ISBN: 9780136870388, 0136870384

(Bolded ones are more useful)

Notes are also available, papers may be provided periodically, when possible

TAs

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One more TBD