HANDBOOK

FOR

GRADUATE POLYMER PROGRAMS

Effective Fall 1999

Chemical Engineering
Materials Science and Engineering
Textile and Fiber Engineering

Polymer Education and Research Center
GEORGIA INSTITUTE OF TECHNOLOGY

GRADUATE POLYMER PROGRAMS
POLYMER EDUCATION AND RESEARCH CENTER
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INTRODUCTION

In response to the need for scientists and engineers with advanced training in polymers, Georgia Tech offers M.S. and Ph.D. programs in Polymers. These degrees are currently offered through three schools – Chemical Engineering, Materials Science and Engineering, and Textile & Fiber Engineering. The core requirements for the polymer degrees are the same in each school. This core is designed to provide a balanced treatment of chemistry, physics and engineering, with additional emphasis on advanced aspects of either chemistry or engineering of polymeric materials. In addition, the wide range of elective courses and research projects available permits the students to develop an in-depth knowledge of a particular area of polymer science or engineering. This combination of breadth and depth of study is vital to the successful performance of polymer science and engineering graduates.

Graduate research in polymers is also conducted by students majoring in the disciplines of Chemical, Electrical, Materials, Mechanical, and Textile & Fiber Engineering, as well as Chemistry and Physics.

ADMINISTRATION

The student's program is administered by the school of residence. The research and educational activities of the different schools in Polymers are coordinated through the Office of the Director of Polymer Education and Research Center (**PERC**).

Admissions Information

All correspondence regarding admission for graduate study in polymers should be addressed to the Director of PERC. The application should indicate the student's desired school of residence. These applications will be reviewed by a PERC committee and forwarded, with the appropriate recommendation, by the director of PERC to the school of residence desired by the applicant. Admission to the graduate degree programs requires the approval of PERC *and* the school of residence. **The final decisions regarding admission and financial aid are made by the school of residence.** Since the requirements for the polymer program are the same in each school, applicants should consider the research projects available in each school. If admission or financial aid is denied by the intended school of residence to an applicant who receives positive recommendation from PERC, consideration will be given by the other schools participating in the Graduate Polymer Degree Programs.

MASTER OF SCIENCE IN POLYMERS

Course descriptions for the referenced polymer courses appear in Appendix A.

Prerequisites

1. B.S. in science or engineering
2. *Demonstrated ability in heat/mass transfer*
3. *Demonstrated ability in fluid flow (Materials Science Track)
4. *Introductory material science*
5. Undergraduate chemistry, physics, and math
6. Demonstrated ability in physical and organic chemistry
7. ***Undergraduate polymer science and engineering** (Polymer Science and Engineering I, CHEM/CHE/ME/MSE/TFE 4775 and Polymer Science and Engineering II: Analysis, Processing & Laboratory, CHEM/CHE/ME/MSE/TFE 4776)*

* Students who do not possess these courses in their academic background can take them at Georgia Tech without receiving graduate credit.

Requirements

1. Curriculum:

A. Core courses (12-13 credit hours at 6000+ level) - these courses are the basis for the PhD qualifying examinations.

B. At least 9 additional semester credit hours of courses at the 4000 level or above **and approved by the school of residence.** Students in the Polymer Materials Science Track must take Polymer Characterization (TFE 6752) as one of these. For students in the Polymer Chemistry Track, six hours have to be chosen from one of the following pairs of courses.

Organic Chemistry (CHEM 6372, 6373)
Physical Chemistry (CHEM 6471 & 6482) / (CHEM 6471 & 6481) / (CHEM 6472 & 6491)
Analytical Chemistry I and II (CHEM 6271, 6272)
Biochemistry I and II (CHEM 6501, 6502)

Polymer Materials Science Track	h	Polymer Chemistry Track	h
CORE COURSES:		CORE COURSES:	
Polymer Structure, Physical Properties and Characterization (TFE 6768)	3	Preparation and Reaction of Polymers (TFE 6750)	3
Mechanics of Polymer Solids and Fluids (TFE 7771)	3	Physical Chemistry of Polymer Solutions (TFE 6751)	3
Physical Chemistry of Polymer Solutions (TFE 6751)	3	Polymer Characterization (TFE 6752)	4
Theoretical Chemistry of Polymers (TFE/Chem 6755)	3	Theoretical Chemistry of Polymers (TFE/Chem 6754)	3
REQUIRED NON-CORE COURSES:		REQUIRED NON-CORE COURSES:	
Polymer Characterization (TFE 6752)* *May be used as the substitute if TFE/Chem 6755 is not offered.	4	Organic Chemistry (CHEM 6372, 6373) or Physical Chemistry (CHEM 6471 & 6482) / (CHEM 6471 & 6481) / (CHEM 6472 & 6491) or Analytical Chemistry I and II (CHEM 6271, 6272) or Biochemistry I and II (CHEM 6501, 6502)	6
Electives: approved by School of residence at 4000 level or above	6	Electives: approved by School of residence at 4000 level or above	3
TOTALS:	22		22

2. Thesis (at least 12 semester credit hours)

Additional Graduation Requirements for M.S.

GPA Requirement	2.7
Total Credit Hours required (Min.)	30
Course Hours at 6000 level or higher (Min.)	12
Thesis (CHE/MSE/TFE 7000) Hours (Min.)	6
Max. Hours of Pass/Fail Coursework	3
Max. Transfer credit hours allowed	6
Maximum Time allowed for Degree Completion	6 years
Prior approval of program of study required	yes

First Year Suggested Course Sequence

Polymer Materials Science Track		**Polymer Chemistry Track**	
Fall	**Spring**	**Fall**	**Spring**
4775	6768	4775	6751
4776	TFE 6755/Chem 6754	4776	6752
7771	6751	6750	TFE 6755/Chem 6754
CHE/MSE/TFE 6790, if required		CHE/MSE/TFE 6790, if required	

PH.D. IN POLYMERS

Requirements for Admission to Candidacy

1. Normally an M.S. in science or engineering.
2. The equivalent of the core curriculum for M.S. in Polymers.
3. Passing the following three-part qualifying examinations.
4. Passing the Ph.D. proposal defense.
5. Filing with the Chair of the school of residence a formal statement naming the Thesis Advisor and the Thesis Reading Committee, and setting forth the topic selected for research. This statement should be followed by a written research proposal containing a statement of purpose and methods of investigation of the research, supported by literature references where appropriate. The student must circulate this statement to the faculty of the school of residence and the Polymer Faculty, along with an announcement of the time and place for the comprehensive oral examination.
6. The comprehensive oral examination must be passed. The subject matter is primarily based on, but not limited to, the applicant's research proposal. The examination is conducted by the Thesis Reading Committee and is open to the faculty and students of Georgia Tech.
7. Upon satisfactory completion of Items 1 through 5, the applicant's Thesis Advisor informs the School Chair who notifies the Dean of the Division of Graduate Studies and requests that the applicant be formally admitted to candidacy for the Ph.D. degree.

Ph.D Qualifying Examinations

PART I: Fundamentals Exam (Undergraduate level; based on Polymer Science & Engineering)	
PART II (Materials Science Track) Structure and Properties of Polymers (graduate level; based on 6768, 6751 and *prerequisites*)	**PART II (Chemistry Track)** Polymer Synthesis, Structure, & Analysis (graduate level; based on 6750, 6752, and *prerequisites*)
PART III (Materials Science Track) Advanced Aspects of Polymeric Materials, Processes and Properties (graduate level; based on 7771, TFE 6755/Chem 6754, and *prerequisites*)	**PART III (Chemistry Track)** Polymer Physical Chemistry (graduate level; based on 6751, TFE 6755/Chem 6754 and *prerequisites*)

- Each student will be allowed a maximum of two attempts to pass the qualifying examinations.
- All three parts must be successfully completed within the first 18 months of residence in the graduate polymer program.

Requirements for the Ph.D. Degree

1. Admission to candidacy
2. A 9-credit hour minor approved by the Ph.D. committee and the school of residence. Students in the Chemistry Track have to minor in Organic Chemistry or Physical Chemistry or Analytical Chemistry or Biochemistry.
3. Additional courses required by the Ph.D. committee
4. Completing the thesis research, preparation of a written dissertation and passing an oral examination on the thesis and the field in which it lies.

In addition, there are a number of requirements imposed by the Institute. These include:

GPA Requirement	3.0
Minimum time in PhD program at Georgia Tech	2 years
Minimum Full-time enrollment in residence	2 semesters
Time limit for completion of degree after admission to candidacy (Max)	5 years
Prior approval of dissertation topic	yes
Public defense of dissertation	yes

Appendix

POLYMER COURSE OUTLINES

Core Courses:

- Polymer Science and Engineering I: Formation and Properties, CHEM/CHE/ME/MSE/TFE 4775
- Polymer Science and Engineering II: Analysis, Processing and Laboratory, CHEM/CHE/ME/MSE/TFE 4776
- Preparation and Reactions of Polymers, CHE/CHEM/TFE 6750
- Physical Chemistry of Polymer Solutions, CHEM/CHE/MSE/TFE 6751
- Polymer Characterization, CHEM/CHE/MSE/TFE 6752
- Theoretical Chemistry of Polymers, CHE/MSE/TFE 6755/CHEM 6754
- Polymer Structure, Physical Properties and Characterization, CHE/ME/MSE/TFE 6768
- Mechanics of Polymer Solids and Fluids, CHE/ME/MSE/TFE 7771

Optional Courses:

- Natural Polymers, TFE 6301
- Materials in Environmentally Conscious Design & Manufacturing, AE/ECE/CEE/CHE/ISYE/MSE/ME/TFE 6759
- Introduction to Biomaterials, BMED/CHE/ME/TFE 6778
- Mathematical, Statistical and Computational Techniques in Materials Science, AE/CEE/CHE/ME/MSE/TFE 6790
- Structure-Property Relations in Materials, AE/CEE/CHE/ME/MSE/TFE 6791
- Thermodynamics and Kinetics of Microstructural Evolution, AE/CEE/CHE/ME/MSE/TFE 6792
- Advanced Principles of Fiber Formation & Structure, TFE 7100
- Damage, Failure & Durability of Composite Materials, AE/CHE/CEE/ESM/MSE/ME/TFE 7791
- Advanced Mechanics of Composites, AE/CEE/CHE/ESM/MSE/ME/TFE 7792
- Manufacturing of Composites, AE/CEE/CHE/ESM/MSE/ME/TFE 7793

POLYMER SCIENCE AND ENGINEERING I: FORMATION AND PROPERTIES CHEM/CHE/ME/MSE/TFE 4775

Course coordinators: Dr. A. S. Abhiraman (ChE)

Prerequisites:
1 year organic chemistry, I year physics and 1 semester physical chemistry or consent of instructor

Proposed Catalog Description:
An introduction to the chemistry, structure and formation of polymers, physical states and transitions, physical and mechanical properties of polymer fluids and solids.

Course Justification:

The learning objectives for the course are as follows:

1. Learn essential concepts of formation, physical chemistry, structure and properties of polymers
2. Provide a foundation for industrial practice in polymer science and engineering
3. Provide a foundation for graduate courses and research in polymer science and engineering

Students shall learn an integrated approach to polymer formation, structure and properties. The course materials have been taught highly successfully at Georgia Tech at least twice a year for 18+ years. Extensive resources have been developed at Georgia Tech to aid in problem solving and integration of all aspects of prerequisite materials in the teaching of Polymer Science. These include numerous solved problems and Web-based material. The latter permits conveying of not only static information (text, equations, graphs and figures) but also dynamic information and intuition-building and analytical skills (through problem solving).

Text: at the level of *Fundamental Principles of Polymeric Materials,* S.L. Rosen

Topical Outline

1. General Introduction
Polymers; bonding in polymers; conformation and configurations of polymers; branches and networks in polymers; transitions in polymers; molecular weight distributions and averages; solid state structure; plasticization.

2. Polymer Formation
Polymerization: kinetics of step growth; Polymerization: kinetics of chain growth; Free radical and ionic polymerizations; Stereoregular polymerization; Ring-opening polymerization; Copolymerization

3. Polymerization Processes
Bulk, Solution, Suspension, Emulsion Polymerization

4. Flow
Dilute solutions and intrinsic viscosity; effect of concentration, molecular weight, temperature and pressure on viscosity; models of non-Newtonian viscosity; measurement of viscosity; elasticity in polymer fluids

5. Mechanical Properties
Thermodynamics of deformation and rubber elasticity
Mechanical Properties (phenomenological): creep; stress relaxation; viscoelastic behavior and models; dynamic mechanical properties; time and temperature effects
Structure - property relations

6. Ultimate Properties; General Properties

POLYMER SCIENCE AND ENGINEERING II: ANALYSIS, PROCESSING AND LABORATORY, CHEM/CHE/ME/MSE/TFE 4776

Course coordinators: Dr. Haskell Beckham (TFE), Dr. John D. Muzzy (ChE)

Prerequisite/Corequisite: CHEM/CHE/ME/MSE/TFE 4775

Proposed Catalog Description:
Polymer fabrication processes and methods of characterization and identification of polymers are presented. Experiments in polymerization, processing, and property evaluation of polymers.

Course Justification:

The learning objectives for the course are as follows:

1. Learn essential concepts of physical chemistry, characterization, and processing of polymers
2. Provide a foundation for industrial practice in polymer science and engineering
3. Provide a foundation for graduate courses and research in polymer science and engineering

There is a tight integration between the materials in the companion course (CHEM/CHE/ME/MSE/TEX 4775), the lecture materials in the proposed course and the laboratory experiments. Further, the laboratory reports (executive report and technical report styles) are also graded for written communication and presentations of results for oral communication skills providing students with field relevant communication skills. The course materials have been taught highly successfully at Georgia Tech for 18+ years.

Text: at the level of *Principles of Polymer Systems,* F. Rodriguez

Topical Outline

1. Chapters 6: Methods of Molecular Weight Determination

colligative properties, osmometry, light scattering, dilute solution viscometry, size exclusion chromatography

2. Chapters 15: Methods of Polymer Analysis

thermal analysis, vibrational spectroscopy, NMR spectroscopy, x-ray diffraction, optical microscopy, electrical and dielectric properties

3. Chapter 12: Polymer Fabrication Processes

Extrusion, injection molding, blow molding, film blowing, and fiber spinning

Laboratories:

a. Polymer Synthesis: condensation polymerization
b. Polymer Synthesis: emulsion polymerization
c. Polymer Analysis: steady and dynamic shear flow rheology
d. Polymer Analysis: dilute solution viscometry, size exclusion chromatography
e. Polymer Analysis: infrared spectroscopy
f. Polymer Analysis: differential scanning calorimetry, thermogravimetric analysis
g. Polymer Analysis: x-ray diffraction
h. Polymer Analysis: optical microscopy
i. Polymer Analysis: electrical and dielectric properties
j. Polymer Processing: film extrusion
k. Polymer Processing: injection molding
l. Polymer Processing: fiber extrusion and capillary rheology
m. Polymer Properties: mechanical testing - tensile and impact testing

PREPARATION AND REACTIONS OF POLYMERS
ChE/CHEM/TFE 6750

Course coordinators: Dr. David Collard (Chemistry) and Dr. Malcolm Polk (TFE)

Prerequisites: CHEM/CHE/ME/MSE/TFE 4775, and Graduate standing or consent of instructor

Proposed Catalog Description:
A detailed treatment of the reactions involved in the synthesis of both man-made and natural polymers, including preparation and degradative reactions of polymer systems.

Course Justification:

The learning objectives for the course are as follows:

1. Learn essential concepts of formation and reactions of polymers focusing on the organic chemistry and mechanisms of reactions
2. Prepare students for research in the field of polymer synthesis

Students shall learn an integrated approach to polymer synthesis and reactions. The course lecture materials have been taught at Georgia Tech for a number of years.

Text: at the level of *Principles of Polymerization*, G. Odian and references from literature.

Topical Outline

1. Introduction to Polymer Synthesis

2. Step Growth Polymerization
   A. Heterocyclic Polymers (Odian)
   Polyimides (Handout): Mechanism, Kinetics, New Methods
   B. Polyurethanes (Odian)
   C. Phenol-Formaldehyde and Amine-Formaldehyde Polymers (Odian)
   D. Oxidative Coupling (Odian)
   E. Oxidative Coupling (Odian)
   F. Polyethers, Polysulfides, and Related Polymers (Odian)
   G. Ring-Opening Polymerization (Odian)
   H. Starburst Dendrimers (Handout)
   I. Inorganic Polymers (Odian)
   Polysiloxanes, Polysilanes, and Phosphonitrilic Polymers

3. Chain Growth Polymerization
   A. Free Radical Polymerization
   Living Free Radical Polymerization (Literature)
   New Methods for Controlling Structure and Stereochemistry (Literature)
   B. Living Cationic Polymerizations (Literature)
   C. Anionic Polymerization
   Traditional Methods (Odian)
   Group Transfer Polymerization (Odian)
   D. Coordination Polymerization
   E. New Methods for Ziegler-Natta Polymerization (Literature)
   F. Metathesis Polymerization (Odian)
   G. Metallocene Complexes of Group 4 Elements in the Polymerization of Monoolefins (Literature)

4. Reactions in Polymer Systems (Odian)

5. General Mechanisms of Degradation and their Effect on Structure (Literature)

Polymer Structure - Property Relationships; General Degradation Mechanisms - Thermal, Thermo-oxidative, photo-oxidative, chemical; General Mechanisms of Stabilization

PHYSICAL CHEMISTRY OF POLYMER SOLUTIONS
CHEM/CHE/MSE/TFE 6751

Course coordinators: Dr. S. Michielsen (TFE), Dr. S. Kumar (TFE), Dr. A. S. Abhiraman (ChE)

Prerequisites: 1 semester physical chemistry and CHEM/CHE/ME/MSE/TFE 4775, 4777 or equivalent or consent of instructor

Proposed Catalog Description:
Study of polymer solutions, polymer miscibility, adsorptions, sorptions, plasticization, molecular weights, molecular weight distributions, and interfacial phenomena using thermodynamics and statistical mechanics.

Course Justification:

The learning objectives for the course are as follows:

1. Learn essential concepts of the physical chemistry vis-a-vis properties of polymer solutions.
2. Provide a foundation for accessing advanced literature in polymer solution theory.
3. Provide a foundation for advanced graduate research in polymer solutions and phase behavior.

Students shall learn an integrated approach to polymer solutions from dilute to concentrated, from small molecule solvents to polymeric ones as well as characterization methods that rely on polymer solutions. The course materials have been annually taught highly successfully at Georgia Tech for more than 7 years. Extensive printed classroom notes have been prepared so that the student can concentrate on the concepts rather than the mathematics. Industry was polled in developing this course to determine the most important concepts required by industry today.

Text: at the level of *Macromolecules in Solution* by H. Morawetz

Topical Outline

1. Review emphasizing solutions: Thermodynamics, Statistical thermodynamics
Review zeroth – third laws of thermodynamics. Phase equilibria. Introduction to quantum mechanics. Statistical thermodynamics

2. Conformations and spatial configurations of polymer chains
Configuration statistics of chain molecules. Scaling Concepts in Polymer Solutions (including static & dynamic flexibility). Rotational Isomeric State theory

3. Dilute polymer solutions: viscosity, light scattering, colligative properties.
Ideal solutions, lattice model, Flory-Huggins, phase behavior, osmotic pressure, Light Scattering – Classical & Dynamic, Neutron & X-ray scattering, Frictional Properties – Diffusion of polymers in solution, Viscosity

4. Concentrated solutions, plasticization, miscibility
Excluded volume, rigid rod polymers, plasticizers, polymer-polymer phase behavior, Frictional Properties – Reptation

5. Polymers at Interfaces
Loops, trains, and tails. Mushrooms, pancakes and brushes.

6. Analytical applications of polymer solutions
GPC with multidetectors, analyzing block copolymers, analyzing polymer blends

7. Industrial applications of polymer solutions
Wet, dry and flash spinning of fibers, polymer coatings.

8. Student papers

POLYMER CHARACTERIZATION
CHEM/CHE/MSE/TFE 6752

Course coordinators: Dr. Haskell Beckham

Prerequisites:
1 semester physical chemistry and CHEM/CHE/ME/MSE/TFE 4775 or 4777 or equivalent, or consent of instructor

Proposed Catalog Description:
This course introduces the student to surface, near-surface and structural methods of polymer characterization. Specialized techniques critical to physical structure are emphasized.

Course Justification:

The learning objectives for the course are:
1. Learn essential concepts of techniques for structural characterization of polymers
2. Learn techniques for characterization of polymer surfaces
3. Gain proficiency in use of characterization equipment
4. Prepare students for research in the field of polymer process-structure-property relationships

The course lecture materials have been taught at Georgia Tech for 9 years. A drawback of the current course is that there is no accompanying laboratory. The semester course corrects that deficiency.

Text: No suitable text exists. A "notebook" has been developed as instructor prepared handouts. This will be supplemented with papers from literature.

Topical Outline
1. Introduction
2. Thermal Analysis
   DSC/DTA; TGA; TMA; DMTA (DMS)
3. Diffraction and Scattering
   Wide Angle X-ray Diffraction (WAXD)
   Small Angle X-ray & Neutron Scattering (SAXS, SANS)
   Small Angle Light Scattering (SALS)
4. Fourier Transform IR (FTIR) & Raman Spectroscopy
5. Nuclear Magnetic Resonance (NMR)
   Solution & Solid State NMR
6. Electron Microscopy
   SEM; Electron Diffraction (SAED) and Imaging (TEM); Energy Dispersive X–ray Analysis (EDS/EDAX)
7. Surface Characterization of Solid Polymers:
   X-ray Photoelectric Spectroscopy (XPS/ESCA); Auger Electron Spectroscopy (AES); Secondary Ion Mass Spectroscopy (SIMS)
8. Scanning Probe Microscopy Techniques:
   STM, AFM
9. Laboratories in:
   i. DSC/DTA/TGA
   ii. DMS
   iii. WAXD: Identification, Crystallinity, Crystal Size
   iv. WAXD: Orientation; SAXS
   v. WAXD, SAXS: photography/imaging techniques
   vi. FTIR: Identification, Phase Analysis
   vii. Raman: Identification, Phase Analysis
   viii. FTIR/Raman: Polarized – Structural characterization
   ix. NMR: Solution state – identification, stereochemistry
   x. NMR: Solid state – identification, molecular mobility
   xi. SEM: topography
   xii. STM/AFM: topography

THEORETICAL CHEMISTRY OF POLYMERS
CHE/MSE/TFE 6755/ CHEM 6754

Course coordinator: Dr. Rigoberto Hernandez (Chem)

Prerequisites: CHEM/CHE/MSE/TFE 6751, CHEM 6422 or consent of instructor

Proposed Catalog Description:
Thermodynamics and microscopic dynamics of polymers. Fundamental concepts, including scaling concepts, governing anisotropy of polarizability, phase transitions, morphology, time-dependent correlations, etc. are discussed.

Course Justification:

1. Learn the foundation of continuum and statistical mechanics, and specially as it pertains to polymers.
2. Learn the use of scaling laws to describe material properties near phase transitions
3. Learn the algorithms and theory behind computer models of polymerization

A characterization of the dynamics of polymers is generally not discussed within physical chemistry courses as the material is often reserved for specialists. This course will integrate this discussion with that of the usual equilibrium models in order to bring in modern perspectives. This will prepare students to address non-equilibrium properties of polymers. Computer visualization will be used to represent the morphologies described by the theory and/or observed by experiment.

Text:
The course can use a combination of the textbooks: "Introduction to Modern Statistical Mechanics," by David Chandler (Oxford, New York, 1982), and "The Theory of Polymer Dynamics," by Masao Doi and Sam F. Edwards (Oxford, New York, 1986). Book chapters from these books will be referred to below as SM and TPD, respectively. These will be supplemented with papers from literature.

Topical Outline

Material to be covered	**Description**
Introduction & Preliminaries	Motivation & classical mechanics
SM 3, Statistical Mechanics	General ensembles: fundamentals & thermodynamic connections
SM 5, Phase Transitions & Morphology	Ising systems, mean field & renormalization group theory
TPD 2, Static Properties of Polymers	Equilibrium Models, Excluded Volume
Molecular Dynamics	Ab initio quantum force and semi-empirical force fields
SM 8, Non-Equilibrium Systems	Fluctuation-dissipation theorem, and Langevin equations
TPD 3, Dissipative Dynamics of Polymers	Smoluchowski Equation, etc.
TPD 4, Dynamics of Dilute Polymers	Rouse & Zimm Models, dynamical scaling, calculating observables
TPD 5, Many Chain Systems	Scaling Theory
TPD 6, Dynamics in Amorphous Systems	Reptation & Length Fluctuations
Polymer Dynamics	Correlation Functions & Measurement
Special Topics	e.g., Reactions, birefringence, DLS, etc.

POLYMER STRUCTURE, PHYSICAL PROPERTIES AND CHARACTERIZATION CHE/ME/MSE/TFE 6768

Course coordinator: Dr. A. S. Abhiraman (ChE)

Prerequisites:
CHEM/CHE/ME/MSE/TFE 4776, and Graduate standing or consent of instructor

Proposed Catalog Description:
Formulations and analysis of molecular and phenomenological models of elastic and viscoelastic behavior, development and description of structure, and fundamental aspects of structure-property relations in the solid state of polymers.

Course Justification:

The learning objectives for the course are as follows:

1. Learn phenomenological and molecular models of phase transitions in bulk polymers
2. Learn molecular and phenomenological models of rubber elasticity and viscoelasticity
3. Learn the foundations of structure-property relations in anisotropic bulk polymers
4. Prepare students for research in the field of polymer process-structure-property relationships

The course will demonstrate the importance of sound principles in physics and chemistry to model polymers through examples of proper approaches as well as some (widely practiced) mistakes in the field. It will make extensive use of current literature and show connections between phenomenological and molecular approaches. The course materials have been refined and taught at Georgia Tech for 15+ years as parts of two courses.

Text: No suitable single text exists. The books listed below will be used as references. These will be supplemented with papers from literature.
Ward & Hadley: *An introduction to the mechanical properties of solid polymers*; Bueche: *Physical properties of polymers*; Treloar: *Physics of rubber elasticity*; Flory: *Statistical mechanics of chain molecules*; Ferry: *Viscoelastic properties of polymers*; Aklonis, et al.: *An introduction to viscoelasticity in polymers*; Schultz: *Polymer materials science*.

Topical Outline

1. Structure and states
   A review of structure and physical states of polymers

2. Conformations and spatial configurations: Principles and models
   Review of equilibrium and statistical thermodynamics; partition functions for polymer chains; freely orienting chain analogs for flexible polymer chains

3. Rubber elasticity: Advanced Models
   1-, 2-, and 3-D models of elasticity in isolated chains; single chain to network extensions; non-ideal rubbers

4. Viscoelasticity
   a. linear viscoelasticity and superposition
   b. time-temperature superposition of modulus and viscosity functions
   c. experiments in viscoelasticity
   d. viscoelastic transitions and structure
   e. molecular origins of viscoelastic behavior of polymers
   f. nonlinear models

5. Fundamental Aspects of Process-Morphology Relations
   a. thermodynamics of melting/crystallization
   b. kinetics and modes of crystal growth
   c. energetics of crystal nucleation phenomena

d. process - morphology relations (phase separating transitions in solutions and bulk polymers; flow and orientation; crystallization in anisotropic polymers; stress field and crystallization; crystallization in copolymers and blends)

6. Principles and techniques for analysis of anisotropy in polymers
   principles governing birefringence, sonic pulse propagation and infra-red dichroism

7. Structure-mechanical property relations
   two- and three- phase models of polymer morphology and physical properties

8. Viscosity and Diffusion in Polymers
   segmental jumps, viscosity and diffusion in polymers

9. Special Topics
   students' research reports on current literature

MECHANICS OF POLYMER SOLIDS AND FLUIDS
CHE/ME/MSE/TFE 7771

Course coordinators: Dr. A.S. Abhiraman (ChE), Dr. Karl Jacob (TFE)

Prerequisites:
Undergraduate training in solid and fluid mechanics and CHE/TFE 4776; 6768; or consent of instructor

Proposed Catalog Description:
Continuum mechanics of solids and fluids; deformation, yield, fracture and fatigue of anisotropic polymers; experimental response and constitutive models of non-Newtonian viscous/viscoelastic polymer fluids.

Course Justification:

The learning objectives for the course are as follows:

1. Learn the foundations of mechanics of large deformations in solids and non-Newtonian flow of fluids
2. Learn the foundations in mechanics for developing structure-property relations in anisotropic bulk polymers
3. Learn phenomenological continuum constitutive models in polymer fluids and solids
4. Learn the distinctions between polymers and small molecular materials in critical mechanical phenomena (yield, fracture, fatigue, etc.)

We have taken the approach of integrating the mechanics of solids and fluids in a single course It is rigorous and yet explicitly cognizant of the essential empiricism in modeling the behavior of polymer solids and fluids. The "continuity" of solid- and fluid-like states of polymers can be best appreciated through this approach. The course materials have been refined and taught at Georgia Tech for 15+ years as parts of two courses. Students have historically found the materials in these courses difficult to assimilate. The problem is often compounded by the absence of a uniform notation in books and papers. However, this subject is one that will benefit from the semester-long coverage.

Text: Reference Texts: Ward*: Mechanical properties of solid polymers*; Bird et al.: *Dynamics of polymeric liquids - Fluid dynamics*; these will be supplemented with papers from literature.

Topical Outline

1. Analysis of stresses in a medium
2. Analysis of deformation in a medium

a. finite strain

b. small strain

3. Linear and non-linear elasticity

Constitutive relations for large elastic deformations; strain energy function and its relationship to stress tensor for large deformations; Relationships between continuum and molecular models of rubber elasticity

4. Symmetry relations and material constants

Covering operations for material symmetry; common symmetries in polymeric materials

5. Anisotropic mechanical behavior of polymers

Consequences of local and global symmetries in polymer morphology

6. Yield behavior

Classical theories of yielding; Hill's yield criterion; brittle and ductile failures in polymers; molecular theories of yielding and cold drawing

7. Breaking phenomena

Classical theories of fracture; critical strain energy release rates in polymer fracture; crazing in polymers; molecular theories of fracture in polymers

8. Fatigue

Static and dynamic fatigue in polymers; empirical formulations; rate theories

9. Framework of fluid dynamics

Introduction to viscous Newtonian and non-Newtonian fluids

10. Material functions for polymer fluids

The concept of simple fluids; viscometric flows of simple fluids

11. Flow phenomena in polymer fluids

Experimental aspects of viscometric functions; flow phenomena on viscoelastic polymer fluids

12. Generalized Newtonian fluids

Ellis, power-law and other models; determination of shear viscosity function through capillary flow

13. Linear viscoelastic fluids

Simple and generalized Maxwell fluids; frame invariance requirements for constitutive equations

14. Co-deformational and corotational models

Maxwell-Oldroyd and Maxwell-Jaumann fluids; various modifications

15. Dimensional analysis vis-a-vis non-Newtonian fluids
    Constitutive equations vis-a-vis dimensionless groups; applications to non-Newtonian viscous and viscoelastic fluids