

Structure and Dynamics of Polymers (E068900)

Course size (nominal values; actual values may depend on programme)

Credits 6.0 Study time 180 h Contact hrs 60.0 h

Course offerings and teaching methods in academic year 2018-2019

A (semester 1)	Dutch	practicum	25.0 h
		excursion	5.0 h
		guided self-study	30.0 h
B (semester 1)	English	excursion	5.0 h
		lecture	30.0 h
		practicum	25.0 h

Lecturers in academic year 2018-2019

De Clerck, Karen	TW11	lecturer-in-charge
D'hooge, Dagmar	TW11	co-lecturer

Offered in the following programmes in 2018-2019

	crdts	offering
Bridging Programme Master of Science in Sustainable Materials Engineering	6	B
Bridging Programme Master of Science in Materials Engineering	6	A
Master of Science in Electromechanical Engineering (main subject Control Engineering and Automation)	6	B
Master of Science in Electromechanical Engineering (main subject Electrical Power Engineering)	6	B
Master of Science in Electromechanical Engineering (main subject Maritime Engineering)	6	B
Master of Science in Electromechanical Engineering (main subject Mechanical Construction)	6	B
Master of Science in Electromechanical Engineering (main subject Mechanical Energy Engineering)	6	B
Master of Science in Chemical Engineering	6	B
Master of Science in Sustainable Materials Engineering	6	B
Master of Science in Materials Engineering	6	A
Master of Science in Chemical Engineering	6	A

Teaching languages

Dutch, English

Keywords

Polymer crystallinity, melting behavior, orientation, polymer (thermo)dynamics in solution/melt, rheology, viscoelasticity, phase separation, structure-property relations for polymers, chain dimensions, Flory-Huggins interaction parameter, polymer physics, Poiseuille flow, mechanical properties, molecular interaction, simulation of polymer flow in basic geometries

Position of the course

Detailed study of the fundamentals of the structure and the (thermo)dynamics of polymers and polymer solutions (including melts), considering different length scales and covering both detailed experimental characterization and modeling tools. With respect to the study of the structure of polymers, aspects such as semi-crystallinity, crystalline state, melting behavior, orientation, and structure-property relations are discussed. With respect to the study of the (thermo)dynamics of polymers, aspects such as segment/solvent interactions, diffusivity and basic behavior under flow

conditions (melt and solution) are discussed. Important aspects are also highlighted by case studies.

Contents

- Introduction to polymer physics and different polymer length scales
 - Nanoscale: mathematical description root mean square end-to-end distance and radius of gyration
 - Ideal case: freely-jointed/Gaussian chains
 - Extension 1: bond angle and short-range restrictions
 - Extension 2: long-range steric interactions, highlighting the necessity to study thermodynamical properties
 - Extension 3: coarsened grain molecular dynamics: Lennard Jones and Coulomb contribution
 - Micro- and macroscale
 - Overview on the main polymer properties (e.g. average molar mass, friction, elasticity, crystallinity, viscoelasticity...) that are covered later on in the course in detail
 - Relevance in a broader context of polymer processing: basic insights
- Thermodynamical properties
 - Simplified case of ideal solution: main theory
 - Gibbs free energy of mixing
 - Importance of temperature and composition
 - Extension to polymer solutions: Flory-Huggins theory
 - Gibbs free energy of mixing
 - Chemical potential of solvent and polymer
 - Special case of diluted solutions: concept of theta conditions
 - Comparison with solubility parameter approach
 - Phase separation: concept of replacement chemical potential: spinodal line and coexistence curve
- Number average molar mass as basic polymer property
 - Definition
 - Relation with Flory-Huggins theory and parameters under diluted conditions
 - Membrane osmometry
 - Vapour osmometry
- Frictional properties
 - Intrinsic viscosity
 - Definition
 - Mathematical descriptions: Huggins equation, Kramer equation, and Mark-Houwink-Sakurada equation
 - Extension toward diffusivity of monomer/solvent/polymer mixtures
 - Cohen and Turnbull basic equation
 - Vrentas and Duda free volume theory: detailed description
- Phase structure and morphology
 - Amorphous state
 - Glass transition
 - Factors influencing the glass transition temperature
 - Crystalline state
 - Determination of crystal structure
 - Polymer single-crystals
 - Semi-crystalline polymers
 - Liquid-crystalline polymers
 - Defects
 - Crystallization kinetics and molecular mechanisms
 - Melting: differential scanning calorimetry (DSC) and factors influencing the melting temperature
 - Relation between glass transition and melting temperature
- Elastic deformation
 - Stress and strain: general aspects
 - Deformation of polymer chains and polymer crystal moduli
- Yield and crazing
 - Yield: general aspects
 - Yield criteria: Tresca, Von Mises and pressure dependent yield behavior
 - Deformation mechanism
 - Crazing: craze yielding and criteria
- Fracture and toughening
 - Fundamentals of fracture: theoretical tensile strength and molecular failure process
 - Mechanics of fracture: brittle and ductile fracture
 - Fracture phenomena
 - Toughened polymers
- Viscoelastic properties and rheological behavior
 - Basic models based on constant strains or stresses
 - Limitations of models (e.g. Maxwell and Voigt model)

- Extension to Boltzmann superposition principle
- Dynamic testing to assess key polymer properties
 - Frequency dependency of viscoelastic behavior
 - Transitions and polymer structure
 - Time-temperature superposition
 - Effect of entanglements
 - Main rheological measuring techniques
- Fundamentals of polymer melt flow
 - Chain flexibility and diffusivity in the melt
 - Conservation laws to describe transport of isothermal polymer melts: mass and momentum
 - Effect of shear rate on main rheological properties: shear thinning
 - Flow pattern of polymer melts in basic geometries: Poiseuille flow
 - Extension for multicomponent systems
 - Extension for reactive polymer flow: basic principles
 - Indication of importance for polymer processing at macro/industrial scale, including design of die (basic principles)
- Case studies
 - Electrospinning: principle and description of chain dimensions
 - Construction of drug-polymer thermodynamical phase diagram
 - Performance of polymer solar cells
 - Simplified description of polymer processing units
 - combined drag and pressure flow for extrusion
 - non-parallel plate drag flow for knife coating applications
 - Determination of virial equation of a standard polymer
 - Crystalline state for fibers with DSC and XRD
 - Toughening via polymer composites
 - Evaluation of polymer-solvent affinity and intrinsic viscosity of polyelectrolytes

Initial competences

This course builds on basic knowledge of organic chemistry and polymers

Final competences

- 1 Knowledge: describing and defining the following concepts: amorphous and semi-crystalline polymers; crystalline state/melting behavior; orientation; structure-property relations; polymers in solution; polymer rheology; multicomponent systems; diffusion of polymer molecules
- 2 Skills: being capable to relate the polymer microstructure to the polymer properties, understanding the relevance of the Flory-Huggins parameter in describing molecular interactions, understanding the effect of process conditions (such as temperature and pressure) on diffusivity of polymers in melt and solution, being able to relate the polymer structure and polymer dynamics to the basic steps of polymer processing, being capable to describe isothermal polymer flow in basic geometries using the conservation law of mass and momentum, recognizing the relevance of different length scales and molecular interactions.
- 3 Attitude: being capable to solve independently and in group problems in the field of structure and dynamics of polymers

Conditions for credit contract

Access to this course unit via a credit contract is determined after successful competences assessment

Conditions for exam contract

This course unit cannot be taken via an exam contract

Teaching methods

Guided self-study, excursion, lecture, practicum

Extra information on the teaching methods

Classroom lectures, practical sessions, company visit

Learning materials and price

Handbook: Introduction to Polymers, Robert J. Young and Peter A. Lovell, CRC Press, ISBN: 978-0-8493-3929-5.
Slides and handouts.

References

see course material

Course content-related study coaching

Evaluation methods

end-of-term evaluation

Examination methods in case of periodic evaluation during the first examination period

Written examination, oral examination

Examination methods in case of periodic evaluation during the second examination period

Written examination, oral examination

Examination methods in case of permanent evaluation

Assignment

Possibilities of retake in case of permanent evaluation

not applicable

Extra information on the examination methods

Periodic evaluation: oral closed-book exam, written preparation; excercises: written examen (closed-book)

Non-periodic evaluation: report or presentation on work practicals

Calculation of the examination mark

Periodic evaluation: 16/20 with 14 points (theory) and 2 points (excercises)

Non-periodic evaluation: 4/20