



5.00 credits

45.0 h + 15.0 h

Q1

Teacher(s)	Demoustier Sophie ;Jonas Alain (coordinator) ;Van Ruymbeke Evelyne ;
Language :	English
Place of the course	Louvain-la-Neuve
Main themes	<p>Two main themes will be discussed :</p> <ul style="list-style-type: none"> • The first theme deals with the physics of polymer materials, and presents the main properties of these materials while establishing in a formal way the relationship with the physical characteristics of the chains at the molecular scale. • The second theme is an introduction to the chemistry of these materials, which presents the main classes of polymerization reactions, and relates the resulting molecular structure and the properties of the materials.
Learning outcomes	<p>At the end of this learning unit, the student is able to :</p> <p>Contribution of the course to the program objectives</p> <p>With respect to the program of the Master in Chemical and Materials Science Engineering, this course contributes to the development and the acquisition of the following learning outcomes:</p> <p>LO 1.1. Identify and use concepts, laws, and reasoning related to a problem of limited complexity.</p> <p>LO 1.2. Identify and use modelling and computational tools to solve this problem.</p> <p>Specific learning outcomes of the course</p> <p>At the end of this course, students will be able to :</p> <ul style="list-style-type: none"> • Determine the parameters required to model a macromolecular chain by a freely-jointed chain model, a wormlike model, or a model of rotational isomeric states; explain using statistical physics how these parameters vary with molar mass, temperature or chemical nature of the repeat unit; • Use statistical physics and a freely-jointed chain model to compute the retraction force resulting from increasing the distance between the chain ends of a polymer chain; explain the main characteristics of this force; derive the stress/strain curve of a rubber band, starting from equations describing the statistical behavior of its chain segments, and from the environmental constraints of the experiment; • Describe phenomenologically the glass transition of polymers and the relaxation phenomena associated with it, on the basis of the notion of free volume. Use this approach to explain how the glass transition is sensitive to the temperature and the rate of measurement; • Describe the morphology of a semicrystalline polymer at different scales, and draw a scheme of this morphology; state how this morphology controls the properties of the material; enumerate the parameters which control the melting temperature of a polymer; derive the equation relating this melting temperature and the lamellar thickness; list the main experimental facts that must be included in any theory of polymer crystallization, and present briefly some kinetic theories able to explain these facts; • Derive the principle of time/temperature equivalence for the elastic modulus of polymers, and describe its practical consequences for the use of such materials; quantify these effects by the Williams-Landel-Ferry equation; • Define and explain different concepts related to the molecular structure of polymers (topology, repeating units linking, configurational structures, average molecular weights and dispersity) ; • Describe and explain the mechanisms of the main methods of polymer synthesis : chain-reaction polymerizations (free radical polymerization, controlled radical polymerizations, coordinative polymerization and ionic polymerizations) and step-reaction polymerization; list and give the impact of the main parameters that govern the kinetics for each polymerization method ; establish relations between the polymerization method and the resulting molecular characteristics (architecture of the chain, regioselectivity, tacticity, molecular weight distribution, ...) of the polymer chains; • Describe the structure of the main types of copolymers (random, alternating, graft and block copolymers) and discuss about the synthesis method and conditions in which each type of copolymer can be obtained; predict and justify the global composition of random copolymers based on the reactivity ratios of a given couple of monomers ; • Select and describe an appropriated polymerization method of a given monomer in order to obtain a polymer with specific molecular characteristics ; • Describe different polymerization processes (bulk polymerization, polymerization in solution, in suspension, in emulsion and interfacial polymerization) and state the advantages and drawbacks of each process.

Evaluation methods	<p>Written exam at the end of the course, comprising small exercises and questions on the main concepts of the course. Part of the final grade will consist of a continuous evaluation led over the semester for (some parts of) the course. This part of the grade will be used in each exam session; the continuous evaluation cannot be presented again.</p> <p>Final grade: let x_1 be the grade on 20 obtained for the continuous evaluation in the part of A. Jonas, let x_2 be the grade on 20 for the exam on the part of A. Jonas, let y be the grade on 20 obtained for the exam on the part of E. Van Ruymbeke, and let z be the grade on 20 obtained for the exam on the part of S. Demoustier, then the final grade on 20 will be $\max(x_2/20 \cdot 8, (x_1/20 \cdot 4 + x_2/20 \cdot 4)) + y/20 \cdot 3 + z/20 \cdot 9$, rounded to the closest integer, except if the grade is between 9 and 10 in which case it is rounded to the lowest nearest integer.</p>
Teaching methods	<p>The course mixes formal presentations by the teachers with exercises done by the students. These exercises serve either to raise questions, or to solve issues. The course will be in flipped classroom format for some parts.</p>
Content	<ol style="list-style-type: none"> 1. Physics part : <ol style="list-style-type: none"> 1.1. Main characteristics of macromolecular chains 1.2. Elasticity of macromolecules, and elasticity of elastomer materials 1.3. The glassy state and the glass transition of polymer materials 1.4. Viscoelasticity and rheology of polymers 1.5. Semicrystalline polymers and polymer crystallization 2. Chemistry part : <ol style="list-style-type: none"> 2.1. Step polymerization 2.2. Free radical polymerization 2.3. Coordinative polymerization 2.4. Copolymerization 2.5. Ionic polymerization 2.6. Controlled radical polymerization
Inline resources	<p>Moodle web site of the course.</p> <p>For the physics part: lecture notes and video sequences are available on the Moodle website.</p> <p>For the chemistry part: copies of slides are available on the Moodle website.</p>
Bibliography	<p>L'ouvrage de référence suivant peut être utile, mais n'est pas obligatoire / the following textbook might be useful, but is not compulsory:</p> <p>Paul C. Hiemenz & Timothy P. Lodge, Polymer Chemistry, 2nd edition, CRC Press: Boca Raton, 2007.</p>
Other infos	<p>This course requires to have a knowledge of thermodynamics, statistical physics and organic chemistry.</p>
Faculty or entity in charge	FYKI

Programmes containing this learning unit (UE)				
Program title	Acronym	Credits	Prerequisite	Learning outcomes
Master [120] in Chemical and Materials Engineering	KIMA2M	5		
Master [120] in Biomedical Engineering	GBIO2M	5		
Master [120] in Chemistry and Bioindustries	BIRC2M	5		