lmapr2019

2023

Polymer Science and Engineering

5.00 credits	45.0 h + 15.0 h	Q1

Teacher(s)	Demoustier Sophie ;Jonas Alain ;Van Ruymbeke Evelyne ;
Language :	English > French-friendly
Place of the course	Louvain-la-Neuve
Main themes	Two main themes will be discussed : • 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	**At the end of this learning unit, the student is able to :** **Contribution of the course to the program objectives** 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: LO 1.1.Identify and use concepts, laws, and reasoning related to a problem of limited complexity. LO 1.2. Identify and use modelling and computational tools to solve this problem. **Specific learning outcomes of the course** At the end of this course, students will be able to : 1 • 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	In the first session, the students will pass an oral exam in front of the three teachers, during which they will present their approach to a general issue or problem proposed during the course by the teachers, or proposed by themselves; they will be asked questions on the concepts of the course linked to the solution of this issue or problem. Mentoring sessions on the problems will be organized during the course. Additionally to this oral exam, a continuous evaluation of the progresses of the students will be organized during the course. Let x_1 be the grade (over 20) received for the continuous evaluation of the part delivered by A. Jonas (physics), x_2 the same for the part delivered by E. Van Ruymbeke (rheology), x_3 the same for the part delivered by S. Demoustier (chemistry), and y the grade obtained for the final exam (over 20), then the final note (over 20) will be max(y, $y/2$ + ($0.5*x_1$ + $0.1*x_2$ + $0.4*x_3$)/2), roundest to the nearest integer except if it is between 9 and 10 in which case it is rounded to the lower integer.
	In the second session, the exam will be a closed-book written exam comprising small exercises and the reproduction of the reasoning on some concepts of the course. The final note will be computed by a formula identical to the one used in the first session. The continuous part of the evaluation cannot be passed again.
	For students taking only LMAPR2019A, the formula is adapted to neutralize the missing x_3 value.
	For the continuous evaluation and the preparation of the problem for the oral exam, a critical use of generative artificial intelligences is accepted. Artificial intelligence will not be authorized for the other parts of the evaluation, unless stated otherwise.
	If, for one part of the continous evaluation process, a student does not abide to the methodological instructions defined on moodle by the teachers, including the use of online resources and student collaborations, all the continuous evaluation will obtain a grade of 0.
Teaching methods	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.
Content	1. Physics part : 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 : 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	Moodle web site of the course. For the physics part: lecture notes and video sequences are available on the Moodle website. For the chemistry part: copies of slides are available on the Moodle website.
Bibliography	L'ouvrage de référence suivant peut être utile, mais n'est pas obligatoire / the following textbook might be useful, but is not compulsory: Paul C. Hiemenz & Timothy P. Lodge, Polymer Chemistry, 2nd edition, CRC Press:Boca Raton, 2007.
Other infos	This course requires to have a knowledge of thermodynamics, statistical physics and organic chemistry.
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		🔍