Course Package

Materials Science

Name module	Materials Science - 1B
Educational programme	MSc Chemical Engineering
Period	Second block of first semester (block 1B)
Study load	15 ECTS
Coordinator	C. C. Diepenmaat

Materials Science			
block 1A	**block 1B**	**block 2A**	**block 2B**
	AMM Organic Materials Science 193700030 (5 EC)		
	Advanced Molecular Separations 201300049 (5 EC)		
	Electives: (1 of the 5 EC or 2 of the 2,5 EC)		
	Electrochemistry Fundamentals and Techn. - 201800014 (5 EC)		
	Advanced Ceramics - 193737010 (5 EC)		
	Ion Transport in Fluids - 201800327 (2,5 EC)		
	Statistical Thermo - 201800332 (2,5 EC)		

Required preliminary knowledge: To do this course package you need to have completed at least the first two years of your BSc. This is an advanced-level graduate course, thus basic knowledge of Organic Chemistry and Polymer Science taught in the bachelor curriculum is a prerequisite and will be assumed. Basic knowledge of Catalysis and Kinetic, Basics of Physical Chemistry, Organic and Inorganic Chemistry, Material Science and Molecular Biology, Basic knowledge of Thermodynamics, Advanced knowledge of Characterization Method, Chemistry & Technology of Organic Materials, basic knowledge of chemical engineering or advanced technology. If you choose to do Statistical Thermo and Molecular Modelling you need to have a knowledge of Statistics and Matlab.

* Statistical Thermo is a required course if you'd like to do Molecular Modelling. For the students who are applying for a full academic year.

Please note: choose 5 ECTS worth of electives for the normal workload.

193700030 - AMM Organic Materials Science

Organic materials feature enormous variations in their physical properties as a result of the tremendous wealth of the different possible existing molecular structures of carbon based compounds. The consequence of this plethora of properties is that function and use of organic materials can be tailored by controlling molecular structure virtually at will by using modern synthetic approaches, allowing one to realize many advanced applications, which belonged to the realm of phantasy just a few decades ago. In this lecture molecular structure-property relations will be discussed for the different types of (advanced) synthetic and natural (macromolecular)organic materials, including man-made polymers, liquid crystals, carbon allotropes (nanotubes,fullerenes and graphenes), dendrimers, nucleic acids, proteins and polysaccharides.Materials selection diagrams will be used to compare organic, inorganic, metallic and other materials,focusing on mechanical properties. Similarities and differences on the basis of molecular/atomicstructures among the different classes of materials will be elucidated. Approaches will be treated which allow materials engineers to quantitatively estimate physical properties based on the molecular structure (by the so-called group contribution techniques). Effects of processing on structure (texture) and hence on properties will be demonstrated. A description and comparison of the major classes of the most frequently used industrial polymers for different function will complement this course. This is an advanced level graduate course, thus basic knowledge of organic chemistry, materials science and polymer science taught in the bachelor curriculum is aprerequisite and will be assumed.

- Introduction (course overview, keywords of knowledge required, exam expectations,recommended literature) (lecture notes)
- Overview of structures of the major classes of organic materials (polymers, liquidcrystals, carbon allotropes (nanotubes, fullerenes and graphenes), dendrimers, nucleicacids, proteins and polysaccharides (lecture notes)
- Materials selection diagrams, organic, metallic and ceramic materials contrasts and similarities (M.F. Ashby, Materials Selection in Mechanical Design)
- Carbon allotropes as molecular building blocks (fullerenes, carbon nanotubes and graphenes)
- Dendrimers and hyperbranched structures- Elastomers, rubber and hydrogels
- Liquid crystals as functional materials
- Relationships between polymer structure and properties Part I: main chain effects(H.R.Allcock et al., Contemporary Polymer Chemistry, 3rd Ed. Chapter 22)
- Relationships between polymer structure and properties Part II: side chain effects(H.R.Allcock et al., Contemporary Polymer Chemistry, 3rd Ed. Chapter 22)
- Group contribution techniques for estimating properties based on molecular structure (D.W. van Krevelen, Properties of Polymers); Calculation examples
- Industrial polymers (H. Ulrich, Introduction to Industrial Polymers)
- Influence of processing, texture and anisotropy Part I.(I.M.Ward, Editor, Structure and Properties of Oriented Polymers)
- Influence of processing, texture and anisotropy Part II.(I.M.Ward, Editor, Structure and Properties of Oriented Polymers)
- Electroactive organic materials
- Photonic organic materials (solar cells, light emitting organics, photochromism, photonicband gap materials)- Natural organic engineering materials

201300049 - Advanced Molecular Separations

In Advanced Molecular Separations, separation technology is discussed starting from molecular properties up to full scale processes. The focus is on choosing a separation technology for given molecular properties, and the subsequent molecular design of more advanced separation technologies. For two separation technologies, fluid separations and membrane technology, the molecular design and separation process are treated in much greater detail, including a discussion on useful models to describe thermodynamics and mass transfer. The course will include two tests, one on fluid separations and one on barrier separations, but will also include two assignments on selecting the right separation technology for a given separation case.

Electives: (1 of the 5 EC or 2 of the 2,5 EC)

201800014 - Electrochemistry Fundamentals and Techn.

Electrochemistry deals with chemical changes caused by electrical energy. Electrochemical processes are highly used in various branches of the industry and have an ever-increasing impact in our everyday life. Think, for example, of consumer products like batteries (e.g., in notebooks, smart phones or cars), electrosynthesis (or electrochemical conversion), electroplating or production of hydrogen by electrolysis of water. With more electrical energy being produced from solar and wind energy, a sustainable electricity supply will rely on storage. Additionally, noting that fossil-based fuels will be phased out, production of chemicals and fuels by alternative means will be required. Here, electrochemistry offers sustainable solutions, but further improvement of current and emerging electrochemical conversion techniques is certainly needed.

The course consists of three parts:

- Lectures and tutorials deal with the fundamental principles of electrochemistry, including thermodynamics, double layer structure, electrode reactions, and mass transport in electrochemical systems. Main experimental techniques for the study of electrode reactions will also be discussed.
- The students (e.g. in groups of 4 students) will carry out two practical (experimental) projects and prepare reports discussing and interpreting the obtained results. The report will be structured in the form of a research article. This allows students to familiarize with learned fundamentals and to apply theoretical concepts to laboratory experiments and case studies in electrochemistry.
- Topical lectures (1x or 2x, if time allows) will expose students to relevant electrochemical research activities carried out by researchers within our faculty/in the Netherlands.

193737010 - Advanced Ceramics

Several steps in the fabrication process of ceramic materials are discussed and the importance to understand the effects of processing variables on the evolution of microstructural parameters is emphasized. Basic processes are treated like powder preparation, powder treatments (milling and mixing), forming into a green shape and sintering. Basic phenomena are e.g.: particle size, interaction between particles, nucleation/crystallization, solid state reactions and transport phenomena in solid state systems.

The objective in materials process engineering is to find relations between (desired) materials properties and relevant microstructural parameters on one side and to understand which process parameter changes a certain microstructural parameter on the other hand.

The basic processes and phenomena, as indicated above, will be treated in lecture notes and tutorials. An important aspect of the course is the in-depth treatment by the student of a specific part of a ceramic fabrication process. This project will be presented by means of a literature and a presentation essay.

201800327 - Ion Transport in Fluids

Starting from the electrochemical potential, the Nernst-Planck equation will be derived and then used to understand the relative contribution of electromigration and diffusion. The validity of assuming electroneutrality in a fluid phase is discussed and investigated by introduction of the Poisson equation. In double layers and interfaces, the potential and ion distributions can be studied further. Next, the effect of fluid transport on ion transport and vice-versa will be introduced by combining the Poisson-Nernst-Planck equations with the Navier-Stokes equations. From this, electrokinetic mechanisms such as electro-osmosis can be derived. Finally, the use of these frameworks in relevant industrial processess where ion transport plays a crucial role is explored.

201800332 - Statistical Thermo

Statistical thermodynamics provides the fundamental concepts that allow us to predict macroscopic thermodynamic variables and materials properties. Via many applied examples from organic and inorganic material science, you will get a microscopic understanding of entropy, you learn how to work within different ensembles, you will learn how to work with partition functions as well as out-of-equilibrium thermodynamics.