GHENT UNIVERSITY

# Course Specifications

Valid in the academic year 2018-2019

## Materials Science Thermodynamics (E066190)

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 | seminar | 20.0 h |
| | | guided self-study | 15.0 h |
| | | seminar: practical PC room classes | 20.0 h |
| | | practicum | 5.0 h |
| B (semester 1) | English | practicum | 5.0 h |
| | | lecture | 15.0 h |
| | | seminar: practical PC room classes | 20.0 h |
| | | seminar | 20.0 h |

Lecturers in academic year 2018-2019

| | | |
|---|---|---|
| De Graeve, Iris | TW11 | lecturer-in-charge |

| 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 Sustainable Materials Engineering | 6 | B |
| Master of Science in Materials Engineering | 6 | A |

### Teaching languages

Dutch, English

### Keywords

Electrochemistry, thermodynamics, potential functions, metallic solutions, phase diagrams, slag systems, thermodynamic databases.

### Position of the course

This course is split in two related parts.
One part deals with Electrochemistry. It contains the fundamental basic concepts.This part of the course forms the base for the later courses on corosion and surface technology.
The second part of the course deals with the fundamental aspects concerning the thermodynamics of metallurgical processes (pyro, hydro and electrometallurgy) with an emphasis on the applications. The course forms the basis for later courses on extractive metallurgy.

### Contents

For the part on Electrochemistry:

- Fundamental principles and concepts:
  - Electrodes and electrochemical reactions, oxidation and reduction,
  - Definition of equilibrium cell potential, standard electrode potential, Nernst equation, activity versus concentration, reference electrodes, galvanic cell, Pourbaix diagram,
  - Flux equation: diffusion, migration and convection of ions in solution,
  - Concepts and models of the double layer,
  - Kinetics and mechanisms of electrode processes: rate sconstants, electron charge transfer and current density, Butler-Volmer equation, kinetic factors (charge

transfer coefficient and exchange current density), polarization curve, overpotential, influence of mass transfer (concepts limiting current and mixed kinetics).
- Methods:
  - Global methods: polarization curves or linear sweep voltammetry (LSV), cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS),
  - Local methods: micro-cell, scanning vibrating electrode technique (SVET), scanning elektrochemical microscopy (EIS),...
- Applications and examples:
  - Examples of corrosion,
  - Production of aluminium,
  - Batteries and fuel cells.

For the part on Thermodynamics:
- General definitions used in thermodynamics, the first, second and third law of thermodynamics
- Thermodynamic functions: Equilibrium constant and thermodynamic functions, Heat content and enthalpy of formation, Temperature dependence of the reaction enthalpy, Entropy, Gibbs free enthalpy and reaction equilibrium
- Phase equilibrium: Two phase equilibrium, Law of Clausius Clapeyron, Multicomponent systems, Gibbs phase rule, Ellingham diagrams (with nomographic scales and limitations)
- Metallic solutions: Partial molar quantities and integral molar quantities, The chemical potential, Ideal solutions and Raoult's law, Standard states and activities, Non-ideal solutions and activity coefficients, Non ideal solutions and Henry's law, relation between ideal Raoult behavior and ideal Henry behavior, Transformation between different standard states, Integration of Gibbs Duhem's equation for binary solutions, Thermodynamic functions of mixing, Exces quantities, "Regular solutions", Sieverts' law
- Thermodynamic treatment of metallurgical processes

Initial competences

basic knowledge chemistry (bachelor)

Final competences

1 Understanding of the concepts of electrochemical processes; thermodynamics; phase equilibria and kinetics
2 Application of the concepts of electrochemical processes; thermodynamics; phase equilibria and kinetics
3 Use and interpretation of thermodynamic databases and knowledge of their limitations
4 Experimental skills on electrochemical processes
5 Experimental skills on pyrometallurgical processes

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, lecture, practicum, seminar, seminar: practical PC room classes

Learning materials and price

Syllabus "Material Science Thermodynamics".
Lecture slides.

References

- GASKELL D.R., 'Introduction to the thermodynamics of materials', Taylor&Francis, 2003
- BRETT C.M.A.,BRETT A.M.O., ‘Electrochemistry: Principles, Methods and Applications’, Oxford Science Publications, 1993

Course content-related study coaching

In person: after the lectures + after electronic appointment.

Evaluation methods

end-of-term evaluation and continuous assessment

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

Participation, skills test, report

Possibilities of retake  in case of permanent evaluation

examination during the second examination period is possible in modified form

Extra information on the examination methods

During examination period: oral closed-book exam, written preparation + written closed-book exam.
During semester: graded lab sessions and reports + assessment of PC-exercise.

Calculation of the examination mark

For both parts (thermodynamics and electrochemistry) a score is obtained during the semester and one during the examination period. If a student does not take part in 1/more evalutaion parts, it is no longer possible to pass the entire course unit. The final score is calculated based on the four subscores obtained. A score of 7/20 is needed for every subscore to be able to pass this course. If this is not the case and the final score is 10 or more out of 20, this will be reduced to the highest non-passing mark (9/20).