GHENT UNIVERSITY

Course Specifications

Valid in the academic year 2022-2023

Materials Science Thermodynamics (E066190)

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

Credits 6.0 **Study time 180 h** **Contact hrs** 60.0h

Course offerings and teaching methods in academic year 2022-2023

A (semester 1)	Dutch	Gent	seminar	15.0h
			seminar: practical PC room classes	15.0h
			practicum	5.0h
B (semester 1)	English	Gent	seminar: practical PC room classes	15.0h
			seminar	15.0h
			lecture	25.0h
			practicum	5.0h

Lecturers in academic year 2022-2023

Bellemans, Inge	TW11	lecturer-in-charge

Offered in the following programmes in 2022-2023	**crdts**	**offering**
Bridging Programme Master of Science in Materials Engineering	6	A
Bridging Programme Master of Science in Sustainable Materials Engineering	6	B
International Master of Science in Sustainable and Innovative Natural Resource Management	6	B
Master of Science in Materials Engineering	6	A
Master of Science in Sustainable Materials Engineering	6	B

Teaching languages

English, Dutch

Keywords

Thermodynamics, potential functions, metallic solutions, phase diagrams, non-ideality, slag systems, thermodynamic databases, electrochemistry, electrochemical kinetics and the influencing factors.

Position of the course

This course deals with the fundamental aspects concerning the thermodynamics of metallurgical processes (pyro, hydro and electrometallurgy) with an emphasis on phase diagrams (pyro and hydro), Ellingham diagrams, Pourbaix diagrams, activities, non-idealities and Butler-Volmer kinetics of electrochemical processes (Evans diagrams) and their applications. The course forms the basis for later courses on extractive pyro-, hydro- and electrometallurgy.

Contents

- General definitions used in thermodynamics, the first, second and third law of thermodynamics with also a link to electrochemistry: electrodes and electrochemical reactions, oxidation and reduction, definition of equilibrium potential, Nernst equation, flux equation
- 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, Phase diagrams (binary and ternary), Ellingham diagrams (with nomographic scales and limitations), Pourbaix diagrams

- 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
- Kinetics and mechanisms of electrode reactions: rate constants, 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).

Initial competences

basic knowledge chemistry (bachelor)

Final competences

1 Understanding of the concepts of thermodynamics, phase equilibria and electrochemical processes
2 Application of the concepts of thermodynamics, phase equilibria and electrochemical processes
3 Use and interpretation of thermodynamic software and knowledge of itslimitations
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

Practicum, Seminar, Lecture, Seminar: practical pc room classes

Extra information on the teaching methods

Due to COVID-19, the teaching methods may vary if the situation requires this.

Learning materials and price

Syllabus and lecture slides (both no charge).

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.

Assessment moments

end-of-term and continuous assessment

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

Written examination

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

Written examination

Examination methods in case of permanent assessment

Skills test, Report, Participation

Possibilities of retake in case of permanent assessment

examination during the second examination period is possible in modified form

Extra information on the examination methods

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

Calculation of the examination mark

The score for this course has three components: practical sessions (during semester; accounts for 2/20 of the total mark), PC-exercises (during semester; accounts for 6/20 of the total mark) and examination (accounts for 12/20 of the total mark). If a student does not take part in 1/more

evaluation parts, it is no longer possible to pass the entire course unit. The final score is calculated based on the three 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).
With regard to the examination during the second examination period, transfer of subscores is possible, as long as the student obtained at least 10/20 for this subscore.