

Thermodynamics for complex systems

ECTS	Course (h)
3	18

Mention du master transmettant la fiche UE :	Chimie et Sciences des Matériaux
Composante de gestion de l'UE :	Faculté des Sciences – Département de Chimie
Responsable de l'UE :	O. DEZELLUS
Statut du responsable :	MCF

REQUIREMENTS

A good knowledge of reading and using equilibrium phase diagrams for binary systems.
Basic notions in thermochemistry: classical thermodynamic functions (G, H, S), chemical potentials.
General knowledge in materials science: crystallography, metallurgy, solid state physics...

PROGRAM

Program in two parts:

- The first one is devoted to ternary phase diagram and their use for synthesis of materials and especially crystal growth. The different kind of sections (isothermal and isoplethic) as well as projections are detailed.
- The second part deals with computational thermodynamic. First, the principles of Calphad method are shortly introduced: modeling of thermodynamic functions using experimental data and constitution of databases. Next, the use of databases with ThermoCalc software to illustrate the use of computational thermodynamic as a support for materials synthesis and development.

SPECIFIC SKILLS

Learning outcomes are the followings:

- Understanding and reading of ternary phase diagrams
- Evaluation of experimental data for determination of thermodynamic characteristics
- Understanding different models of phases
- Define a calculation strategy well suited to solve a materials science problem
- Using ThermoCalc software as a beginner