Course code	Course title
METRO 004	Numerical Modelling

Course summary

The aim of the course is to present a review of mathematical modelling of phase change problems and describes fundamentals of numerical methods used for simulating solidification problems, with a focus on solidification coupled to convective flow too.

Lectures list

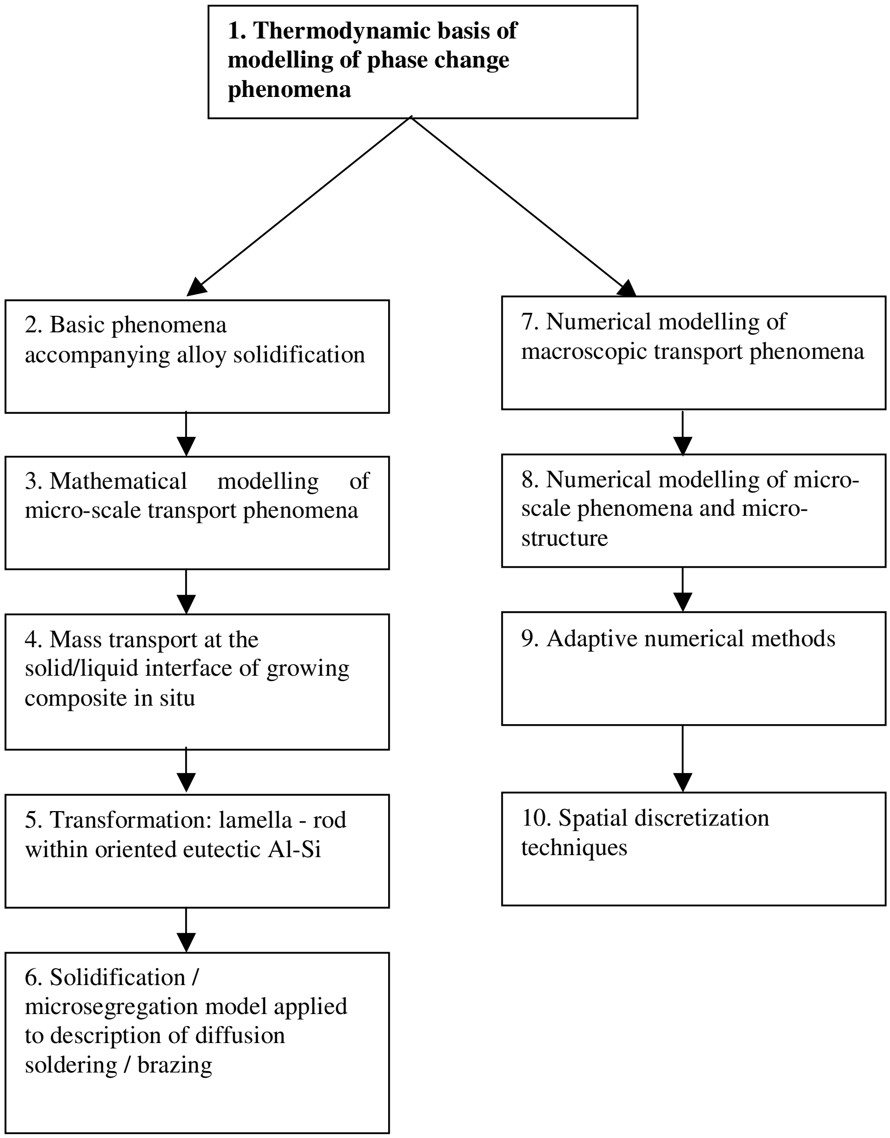
n.	Title	Summary	Lecturer	Duration
1	Thermodynamic basis of modelling of phase change phenomena	**Thermodynamic basis of modelling of phase change phenomena**: *equilibrium phase transitions (equilibrium solidification), solidification temperature depression, the lever rule, eutectic temperature, cooling curves, solubility, insolubility and partial solubility of components in binary systems, peritectic phase diagrams, phase diagrams for binary systems containing compounds, ternary diagrams.*	Dyja Robert	1h 37’
2.	Basic phenomena accompanying alloy solidification	**Basic phenomena accompanying alloy solidification**: *surface energy and surface tension, surface energy and impurity segregation at interfaces, influence of curvature on the solidification temperature and solubility, nucleation (homogeneous and heterogeneous),size distribution of nuclei, rate of nucleation, non-equilibrium phenomena (stability of the solid/liquid interface - dendrites)* The notions as surface energy are introduced and its role in nucleation of the new phase, eg. formation of solid grains from the melt, are discussed. Moreover, it is shown how surface energy contributes to instability of the liquid/solid interface. As a result of this instability formation of complex, dendritic microstructure of the solid phase is initialised. Finally interaction between a mould and the solidifying liquid is presented.	Furmański Piotr	50’
3.	Mathematical modeling of micro-scale transport phenomena	**Mathematical modeling of micro-scale transport phenomena**: *basic thermodynamic relationships, modeling of nucleation, modeling of diffusion process in phases and solid/liquid interface, modeling of heat conduction in phases and solid/liquid interface, modeling of heat and species transfer by convection in the liquid phase, modeling of free surface phenomena* Solidification process in pure metals and alloys considered analytically and numerically are discussed on the scale of crystal grains attached to a mould wall or floating in the melt. Various phenomena embracing the nucleation process as well as heat transfer are taken into account. For clarity of presentation the lecture is essentially limited to pure metals and dilute binary alloys, in which one of the components can be treated as a solute and the other as a solvent. However, the presentation can be relatively easy extended to multi-component alloys and non-dilute cases.	Furmański Piotr	35’

4.	Mass transport at the solid/liquid interface of growing composite in situ	**Solidification of eutectics is described**. Modification of the Jackson-Hunt theory dealing with the solute micro-field within diffusion layer of the liquid.	Wołczyński Waldemar	10’
5.	Transformation: lamella - rod within oriented eutectic Al-Si	**The criterion predicting whether lamellae or rods will be formed** for an eutectic alloy is given. It is concluded that criterion is able rather to characterise a given phase diagram and not to describe the transformation: lamella – rod. The threshold growth rate for transformation is determined by using the so-called new criterion together with mechanical equilibrium varying with solidification rate.	Wołczyński Waldemar	16’
6.	Solidification / microsegregation model applied to description of diffusion soldering / brazing	**Model for solidification / microsegregation** and its application to diffusion soldering / brazing is given. New model for general description of solidification / microsegregation is postulated.	Wołczyński Waldemar	10’
7.	Numerical modelling of macroscopic transport phenomena	**Lecture describes fundamentals of numerical modelling** of solidification problems, using fixed grid and two-domain approaches. Basics of discretization methods and boundary condition settings are given. Finite Element method is explained in details. Integration of the Enthalpy Method to phase change problems is introduced. The lecture concludes with few examples of calculations for alloys solidification.	Banaszek Jerzy	1h 15’
8.	Numerical modelling of micro-scale phenomena and micro-structure	**Interface tracking methods and interface non-tracking techniques** are shown. The details of cellular automata and phase field methods are presented and their advantages and drawbacks are highlighted. The lecture starts with a short introduction to the subject. Than, two classifications of the micro-structure modelling methods are introduced. The details of the models are presented for the utilized two types of cellular automata method. Also, the phase field method is shown as an alternative approach. Finally it is shown how to combine two techniques discussed. The lecture is closed by giving some keypoints and sources on which the lecture was prepared.	Wodo Olga	1h 28’
9.	Adaptive numerical methods	**The problem of adaptive solutions is discussed.** It concerns limited accuracy of the finite element method and its convergence rate. The lecture embraces such notions as global measure of the error (like the *infinity norm,* the *L-one* and *L-two norm*s, etc.) error estimators used to find an estimate of the unknown error in terms of the numerical solution itself and of the problem data, mesh refinements and adaptive solutions, adaptive strategies (like, *fixed threshold strategy, fixed fraction strategy, fixed contribution strategy and error equidistribution strategy)*. The methods discussed are illustrated by examples of solidification of a casting.	Nagórka Arkadiusz	1h 20’

10.	Spatial discretization techniques	**The finite difference, the finite element and the finite volume methods** are discussed in order to explain the meaning of spatial discretization techniques nowadays commonly used in solving real word problems. These methods are introduced using an illustrative example of the Dirichlet problem of the Poisson equation. The model problem can describe many steady-state problems such as conductive heat transfer, diffusion, electrostatics, etc..	Nagórka Arkadiusz	1h 27’
				9h 08’

Lectures prerequisites chart

There are two groups of lectures, mathematical description of the solidification problems and numerical implementations. Student can choose one of the paths, or follow all lectures according to their numbering.



Each arrow means a prerequisite.