Course code	Course title
METRO 004	Numerical Modelling

Prerequisites

The course is addressed to advanced students and scientists from engineering and applied sciences, as well as to physicists and mathematicians interested in the fundamentals of the field. There are two groups of lectures, mathematical description of the solidification problems and numerical implementations. For better understanding the first part some basic course of thermodynamics and course of calculus is necessary.

Training Objectives

The course should help students to understand principles of numerical modelling of casting problems, to gain knowledge and allow critical assessment of different numerical approaches, physical models used in the field. Even if some parts of the course may appear difficult, she/he should realise complexity of the problem and possibility for extending her/his knowledge by more profound studies.

Summary

Thermodynamic basis of modelling of phase change phenomena. The lecture explains such terms as 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.

Basic phenomena accompanying alloy solidification. There is introduction given to 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.

Mathematical modeling of micro-scale transport phenomena. The basic thermodynamic relationships are given, 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.

Solidification of eutectics is described. Modifications of the Jackson-Hunt theory dealing with the solute micro-field within diffusion layer of the liquid are described in details.

The criterion predicting whether lamellae or rods formation. The lecture describes criteria for lamellae or rod transition for an eutectic alloy. 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.

Model for solidification / microsegregation
The lecture describes theoretical basis for modelling solidification with microsegragation and its application to diffusion soldering / brazing is given. New model for general description of solidification / microsegregation is postulated.

Fundamentals of numerical modelling. Numerical modelling of flow problems with solidification is introduced, fixed grid and two-domain approaches are discussed. 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.

Interface tracking methods and interface non-tracking techniques. 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.

Adaptive numerical methods. The lecture 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.

The finite difference, the finite element and the finite volume methods. The three fundamental 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..