MTE 687: Microstructure Evolution of Materials

Prerequisites

None

Course Description

The course will cover the fundamentals and state-of-the-art techniques used in mathematical modeling and computer simulation of microstructure formation and control during the solidification and solid state transformations of materials. The concepts and methodologies covered in this course for net-shape casting and ingot remelt processes can be applied, with some modifications, to model other materials processes such as welding, deposition, and heat treatment processes. Modeling and simulation of microstructure evolution requires complex multi-scale computational areas, from computational fluid dynamics macroscopic modeling through mesoscopic to microscopic modeling, as well as strategies to link various length-scales emerged in modeling of microstructural evolution.

Note: Students should have knowledge of physical metallurgy and materials thermodynamics. Students should be familiar with differential and integral calculus and should have some knowledge of statistics.

Objectives

- To gain an insight in the theoretical concepts applicable to the development of materials structure models at various length scales (macro-, micro-, meso and nano-scale)
- To develop the skills in formulating and simulating the materials-related problems such as phase transformations, microstructure evolution during processing and material properties, and
- To develop an appreciation for the powerful role of numerical simulation in the design and development of advanced materials and processes.
- Provide training to (i) use a dedicated microstructure simulation software (ii) interpret and analyze the simulation results for optimum performance.

Outline of Topics

1. Length-Scales and Generations of Modeling Methodologies for Predicting the Evolution of the Solidification Structure

1.2 Length Scales in Modeling of the Solidification Structures

1.3 Generations of Modeling Techniques, Modeling Capabilities and Limitations

2. Deterministic Macro-Modeling: Transport of Energy, Momentum, Species, Mass, and Hydrodynamics During the Solidification Processes

2.1 A Macroscopic Model for Calculating Energy, Momentum, Mass and Species Transport

2.2 Methods for Coupling HT-SK Models

3. Deterministic Micro-Modeling: Mathematical Models for Evolution of Dendritic and Eutectic Phases

4. Stochastic/Mesoscopic Modeling of Microtructures

5. Solute Transport Effects on Microtructure

6. Micro-Solute Transport Effects on Microstructure
6.1 Deterministic Modeling of Secondary Phases

7. Probabilistic (Monte Carlo) Modeling of Microstructure
7.1 Fourth Generation of Solidification and Solid State Modeling

8. Modeling and Simulation of Microtructures in Shaped and Centrifugal Castings
8.1 Shaped Castings
8.1.1 Prediction of Grain Structure in Steel Castings
8.1.2 Gray-to-White Transition in Cast Iron
8.1.3. Modeling of Solidification Structure in Al-based Alloy Castings
8.1.4 Modeling of Solidification Structure in RS5 Alloys
8.2 Centrifugal Castings

9. Modeling and Simulation of Ingot MicroStructure in Primary and Secondary Remelt Processes
9.1 Modeling Approach for Simulation of Remelt Ingots
9.1.1 A Deterministic Macroscopic Model for Calculation of Mass and Energy Transport in Ingots
9.1.2 A Stochastic Mesoscopic Model for Simulation of Structure Evolution in Ingots
9.1.3 Computational Aspects for Modeling of Remelt Ingots
9.1.4 Primary and Secondary Dendrite Arm Spacings in Commercial alloys (Deterministic Modeling)
9.1.5 A Stochastic Model for Modeling Secondary Phases during Solidification of Alloy 718 Ingots
9.2 Simulation Results for Some Commercial Applications
9.2.1 Modeling Parameters
9.2.2 Global Comparison of VAR, ESR, and PAM Processes
9.2.3 VAR Process Modeling
9.2.4 ESR Process Modeling
9.2.5 PAM Process Modeling
9.2.6 Process Optimization
9.2.7 Alloy Systems and Solidification Maps
9.2.8 Prediction of Primary and Secondary Dendrite Arm Spacings
9.2.9 Stochastic Modeling of Secondary Phases
9.2.10 Experimental Technique for Composition Measurements and Estimating the Secondary Arm Spacing in Ti-17 Alloy

10. Practical Techniques with Simulation Examples for Controlling the Microstructure

10.1 Electromagnetic Stirring
- 10.1.1 Mathematical Formulation
- 10.1.2 Solution Methodology and MHD Model Validation
- 10.1.3 Results and Discussion for PAM-Processed Ti-6-4 Ingots

10.2 Micro-Chilling in Steel Castings
- 10.2.1 Use of Steel Powder (Micro-Chills) for Efficient Superheat Removal

10.3 Ultrasonic Vibration
- 10.3.1 Ultrasonic Vibration Effects in Fluids
- 10.3.2 Modeling of Ultrasonic Vibration in Fluids

10.4 Modeling of Electromagnetic Separation of Phases to Produce In-Situ Composites

Required Text

1. L. Nastac, *Modeling and Simulation of Microstructure Evolution in Solidifying Alloys,* Springer, New York, 2004 (ISBN 978-1-4020-7831-6).

Additional recommended reading material:

2. Suhas V. Patenkar, Numerical heat transfer and fluid flow, Taylor and Francis, 1980.

3. D.M. Stefanescu: *Science and Engineering of Casting Solidification*. Springer, 2009.

4. J. Dantzig and M. Rappaz, *Solidification*, EPFL Press, 2009.

Evaluation and Grading

GRADE DETERMINED AS FOLLOWS:		
60% - average of three exams 40% - Special Project	A	90
	B	80
	C	65
	D	50

Schedule of Exams

Exam#1: September 24. 2014

Exam#2: October 29. 2014

Exam#1: November 25. 2014

Exams

Three exams will be given during the semester, and they are listed in the syllabus.

Make-up exams are given only when approval is obtained in advance

Special Project

The Special Project is due no later than the end of the final exam period, which December 12, 2014. If the special project deadline is missed, the student must (1) get an excuse from the Office of Student Services, (2) pay a fee at the Bursar's Office (and get a permit to submit the Special Project), and (3) submit the special project at the beginning of the next term

Attendance policy

Although attendance has no effect on the final grade, students are expected to attend all classes in order to maintain an adequate level of performance on the exams and on the special project.

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Class Day & Hour: TW 2:00 - 3:15 pm
Office Hours: MW 1:00 - 2:00 pm.