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

   2.1 A Macroscopic Model for Calculating Energy, Momentum, Mass and Species Transport
2.2 Methods for Coupling HT-SK Models


4. Stochastic/Mesoscopic Modeling of Microstructures

5. 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 Microstructures 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


Additional recommended reading material:


Evaluation and Grading

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<th>GRADE DETERMINED AS follows:</th>
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<tr>
<td>60% - average of three exams</td>
<td>A 90</td>
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<tr>
<td>40% - Special Project</td>
<td>B 80</td>
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<td>C 65</td>
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Schedule of Exams

Exam#1: September 23, 2015
Exam#2: October 28, 2015
Exam#3: November 24, 2015
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 11, 2015. 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.

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