(1a)	**(2)**	**(1b)**
MECH 866*/3.0		Advanced Phase Transformations

This course focuses on the practical aspects and the relevant fundamentals of phase transformations in advanced manufacturing of metal alloys. The course offers a deep theoretical insight into solidification and solid-state diffusional transformations, along with an effective utilization of relevant analytical models to explore/explain the effect of material and processing variables on the evolution (i.e., types and kinetics) of phase transformations.

Course description

This is an elective course with the intent to provide the students with the necessary knowledge and tools to investigate, understand and control phase transformations in metal alloys. This course will emphasize a theoretical-based approach to learning and problem solving in the realm of thermally-activated metallurgical phenomena.

While demonstrating a physical metallurgy, solid state physics and/or physical chemistry background is advantageous for accomplishing the course objectives, it is not a prerequisite. The course is designed to build upon a prior knowledge of essentials/fundamentals of phase diagrams, phase equilibria and thermodynamics. The lectures will provide the detailed theoretical basis that students are required to learn and develop in the course (in reference to relevant textbooks and journal publications). Before, during and after the lectures (through reading materials), the students will familiarize themselves with the main concepts involved in describing and analysis of phase transformations. The students' learning performance and grasp of the theoretical knowledge will be evaluated through "general quizzes". At the same time, throughout the semester, the students will be guided through an individually-customized "assignment", as well as an individual "project", with one-on-one supervision (in-class and/or otherwise). The course will cover the following topics:

1. **Introduction to Phase Transformations**
2. **Diffusion**
3. **Solidification**
4. **Diffusional Transformations in Solids**

1. <u>Introduction to Phase Transformations</u> [~1 week]

- **Basic concepts of metallurgical thermodynamics**
- **Thermodynamics and Phase Diagrams**

This will be a brief introduction to thermodynamics and kinetics of phase transformations, phase equilibria and construction of phase diagrams. The content will be majorly presented from chapter 1 of "*Phase Transformations in Metals and Alloys*", by Porter & Easterling. Themes include thermodynamics and phase equilibria in binary systems, equilibrium in heterogeneous systems, construction of binary phase diagrams and effects of defects/interfaces on equilibrium.

2. <u>Diffusion</u> [~2 weeks]

- **Mathematics of Diffusion**
    - ***Fick's first & second laws***
    - ***Steady-state vs. non-steady-state diffusion***
    - ***Solutions to the diffusion equation***

- **Mechanisms of Diffusion**
    - ***Interstitial diffusion (random jump)***
    - ***Substitutional diffusion (intrinsic/self-diffusion vs. inter-diffusion)***
- **The Thermodynamic Driving Force for Diffusion**

As a prelude to solidification and solid-state transformations, this section will be a short overview of diffusion in general eluding to the most important/relevant concepts, formulas and mechanisms. We will cover chapter 2 of "*Phase Transformations in Metals and Alloys*", by Porter & Easterling, chapters 1 & 2 of "*Phase Transformations*", by JJ Hoyt, as well as some select journal publications. Themes include common solutions to the diffusion equation in a single-phase binary system, interstitial and substitutional diffusion mechanisms, methods of measuring/estimating intrinsic vs. inter-diffusion coefficients and the thermodynamic driving force for diffusion.

3. <u>Solidification</u> [~3 weeks]

- **Fundamentals of Solidification**
    - ***Nucleation & growth***
    - ***Alloy solidification: equilibrium vs. non-equilibrium (no diffusion in solid)***
    - ***Solidification morphology (Planar to Columnar to Equiaxed transitions)***
- **Rapid Solidification Phenomenon**
    - ***Theoretical formulation***
    - ***Effects on a eutectic phase diagram (Solid Solubility & Eutectic Fraction/Composition)***
    - ***Effects on the microstructure and phase morphology***

This section is designed to teach the students essential fundamentals and analytical models of a wide span of solidification phenomena occurring under equilibrium or non-equilibrium conditions; i.e., present during various mainstream and advanced manufacturing processes. We will cover select contents from chapter 4 of "*Phase Transformations in Metals and Alloys*", by Porter & Easterling, chapters 3 & 7 of "*Phase Transformations*", by JJ Hoyt, chapters 2-7 of "*Fundamentals of Solidification*", by Kurz & Fisher, as well as select journal publications. The themes include nucleation & growth mechanisms and kinetics, solute redistribution in solidification of binary alloys, interface instability and cellular/dendritic growth, directional vs. equiaxed solidification and the deviation from equilibrium (i.e., no diffusion in solid vs. non-equilibrium solid-liquid interface).

4. <u>Diffusional Transformations in Solids</u> [~4 weeks]

- **Spinodal Decomposition**
    - ***2nd order phase transformations***
- **Precipitation**
    - ***Second-phase formation (nucleation & growth) via 1st order phase transformations***
    - ***Continuous vs. Discontinuous precipitation***
    - ***Clustering & GP-zone formation***
    - ***Precipitation Kinetics***
- **Grain Growth and Particle Coarsening**
- **Recrystallization**
    - ***Mechanisms***
    - ***Recrystallization Kinetics***
    - ***Competition/Interaction between Precipitation and Recrystallization***

In this section, the students will obtain a deep understanding of the thermodynamic mechanisms and kinetics of second phase formation via diffusion, and will develop the underpinning knowledge required for distinguishing between its various types; i.e., 2nd and 1st order transformations and the subcategories such as continuous vs. discontinuous precipitation (equilibrium phases), clustering and

GP-zone formation (meta-stable phases). Moreover, the content will cover the mechanisms and kinetics of grain and particle coarsening as well as recrystallization, in conjunction with precipitation (as a competing phenomenon). We will cover select contents from chapter 5 of "*Phase Transformations in Metals and Alloys*", by Porter & Easterling, chapters 3, 4 & 5 of "*Phase Transformations*", by JJ Hoyt, chapter 16 of "*The Theory of Transformations in Metals and Alloys*", by JW Christian, chapters 7 & 9 of "*Recrystallization and Related Annealing Phenomena*", by Humphreys & Hatherly, as well as select journal publications.

<u>Assignment</u> [throughout the semester]
The students will perform an individualized assignment on a "diffusional" phase transformation problem using pre-developed analytical models that will be provided to them. The models, written in Matlab and/or Maple, present a number of different metallurgical phenomena including solidification patterning (e.g., columnar to equiaxed transition), rapid solidification, and nucleation and growth in clustering and precipitation. The theme will be decided on a case-by-case, student-by-student basis, depending on their interests and line of research. The idea is to use the core scientific knowledge of a phase transformation phenomenon to explore the effect of material properties (e.g., alloy composition, surface energy, etc.) and processing conditions (e.g., cooling rate, temperature gradient, etc.) on the microstructural outcome of a metallurgical process (e.g., solidification morphology, grain/cell size, phase fractions, etc.). Detailed instructions and supervision will be provided to the students as to how to run the programs in Matlab/Maple, and the students will implement only minor modifications to the codes in order to define specific conditions requested in the assignment.

<u>Project</u> [throughout the semester]
The students will perform an individualized project on a phase transformation problem. The theme will be decided on a case-by-case, student-by-student basis, depending on their interests and line of research. The students will present their projects in a 20 min power point presentation (in the last class), and will also hand in a report. The project can fall under <u>either of the following categories</u>

- An ***experimental work*** or a ***numerical/analytical simulation*** that can be completed in one semester, and may or may not be in line with the students' current research; The student will address/investigate a metallurgical process influenced by any kind of phase transformation (diffusional and/or otherwise), or
- An ***investigative proposal*** detailing a literature review on a phase transformation problem (currently being researched within the materials science community as a hot topic), identifying the main challenges as well as proposing the approach/methodology to address it.

Instruction style

Students will familiarize themselves with the content of the required reading before class (lectures notes will be posted online ahead of each class). Time in the classroom will be spent reinforcing the theoretical concepts (through lecture & discussions), as well as one-on-one guidance/advice required for the assignment and the project, which they will complete on their own. Two quizzes will be held in class time (week 3 and week 12). The assignment and project topics will be decided by the end of week 3, and the students will have the rest of the semester to carry them out.

Grading

Assignment (20%), ***Project Presentation*** (10%), ***Project Report*** (30%), ***Quiz 1*** (10%), ***Quiz 2*** (30%)