THE OHIO STATE UNIVERSITY
COLLEGE OF ENGINEERING

Computational Thermodynamics and Kinetics

MATSCEN 5321

Credit Hours:
2.00 - 2.00

Course Levels:
Undergraduate (1000-5000 level)
Graduate (5000-8000 level)

Course Components:
Lecture
Lab

Course Description:
Comprehensive background on computational thermodynamics and kinetics. Includes focus on CALPHAD (Calculation of Phase Diagram) methodology.

Prerequisites and Co-requisites:
Prereq: 2251 and 3151 or equivs, or Grad standing in MatScEn or WeldEng; or permission of instructor.

Course Goals / Objectives:
- Prepare students to be able to understand the basics of computational thermodynamic and kinetic models.
- Application of modeling to real-life design challenges faced by industries using commercially-available modeling software.

Course Topics:

- Review of thermodynamic equations & the concept of lattice stability
- Introduction to solution thermodynamics & sub-lattice models & Basics of the CALPHAD methodology
- Introduction to Thermo-Calc and CALPHAD software
- Calculation of multi-component phase equilibria, precipitation modeling, segregation of elements, specific heat, latent heat data for solidification modeling, thermodynamic factors for constructing matrices for multicomponent alloys.
- Applications to real materials design such as superalloys, steels, Ti alloys, Al alloys, Mg alloys, Cu alloys, etc.
- Application of CALPHAD in materials joining research. Link computational thermodynamics to microstructure models such as phase-field models and atomistic simulations such as DFT calculations.
- Review of phase transformation modes (1st order and 2nd Order); interface controlled, diffusion controlled, mixed control and displacive transformation
- Diffusion controlled growth: interface equilibrium, review of diffusion equations, the concept of mobility and thermodynamic factor and interface movement
- CALPHAD-type description of the mobility as a function of temperature and composition & Mobility database structure & relation to first principle calculations
- Diffusion in ternary systems and concept of diffusion paths: Intro to DICTRA®: Simulations of binary diffusion couples & Simulations of ternary diffusion couples (single phase to multi-phase) Diffusion involving 2-phases & precipitation reactions
- Case studies of application of DICTRA in problem-solving
- Predicting other modes of phase transformation, link to overall transformation kinetic theories and applications to real materials design such as superalloys, steels, Ti alloys, Al alloys, Mg alloys, Cu alloys and emerging materials
- Experimental Methods to measure kinetic parameters and assumptions
- Group project presentations

Designation:

Elective