

Last Update: 20.6.2021

## 84900-01 Kinetics of Materials I

Prof. Daniel Nesim

Course Type: Lecture

היקף שעות: 1 נק"ז

א' :Semester

2021 :Year

:Course Website

Day & Time: Tuesday 12:00-14:00

### A. Course objectives and purposes:

This course, is modeled after a graduate core course taught at MIT in the Materials Science and Engineering department by Professor Samuel Allen. It is a fundamental course that presents a unified treatment of phenomenological and atomistic kinetic processes in materials. It provides the foundation for the advanced understanding of processing, microstructural evolution, and behavior for a broad spectrum of materials. The course emphasizes analysis and development of rigorous comprehension of fundamentals. Topics include are irreversible thermodynamics, diffusion, nucleation, and phase transformations. The main topic taught during the course is diffusion.

### Course outcomes :

1. Model systems using forces and fluxes
2. Solve any diffusion couple problem, including Kirkendall effect
3. Solve problems involving multi-layer diffusion
4. Solve ionic diffusion problems
5. Understand issues related to thin film diffusion

### B. Course Topics:

#### Rational and topics:

On successful completion of this module, students should be able to think as a materials scientist. The concepts learned will help the student to better plan experiments and to predict their outcome.

**Knowledge:** Concepts of driving forces and fluxes. Fundamentals of solid-state diffusion applied to many examples (e.g., multi-system, ionic crystals, etc.).

**Skills and Competences:** Ability to develop framework of driving forces and fluxes for any experiment involving solid state diffusion. Estimate and to predict the results of experiments involving solid state diffusion.

### **Course meetings:**

The theoretical part of the course is presented in the Moodle learning environment in the form of Oral lectures combined with Power Point Presentation. Tutorials will be attached as PDF documents.

### **Detailed teaching program:**

1. *Introduction*  
Thermodynamics and Kinetics. Averaging. Fields, Variations, and Continuum Limits. Fluxes and Accumulation. Conserved and Non-conserved Quantities.
2. *Principles of Irreversible Thermodynamics*  
Entropy and Entropy Production. Basic Postulate of Irreversible Thermodynamics. Linear Irreversible Thermodynamics. The Diffusion Potential. Onsager's Symmetry Hypothesis.
3. *Driving Forces and Fluxes for Diffusion*  
Diffusion in a concentration gradient. Reference frames for diffusion and marker velocity. Relation of diffusivity to mobility. Self-diffusion, intrinsic diffusion, and interdiffusion.
4. *Interdiffusion*  
Reference frames for describing diffusion. Intrinsic diffusivities. The Kirkendall effect.
5. *Effects of Capillarity and Stress on Diffusion*  
Surface tension and surface free energy. Mean curvature of a surface. Interface motion and changes of interfacial area. Smoothing of a rough surface. Effect of stress on diffusion potential. Equilibration of solute "atmospheres" around edge dislocations. Darcy's Flow.
6. *The Diffusion Equation*  
Flux and divergence. The constant-diffusivity case. Scaling of the diffusion equation. Superposition of solutions. Error function solution. Fundamental point-source solutions.
7. *Solutions to the Diffusion Equation—I*  
Concentration-dependent diffusivity. Time-dependent diffusivity. Anisotropic diffusion.
8. *Solution to the Diffusion Equation—II*  
Steady-state solutions. Time-dependent solutions. Superposition of point sources. Method of images.

9. *Solutions to the Diffusion Equation—III*  
Method of separation of variables. Method of Laplace transforms.
10. *Solutions to the Diffusion Equation—IV*  
Numerical methods for solving differential equations. Treatment of boundary conditions. Examples.
11. *Activated Jump Processes*  
One-particle model. Many-body model. Computer simulations. Mean square displacement from a point source. Diffusion Resulting from Discrete Jumps  
Diffusion and random walks. Diffusion with correlated jumps. Relation of mean square displacement to diffusivity.
12. *Diffusion in Crystals—I*  
Diffusion mechanisms in crystals. Atomic models for diffusion coefficients in metals.
13. *Diffusion in Crystals—II*  
Atomic models for diffusion coefficients in ionic crystals. Intrinsic and extrinsic regimes of diffusion. Nonstoichiometry.
14. *Short-Circuit Diffusion in Crystals*  
The diffusion spectrum. Diffusion along grain boundaries. Diffusion along dislocations.

### **C. Prerequisites:**

Basic solid state chemistry, Advanced physical chemistry  
Recommended but not mandatory: Introduction to X-ray diffraction (XRD)

### **D. Course Requirements:**

Attendance and active class participation are mandatory.

### **E. Final Grading:**

Written examination covering all material taught in the course.

### **F. Bibliography**

All material needed will be provided during the course.

A complete but more complex text is:

Kinetics of Materials, Baluffi, Allen, Carter, John Wiley & Sons.

Other specific books and references to supplement the learning will be shown in class.