MS133. Kinetic Processes in Materials


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**Lectures.** TR 2:30 PM - 3:55 PM in Keck 142

**Sub Lectures.** Chen Xu (highlighted dates)

**Recitation.** TBD

**Office Hours.** TBD

**Website.** [http://jrgreer.caltech.edu/teaching.php](http://jrgreer.caltech.edu/teaching.php). Find the “MS133” tab and download your homework assignments, lecture notes, solutions, and handouts from this website.

**Homework.** There will be weekly problem sets to be turned in on Fridays NO LATER than 5pm. There will be no problem set due the week after midterm and the week before final. NO LATE HOMEWORKS WILL BE ACCEPTED. Collaborative work is encouraged, but homework has to represent everyone’s own individual solutions.

**Exams.** There will be 1 take-home midterm exam and 1 final exam. You are welcome to use any of your notes (no books) during these exams. You **may not** collaborate with others on any of the problems and you **may not** work past the allotted amount of time. Both the midterm and the final exams will last 3 hours.

**Class Schedule (subject to change).**

<table>
<thead>
<tr>
<th>Week/Date</th>
<th>Section</th>
<th>Topic</th>
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<tbody>
<tr>
<td>Wk 1/ April 2</td>
<td>(1) Class notes Ch. 1 (pp. 1-35)</td>
<td>(1) Fick’s Laws and Macroscopic Diffusion. Examples of using Fick’s laws; cylindrical and thin film solution; moving boundary in a eutectic system; concentration-dependent diffusivity. HW1 due 04/10</td>
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<tr>
<td>Wk 2/April 7</td>
<td>(2) Ch. 2 (pp. 55-82)</td>
<td>(2) Atomistic Mechanisms of Diffusion: random walk; diffusivity and hopping rate; equilibrium vacancy concentration; atomic jump frequency; effect of pressure. HW2 due 04/17</td>
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<tr>
<td>Wk 2/April 9</td>
<td>(3) Ch. 3 (pp. 87-94); Handout #1 (vacancy-impurity pairs)</td>
<td>(3) Diffusion in Dilute Alloys: impurity-vacancy interactions; jump frequency; counting vacancy-impurity pairs. (4) Diffusion With a Chemical Gradient: Kirkendall effect, chemical diffusion coefficient, Chemical potential HW3 due 04/24</td>
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<tr>
<td>Wk 3/April 14</td>
<td>(4) Ch. 4 (pp 99-108)</td>
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<tr>
<td>Wk 3/April 16</td>
<td>(5) Ch. 5 (pp 109-116)</td>
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<tr>
<td>Week/Date</td>
<td>Topic</td>
<td>Videos/Assignments</td>
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<td>Wk 4/April 21</td>
<td>(4) Ch. 4 (pp 109-120)</td>
<td>(4) Diffusion With a Chemical Gradient (cont’d): Potential gradients and jump frequencies, Vacancy equilibrium and Kirkendall voids. HW4 due 05/01</td>
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<tr>
<td>Wk 4/April 23</td>
<td>Handout #2 (Kirkendall experiment)</td>
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<tr>
<td>Wk 5/April 28</td>
<td>(5) Ch. 5 (pp 135-151)</td>
<td>(5) Surfaces: Surface energy and stress, thermodynamics of surface defects, entropy Midterm NO HW!</td>
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<td>Wk 5/April 30</td>
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<tr>
<td>Wk 6/May 5</td>
<td>(6) Ch. 6 (pp. 157-176); Handout #2 (g.b. equilibrium)</td>
<td>(6) Solidification: homogeneous and heterogeneous nucleation; nucleation barrier and nucleation rate. HW5 due 05/15</td>
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<tr>
<td>Wk 6/May 7</td>
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<tr>
<td>Wk 7/May 12</td>
<td>(7) Ch. 6 (pp. 177-209)</td>
<td>(7) Growth: atom attachment rate, uniform and non-uniform growth, Gibbs-Thompson effect, dendrites, eutectic solidification HW6 due 05/22</td>
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<tr>
<td>Wk 7/May 14</td>
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<td>Wk 8/May 19</td>
<td>(8) Ch. 7 (pp. 229-245); Handout #3 (grain growth)</td>
<td>(8) Solid-Solid Transformations: chemical concentration of precipitate; nucleation energy contributions; nucleation barrier; growth; isothermal transformation kinetics. Final Exam. No HW!</td>
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<tr>
<td>Wk 8/May 21</td>
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<tr>
<td>Wk 9/May 26</td>
<td>(9) Ch. 7 (pp. 248-259)</td>
<td>(9) Cont’d: time-temperature-transformation diagrams. Spinodal decomposition: spinodal instability, strain effect, decomposition rate.</td>
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<td>Wk 9/May 28</td>
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**Lecture Topic Outline.**

1. Fick’s Laws and Macroscopic Diffusion
   1.1 Introduction
   1.2 Fick’s Laws
      1.2.1 Fick’s First Law
      1.2.2 The Conservation Equation
      1.2.3 Fick’s Second Law
      1.2.4 Cylindrical Example Using Fick’s First Law
   1.3 The Thin Film Solution
   1.4 Other Solutions Based on the Thin-Film Solution
   1.5 Separation of Variables
   1.6 Moving Boundary in a Eutectic System
   1.7 Concentration-Dependent Diffusivity
      1.7.1 Boltzmann-Matano Analysis
      1.7.2 Numerical Methods
      1.7.3 Application of Boltzmann-Matano Method to Numerical Data
2 Atomistic Mechanisms of Diffusion
2.1 Random Walk
2.2 Diffusivity and Hopping Rate
2.3 Atom Jump Mechanisms
2.4 Expression for Diffusivity
2.5 Equilibrium Concentration of Vacancies
   2.5.1 Measurement of Vacancy Concentration by Dilation and Lattice Parameter
2.6 Atomic Jump Frequency
2.7 Correlation Coefficient
2.8 The Effect of Pressure

3 Diffusion in Dilute Alloys
3.1 Impurity-Vacancy Interactions
3.2 Concentration of Vacancy-Impurity Pairs
3.3 Jump Frequency
3.4 Correlation Effects

4 Diffusion With a Chemical Gradient
4.1 Kirkendall Effect
4.2 Chemical Driving Force
   4.2.1 Generalized Flux Equations
   4.2.2 Darken’s Flux Equation
   4.2.3 Relationship Between Tracer and Intrinsic Diffusivities
   4.2.4 Chemical Diffusion Coefficient
   4.2.5 Regular Solution Example
4.3 Potential Gradients and Jump Frequencies
   4.3.1 Chemical Potential as Driving Force
4.4 Vacancy Equilibrium and Kirkendall Voids

5 Surfaces
5.1 Surface Energy
   5.1.1 Surface Stress
   5.1.2 Enthalpy
   5.1.3 Surface Energies from Bulk Parameters
   5.1.4 Entropy
5.2 Thermodynamics of Surface Defects

6 Solidification
6.1 Nucleation
   6.1.1 Nucleation Barrier
   6.1.2 Distribution of Solid Particle Sizes
   6.1.3 Nucleation Rate
   6.1.4 Heterogeneous Nucleation
   6.1.5 Numerical Estimation of Nucleation Rates
6.2 Growth
   6.2.1 Atom Attachment Rate
   6.2.2 Uniform Growth
   6.2.3 Nonuniform Growth Modes
6.2.4 Interface Stability and Dendrite Formation
6.2.5 Gibbs-Thompson Effect
6.2.6 Dendrite Growth Rate
6.3 Alloy Solidification
6.4 Constitutional Undercooling
6.5 Eutectic Solidification

7 Solid-Solid Transformations
7.1 Chemical Concentration of the Precipitate
7.2 Nucleation Energy Contributions
   7.2.1 Transformation Free Energy
   7.2.2 Strain Energy
7.3 Nucleation Barrier
7.4 Growth in Solid-Solid Transformations
7.5 Isothermal Transformation Kinetics
7.6 Time-Temperature-Transformation Diagrams

8 Spinodal Decomposition
8.1 Spinodal Decomposition
   8.1.1 Spinodal Instability
   8.1.2 Estimation of the Gradient Energy Term
   8.1.3 Strain Effect on Spinodal Instability
   8.1.4 Spinodal Decomposition Rate

Books and Notes.

Additional Recommended Texts

2. P. Haasen “Physical Metallurgy”