COMMONWEALTH GRADUATE ENGINEERING PROGRAM
DISTANCE LEARNING COURSE PLANNING SHEET
UNIVERSITY OF VIRGINIA

Course: MSE624 - Kinetics of Solid-State Reactions   Semester: Spring 2007

Instructor: William C. Johnson   Phone No. (434) 982-4884

Office Address: Department of Materials Science and Engineering
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Textbook(s): (Student to purchase)

No textbook required for Spring 2007

Reference(s):

Kinetics of Materials by R.W. Ballufi, S.M. Allen, and W.C. Carter; J. Wiley and Sons

Diffusion in Solids by M.E. Glicksman

Mathematical Methods in the Physical Sciences by M. Boas

Computer Needs:

Computer Capability ______basic______________________________

Software required? ______No__________________ Provided? ________________

Other ____

MSE624 - Kinetics of Solid State Reactions Spring 2007

Instructor: William C. Johnson
Office: 218 Wilsdorf Hall
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Class Time: TR: 8:00-9:15pm.

Office Hours: WF: 1:00-2:00pm and by appointment.

Prerequisite: MSE623 Thermodynamics of Solids; MSE601 Crystallography and Defects; or permission of instructor.

Honor Code Policy: All students must abide by the University of Virginia Honor Code. Violations will be reported to the Honor Committee.

Text: There is no assigned text this semester.

Additional References: *Kinetics of Materials* by R.W. Balluffi, S.M. Allen, and W.C. Carter, J. Wiley and Sons, 2005; *Diffusion in Solids* by M.E. Glicksman; and *Diffusion-Mass Transfer in Fluid Systems* by E.L. Cussler. A useful reference for mathematical techniques is *Mathematical Methods in the Physical Sciences* by M. Boas. Some notes will be posted on the class toolkit web site: http://toolkit.itc.virginia.edu

Grading: Some portions of both examinations will likely be closed-book and closed-notes.
Homework, projects, and class participation (30%)
Midterm Exam (30%)
Final Exam (40%)

Homework: Homework is assigned frequently. Unless otherwise directed, you may consult with your fellow students about any homework problem. However, each student is to hand in his/her own homework solutions. You will be asked to grade some homework assignments yourself using solutions posted on the class website: http://toolkit.itc.virginia.edu. In such cases, you are to work the homework problems before comparing your work with the solutions. If you discover you have made a mistake, you are allowed to put the solutions aside and to rework the problem. If you rework the problem correctly, you may earn full credit for that problem. You may not copy the solution from the website. Homework is due at the beginning of class on the indicated day. Off-ground students in particular frequently encounter unforeseen travel or other professional demands on their time. Please notify me promptly, if you are unable to complete the assignment punctually so that we can work out a mutually agreeable schedule.

Course Objectives: The three primary objectives for this course are to:
1) Serve as an introduction to basic kinetic processes in solid-state materials.
2) Develop basic mathematical skills necessary for research in materials science.
3) Reinforce basic numerical and computer programming skills.

The course will emphasize the formulation and solution of differential equations and boundary conditions used to describe basic solid-state kinetic phenomena including microstructural evolution, heat and mass diffusion, and interfacial reactions.

Course Outline:

I. Field (Phenomenological) Theory - Single Phase Systems
- A. Application of physical laws to develop governing equations
  1. Conservation laws - mass diffusion
  2. Flux (constitutive) equations
     - a. Fick's law
     - b. Variational approaches
     - c. Substitutional alloy
     - d. Interstitial ally
  3. Thermodynamics - thermal diffusion
  4. Diffusion in gravitational field
  5. Diffusion with unsaturable trapping sites
- B. Boundary conditions for diffusion
  1. Insulated boundaries
  2. Local thermodynamic equilibrium
  3. Molecular dissociation at interfaces

II. Analytic solutions to diffusion equations - infinite domain
- A. Mathematical techniques
  1. Boltzmann similarity transformation
  2. Planar sources in one-dimension
  3. Point and line sources
- B. Applications
  1. Diffusion couples and diffusion bonding
  2. Grain boundary adsorption

III. Introduction to Crystalline Diffusion Theory
- A. Random walks
  1. One-dimensional master equations
  2. Relationship to diffusivity
  3. Difference equations for diffusion
- B. Intrinsic diffusivities
- C. Smigelskas-Kirkendall effect and Darken analysis
- D. Inverse problem: Finding diffusivity from composition field
  1. Composition-independent diffusivity
  2. Matano analysis

IV. Introduction to Linear Irreversible Thermodynamics
- A. Entropy production and fundamental postulate
  Thermodynamic restrictions on thermal conductivity-scalar
  Thermodynamic restrictions on diffusivity-second rank tensor
- B. Onsager coefficients

V. More Solutions to the Diffusion Equation
- A. Analytic solutions: semi-infinite domain
  1. Mathematical techniques
     - a. Boltzmann similarity transformation
     - b. Planar sources
  2. Application - Surface hardening

B. Analytic solutions: finite domain
  1. Steady-state problems in one dimension
    a. Cartesian systems
    b. Polar coordinates
    c. Spherically symmetric systems
    d. Composition dependent diffusivities
  2. Steady-state problems in two dimensions
    a. Separation of variables
    b. Sturm-Liouville eigenvalue problem
  3. Time dependent problems in one and two dimensions
  4. Applications
    a. Homogenization
    b. Carburization

C. Numerical solutions
  1. Finite difference technique
  2. Application: binary diffusion couple - finite domain

VI. Kinetics of two-phase systems

A. Establishing interfacial conditions at planar interfaces
  1. Equations of motion - balance laws
    a. Mass
    b. Energy
  2. Boundary conditions
    a. Local thermodynamic equilibrium
    b. Non-equilibrium at interface

B. Solving problems with interface motion - local thermodynamic equilibrium
  1. Two-phase diffusion couple
  2. Growth of surface phase
    a. Quasi-stationary solutions
    b. Linear-gradient (Zener) approximation
  3. Similarity transformation - analytic

C. Interfacial reactions - non-equilibrium at interface
  1. Linear and parabolic growth laws - oxidation of silicon
  2. Composite materials - growth of intermediate phase

VII. Diffusion in Multicomponent (Ternary) Systems

A. Governing equations and diffusivity matrix

B. Steady-state solutions

C. Time-dependent solutions
  1. Eigenvalues and eigenvectors
  2. Infinite systems
  3. Semi-infinite systems
  4. Finite systems