**MSE 6411 – Thermodynamics of Materials**

School of Materials Science and Engineering

Georgia Institute of Technology

Fall Semester 2016

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| Course Objective | To provide students with a fundamental understanding of the thermodynamic and statistical mechanics aspects which govern the behavior of all materials in all states. |
| Learning Objectives  Academic Integrity  Learning Accommodations  Lecture  Instructor  Office  Phone  E-mail  Office Hour | Upon completion of this course, students will be able to:   1. Understand the role of free energies in various chemical and physical material processes and for equilibrium/non-equilibrium states 2. Reduce thermodynamic aspects to the general framework of statistical mechanics 3. Acquire a thorough insight on a comprehensive approach to describe the behavior of assemblies of small molecules and long chain molecules using fundamental thermodynamic and statistical mechanics principles 4. Apply thermodynamics/statistical mechanics approaches to their research projects in materials science and engineering   Students are reminded of the Georgia Tech Academic Honor Code and Student Code of Conduct. Academic dishonesty and violations of the Honor Code will be handled according to the established Georgia Tech policies. If specific polices described for tests and homework are not clear, students should clarify those with the instructors to assure proper compliance with expected policies.  If needed, we will make classroom accommodations for students with documented disabilities. These accommodations must be arranged in advance and in accordance with the Office of Disability Services (<http://disabilityservices.gatech.edu>).  12:05-1:25 T, Th in Love 183  Karl I. Jacob, Arun Gokhale, Mo Li, Robert Speyer, Mohan Srinivasarao  MRDC 4509  (404) 894-2541  [karl.jacob@mse.gatech.edu](mailto:karl.jacob@mse.gatech.edu)  T, Th 3:00-4:00 PM |
| Teaching Assistant | TBD |
| Homework | Problems will be assigned periodically and solutions will be posted a week later. Homework may not be collected or graded |
| Exam/grading | 4 Exams, 25% each at the end of each Part |

**References**

1. Molecular Driving Forces – Statistical Thermodynamics in Chemistry and Biology, Ken A. Dill and Sarina Bromberg, Garland Science, Taylor & Francis Group, 2nd Edition
2. Basic Chemical Thermodynamics (Oxford Chemistry Series), E. Brian Smith
3. Basic Thermodynamics (Oxford Science Publications), Gerald Carrington
4. Fundamentals of Classical and Statistical Thermodynamics, Bimalendu N. Roy, Wiley Pub
5. Physical Chemistry, Peter Atkins, Oxford Uni Press
6. Statistical Physics, Landu and Lifshitz, Butterworth – Elsevier (https://archive.org/stream/ost-physics-landaulifshitz-statisticalphysics/LandauLifshitz-StatisticalPhysics#page/n81/mode/2up )
7. Introduction to Statistical Physics (Graduate Texts in Contemporary Physics), Silvio Salinas, Springer
8. Thermodynamics and Statistical Mechanics, Peter Landsberg, Dover Pub
9. Statistical Mechanics. Donald McQuarrie, University Science Books
10. Statistical Mechanics: A Set of Lectures, Richard Feynman, Westview Press
11. Statistical Mechanics, R. K. Pathria, Academic Press
12. Introduction to Modern Statistical Mechanics, David Chandler, Oxford Univ

**Topical Outline – Thermodynamics of Materials**

**PART I: Fundamentals and Elementary Applications (7 classes for Part I)**

I. Thermodynamics, Entropy, First & Second Laws **(2 classes)**

A. Extremum Principles, Heat, Work, Energy and the First Law (1 class)

B. Free Energies, Temperature, Equilibrium and Ideal Gas (1 class)

II. Introduction to Statistical Mechanics **(5 classes)**

1. Brief Introduction to Probability and Statistics (1 class)
2. Boltzmann Distribution Law, Partition Function, Ensembles, Heat Capacity,

Energy Fluctuations (2 classes)

1. Reduction of thermodynamic variables from partition function (2 classes)

**PART II: Liquids, Mixtures and Phase Behavior (15 classes for Part II)**

III. Phase Equilibria, Thermodynamics of 1-Component Fluids, Chemical Equilibria **(7 classes)**

A. Classic Van der Waals Model: Equation-of-State, Virial expansion, Liquid-Vapor phase transition, Isothermal compressibility, Law of corresponding states (2 classes)

B. Microscopic Lattice Fluid Model: Partition function, athermal limit, mean field

approximation, attractions, connection to van der Waals model (2 classes)

C. Chemical Reaction Equilibria: reaction equilibria and thermodynamics of point defects. (3 classes)

IV. Continuum Fluids: Thermodynamics, Structure **(3 classes)**

A. Hard Sphere Fluids (relevant to atoms, molecules, colloids) (2 classes)

1-dimensional Tonks model, comparison to lattice fluid model

B. Correlation functions, Radial Distribution Function g(r) (1 class)

V. Binary phase diagrams: Two Component Liquid Solutions and Solid Alloys **(3 classes)**

VI. Solutions of long chain molecules and blends **(2 classes)**

1. Flory-Huggins approach: effect of enthalpy, entropy and degree of polymerization (1 class)
2. UCST and LCST behavior (1 class)

**PART III: Thermodynamics of defects, surfaces, and interfaces 6 classes for Part III)**

VIII. Surfaces and Interfaces: Physical Adsorption, Monolayers and Langmuir Isotherm **(6 classes)**