MSE 6411 – Thermodynamics of Materials

Course Objective	To provide students with a fundamental understanding of classical thermodynamics and statistical thermodynamics that govern the behavior of all materials in all states.
Learning Objectives	Upon completion of this course, students will be able to: (1) Understand the role of internal energy, entropy, and free energy in various chemical and physical material processes and for equilibrium/non-equilibrium states (2) Understand statistical thermodynamics and its role in linking processes at atomic/molecular scale to macroscopic thermodynamic behavior of materials (3) Apply thermodynamics approaches to understand behavior of surfaces and interfaces in materials
Academic Integrity	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 instructor to assure proper compliance with expected policies.
Learning Accommodations	Proper accommodation will be provided, in accordance with Georgia Tech's policies, for students with documented disabilities that could affect their performance. Students should inform the instructor at the beginning of the semester if they are seeking such an accommodation.
Lectures	2:00 to 3:15 pm on Tuesdays and Thursdays. The classes will be in Room 299, Love Building
Instructor	Arun Gokhale
Teaching Assistants	TBA
Homework	There will be 10 to 12 Home Assignments in the course. Homework will not be collected or graded
Tests/Exams	There will be 4 tests; all test will be in-person, closed books and closed notes.
Mode of Delivery	The course will be taught in the in-person mode. All lectures and tutorials will be in-person.

Class Attendance	Students are required to attend the in-person lectures and participate in the class discussions

References books

1. *Thermodynamics in Materials Science* by Robert DeHoff, CRC, Taylor & Francis Group, 2nd Edition
2. *Chemical Thermodynamics of Materials* by C.H.P. Lupis, North-Holland, New York
3. *Molecular Driving Forces – Statistical Thermodynamics in Biology, Chemistry, and Nanoscience* by Ken A. Dill and Sarina Bromberg, Garland Science, Taylor & Francis Group, 2nd Edition.

TOPICS

Classical Thermodynamics
Mathematics, probabilities, and statistics background, isolated, closed, and open thermodynamic systems, extensive and intensive properties, state variables and process variables, work, heat, internal energy, enthalpy, entropy and free energy, laws of thermodynamics, Maxwell's relationships, thermodynamics of liquid and solid solutions, chemical potential, conditions of equilibrium in multi-component and multi-phase systems, free energy-composition diagrams, Gibbs phase rule, unary and binary phase diagrams, thermodynamic modeling of phase diagrams.

Statistical Thermodynamics: Statistical behavior of ensembles, microstates and macrostates, Boltzmann's entropy equation, degeneracy of energy states, Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac statistics, equipartition of energy, quantum harmonic oscillators, quantum mechanics based modeling of energy levels, partition function of ensembles, calculation of thermodynamic properties from partition functions, phonons, Einstein and Debye theories of heat capacity, statistical thermodynamics of gases, statistical thermodynamics of solutions.

Thermodynamics of Point Defects, Interfaces, and Surfaces: Equilibrium concentrations of point defects in materials, surface energy and surface tension, thermodynamic surface excess functions, thermodynamic equilibrium in presence of planar and curved surfaces/interfaces, anisotropic surface/interfaces, Gibbs-Wulf construction, effects of interface curvature on chemical potential, solubility, melting point, and vapor pressure of nano-particles, Thompson-Freundlich equation, effects of interface curvature and size on phase boundaries in phase diagrams, Gibbs adsorption equation.