Thermodynamics and Statistical Mechanics in Materials Science
ENG ME/MS 505

Introduction

The goal of this course is to provide graduate students embarking on research in Materials Science and Engineering, and advanced undergraduate students a solid introduction to the applications of thermodynamics in Materials Science. The course will provide a comprehensive treatment of the laws of thermodynamics and their applications to equilibrium and the properties of materials. It will provide a foundation to treat general phenomena in materials science and engineering, some examples of which include chemical reactions, magnetism, and point defect chemistry. Relations pertaining to multiphase equilibria as determined by a treatment of solution thermodynamics will be developed including graphical constructions that are essential for the interpretation of phase diagrams. The treatment will include electrochemical equilibria and surface thermodynamics. The course also weaves in statistical thermodynamics as they relate to macroscopic equilibrium phenomena.

Course Schedule

Monday, Wednesday 12-2 PM

Textbooks

Thermodynamics in Materials: A Classical and Statistical Synthesis, John B. Hudson, John Wiley & Sons (1996) (Required text)

Thermodynamics in Materials Science, Robert DeHoff, CRC Press, Second Edition (2006) (Recommended text)

Modern Thermodynamics: From Heat Engines to Dissipative Structures, Dilip Kondepudi and Ilya Prigogine, Wiley

Instructor

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Approximate Topic Schedule

1. Laws of thermodynamics – 9/3
2. Thermodynamic variables and relationships (Maxwell's relationships) – 9/8 and 9/10
3. Equilibrium and criteria for equilibrium – 9/15 and 9/17
4. Basis for statistical thermodynamics, ensembles, and statistical mechanical basis for equilibrium
5. Connection between statistical and classical thermodynamics, evaluation of allowed energies
6. Ideal Gases
7. Unary heterogeneous systems (Gibbs free energy, chemical potential, phase stability, Clausius Clapeyron equations, simple unary phase diagrams) – 9/22 and 9/24
8. Multicomponent homogeneous nonreacting systems (Solution theory) – 9/29
9. Midterm I - 10/1
10. Multicomponent heterogeneous systems (conditions for equilibrium, Gibbs phase rule, Introduction to phase diagrams) – 10/3 and 10/6
11. Thermodynamics of reacting systems – 10/8, 10/14 and 10/15
12. Thermodynamics of defects in crystals – 10/20 and 10/22
13. Electrochemical measurements - 10/27 and 10/29
14. Thermodynamics of surfaces – 11/3 and 11/5
15. Introduction to statistical mechanics – 11/10 and 11/12
16. Distribution of momenta and velocities (Maxwell's distribution) – 11/17
17. Application of Maxwell distribution – diffusion and effusion – 11/19
18. Midterm II – 12/1
19. Boltzmann distribution (thermionic emission, contact potential) – 11/24
20. Phase space, partition function, and equipartition of energy – 12/3
21. Brief review of quantum mechanics – 12/8
22. Distinguishability, indistinguishability, degeneracy – application of Fermi-Dirac statistics – 12/11

Grading:
Midterms – 50%, Assignment – 5%, In class participation – 5%, Final – 40%

Instructor Office hours:
Thu – 1 to 3 PM