MatE 251 – Advanced Solid State Thermodynamics

MATERIALS ENGINEERING PROGRAM

COLLEGE OF ENGINEERING

Fall 2010, Saturdays 9:00 a.m. to 11:50

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Hours: TBD

Course Description: Advanced study of the thermodynamics of solids as they relate to the application of materials engineering principles in materials selection, materials processing, materials research and process development. Topics include the First, Second and Third Laws of Thermodynamics, Solution Thermodynamics, Statistical Thermodynamics, Ternary Phase Equilibria, Extent of Reactions, Defect Chemistry and Thermodynamics of Surfaces and Interfaces, among others. Students are expected to be completely familiar with all aspects of binary phase equilibria, binary phase diagrams, and the application of these diagrams in problem solving. Emphasis in class will be placed on developing the student's ability to apply the principles of solid state thermodynamics towards solving real world problems.

Objectives: The Learning Objectives for this class are listed separately, in Appendix A.

Required Text: David V. Ragone, Thermodynamics of Materials, Vol I and Vol II, John Wiley & Sons, New York (1995)

References: A partial list of useful references is provided in Appendix B. Students are strongly encouraged to read the relevant sections/chapters in the recommended references to augment their understanding of the subject matter.

Prerequisites: Graduate standing in the Materials Engineering Program. Students who do not have an undergraduate degree in materials or chemical engineering should have completed MatE 115 and MatE 152.

Assignments will be handed out periodically, and will be due in exactly one week. No late assignments will be accepted.

Examinations: There will be one midterm examination and one final examination. The tentative date for the midterm examination is included in the Tentative Lecture Schedule. The final examination will be held on the day and time indicated in the Schedule of Classes. All examinations will be held in class.

Term Project: Completion of a term project is a requirement for this class. A list of potential term project topics are included in Appendix C. Students will work in groups (2 ~ 3 students). The objective of the term project is to develop a laboratory exercise that will demonstrate an aspect of thermodynamics, experimentally and in writing, so that juniors and seniors in a materials engineering curriculum will understand thermodynamics better. Appropriate documentation is required. An example of how the term project should be documented will be provided. An in-class demonstration/presentation is also required. Further details regarding the term project will be provided in class. Students may propose term project topics other than those listed in Appendix C. However, these must be related to the thermodynamics of solids or solutions, and must first be approved by the instructor.

The schedule for completion of the term project will be as follows:

September 11: Students submit group names and requested term project title

September 18: Student groups and term project titles finalized

October 16: Mid-semester status report. (1 ~ 2 pages)

December 4: Term project completed with in-class demonstration and write-up requirements

Grading:

Midterm	20 %
Final Examination	45 %
Homeworks & Quizzes	15 %
Term Project	20%
T O T A L	100

Letter Grades:

Semester aggregate	
> 90:	A
80 ~ 89.9:	B
70 ~ 79.9:	C
60 ~ 69.9:	D
< 60:	F

Office hours: Please feel free to stop by my office during my office hours for any additional help that you may need. If you truly do have a time conflict with my office hours, I will be happy to arrange a mutually convenient time.

Other Notes Of Importance:

- No late assignments will be accepted.
- Absence during examinations and quizzes, without prior approval, will result in a zero. Prior approval will be given only under exceptional circumstances.
- Seating arrangements may be handed out for mid-term and final examinations.
- There will be no make-up examinations.
- There will be no extra-credit assignments.
- Students may collaborate in their efforts in solving home work problems. However, each submission must be individually prepared.
- The University's Academic Dishonesty Policy will be strictly followed. Students who are not familiar with this are encouraged to familiarize themselves with this policy.

You are responsible for understanding the policies and procedures about add/drops, academic renewal, withdrawal, etc. found at http://sa.sjsu.edu/student_conduct.

For expectations about classroom behavior; see Academic Senate Policy S90-5 on Student Rights and Responsibilities.

For a definition of plagiarism, please refer to the website of the Office of Student Conduct and Ethical Development at http://sa.sjsu.edu/student_conduct.

If you would like to include in your paper any material you have submitted, or plan to submit, for another class, please note that SJSU's Academic Integrity policy F06-1 requires approval by instructors. Material that has been, or will be, submitted to another source for credit will not be accepted in this class.

The evacuation plan for the classroom will be discussed during the first class period.

University, College or Department Policy Information

Academic Integrity Statement (from Office of Judicial Affairs)

Academic integrity is essential to the mission of San José State University. As such, students are expected to perform their own work (except when collaboration is expressly permitted by the course instructor) without the use of any outside resources. Students are not permitted to use old tests, quizzes when preparing for exams, nor may they consult with students who have already taken the exam. When practiced, academic integrity ensures that all students are fairly graded. Violations to the Academic Integrity Policy undermine the educational process and will not be tolerated. It also demonstrates a lack of respect for oneself, fellow students and the course instructor and can ruin the university's reputation and the value of the degrees it offers.

We all share the obligation to maintain an environment which practices academic integrity. Violators of the Academic Integrity Policy will be subject to failing this course and being reported to the Office of Student Conduct & Ethical Development for disciplinary action which could result in suspension or expulsion from San José State University.

The policy on academic integrity can be found at http://www2.sjsu.edu/senate/S07-2.htm

Campus Policy in compliance with the Americans with Disabilities Act

If you need course adaptations or accommodations because of a disability, or if you need special arrangements in case the building must be evacuated, please make an appointment with your course instructor as soon as possible. Presidential Directive 97-03 requires that students with disabilities register with DRC to establish a record of their disability.

MatE 251 - Tentative Lecture Schedule

Date	Topic	Reading
Aug 28	Class Organization, First Law	Vol 1, Chap 1
Sept 04	First Law - continued	
Sept 11	Second Law	Vol 1, Chap 2
Sept 18	Property Relationships	Vol 1, Chap 3
Sept 25	Equilibrium & Chemical Equilibrium	Vol 1, Chap 4, 5
Oct 02	Equilibrium & Chemical Equilibrium - continued	
Oct 09	Solutions & Solution Thermodynamics	Vol 1, Chap 7
Oct 16	Solutions & Solution Thermodynamics - continued	
Oct 23	Phase Rule & Phase Diagrams	Vol 1, Chap 8, 9
Oct 30	Ternary Phase Diagrams	Handouts
Nov 06	Ternary Phase Diagrams	
Nov 13	Statistical Thermodynamics	Vol 2, Chap 2
Nov 20	Defects in Solids	Vol 2, Chap 3
Nov 27	Thanksgiving Break	
Dec 04	Surfaces & Interfaces	Vol 2, Chap 4
Dec 11	Term Project Demonstrations	
Dec 18	Final Examination (09:00 ~ 11:50)	

Appendix A

The **Learning Objectives** for this class include the following:

Analyze open and closed systems and be able to distinguish between the two.

Explain intensive and extensive properties and be able to formulate these mathematically.

Explain state functions and their relevance to thermodynamic parameters.

Formulate heat capacity in terms of thermodynamic functions.

Explain the First and Second Laws of Thermodynamics and be able to describe the constraints in the applicability of each.

Calculate enthalpies of formation and enthalpy changes in chemical reactions.

Calculate adiabatic temperature change in chemical reactions.

Explain entropy.

Calculate entropy changes for different systems such as open, adiabatic, reversible and irreversible systems.

Calculate entropy changes in chemical reactions.

Explain the Third Law of Thermodynamics.

Develop mathematical relationships so that thermodynamic functions that are not directly measurable can be expressed in terms of measurable parameters/quantities.

Explain and compare equilibrium in different materials systems.

Explain first-order and second-order phase transformations.

Determine the variation of equilibrium pressure with temperature in first order phase transformations.

Use the Clapeyron Equation to calculate variation in vapor equilibiria.

Determine the variation in vapor pressure with particle size.

Explain and calculate thermodynamic activity of individual species in multicomponent systems.

Explain the kinetic and thermodynamic models of equilibrium.

Explain standard and non-standard reactions and be able to distinguish between the two.

Explain spontaneous and driven reactions and be able to distinguish between the two.

Calculate the Gibbs Free Energy change for reacting systems.

Use the Gibbs Free Energy change as a measure of deviation from equilibrium.

Calculate the activity product for multicomponent systems; determine the variation of the activity product with variations in temperature and variations in activity of reactants and/or products.

Calculate the equilibrium constant for reacting systems, including the variation in the equilibrium constant with variations in total pressure, partial pressures and temperature.

Calculate extent of reaction in multicomponent multiphase reacting systems.

Calculate threshold partial pressures and decomposition pressures for condensed phase-gaseous phase reacting systems.

Assess reacting systems by using Ellingham Diagrams.

Use Sievert's Law to determine the extent of solubility of gases in liquid and solid metals.

Explain partial molar quantities and relative partial molar quantities.

Explain ideal, non-ideal and regular solutions.

Calculate the enthalpy, entropy and free energy of mixing in ideal and regular solutions.

Use the Gibbs-Duhem relationship to determine thermodynamic parameters.

Describe the Gibbs Phase Rule. Use the Gibbs Phase Rule for determining the degrees of freedom for multi-component reacting and non-reacting systems.

Apply the Hume-Rothery Rules for binary alloy systems.

Analyze one-component and multi-component systems using the Gibbs Phase Rule.

Explain solid solution and intermetallic compound formation in binary and ternary alloy systems.

Use phase diagrams to determine the propensity of systems to exhibit Kirkendahl voiding.

Explain entropy from the perspective of "most probable state of existence".

Calculate defect concentration in solids based on knowledge of activation energy for defect generation and solid solubility limits.

Explain intrinsic and extrinsic defects in ionic solids.

Determine the nature and concentration of extrinsic defects generated by different types of solutes.

Determine the effect of defects on electronic properties of elemental and compound solids.

Understand the relationship between surface tension and surface energy.

Determine the effect of surface curvature on the activity and vapor pressure of surfaces.

Use the Young Equation to determine wettability and wetting of surfaces.

Use surface energy to determine impurity segregation at interfaces.

Describe the different types (categories) of phase transformations.

Explain homogeneous and heterogeneous nucleation.

Explain the effect of supercooling on the thermodynamic driving force and critical radius for homogeneous and heterogeneous nucleation.

Explain the effect of surface tension on the free energy barrier for heterogeneous nucleation.

Calculate rates of nucleation.

Explain the development of TTT diagrams.

Appendix B: References

1. Moore, Physical Chemistry, Prentice Hall. (or any other good text in Physical Chemistry)

2. R.E. Dickerson, Molecular Thermodynamics, W.A. Benjamin, Inc. (1969)

3. Coudurier, et al., Fundamentals of Metallurgical Process, Pergamon (1985)

4. Darken & Gurry, Physical Chemistry of Metals, McGraw Hill, (1953)

5. Gaskell, Introduction to Metallurgical Thermodynamics, McGraw Hill (1973)

6. AIME, Electric Furnace Steelmaking Vol II: Theory and Fundamentals, (1963)

7. Pauling, The Chemical Bond, Cornell University Press (1960)

8. Wefmore and Le Roy, Principles of Phase Equilibria, Dover (1951)

9. Mott and Jones, The Theory of the Properties of Metals and Alloys, Dover (1958)

10. Nernst, The New Heat Theorem, Dover (1969)

11. Swalin, Thermodynamics of Solids, John Wiley, (1962)

12. Wagner, Thermodynamics of Alloys, Addison - Wesley (1952)

13. Alcock, Principles of Pyrometallurgy, Academic Press (1976)

14. Richardson, Physical Chemistry of Melts in Metallurgy, Vol I and II, Academic Press, (1974)

15. Bent, The Second Law, Oxford University Press (1965)

16. Shewmon, Diffusion in Solids, McGraw - Hill (1963)

17. Porter & Easterling, Phase Transformations in Metals & Alloys, Van Nostrand Reinhold (1981)

18. Levenspiel, Chemical Reaction Engineering, John Wiley (1972)

19. Crank, The Mathematics of Diffusion, Oxford Press (1956)

20. Kubaschewski and Alcock, Metallurgical Thermochemistry, 5th Edition, Pergamon Press

21. Garrels and Christ, Solutions, Minerals and Equilibria (1965)

22. Butler, Ionic Equilibrium - A Mathematical Approach, Addison - Wesley (1964)

23. Stumm and Morgan, Aquatic Chemistry, Wiley - Interscience (1970)

24. Shewmon, Transformations in Metals, J. Williams Book Co., (1983)

25. Kingery, et al, Introduction to Ceramics, John Wiley, (1976)

Appendix C: Potential Term Project Topics

- Effect of solute additions on contact angle

- Effect of oxidation/aging of copper substrates on solder adhesion

- Prediction of activity coefficients for aqueous systems

- Modification of Hume-Rothery Rules for systems exhibiting limited solid solubility

- Effect of surface-to-volume ratio on dissolution of particles

- Determination of bond energy from latent heat of melting, latent heat of vaporization and coordination number considerations

- Evaluation of Pauling's formulation for enthalpy of formation of ionic compounds:

  $$\Delta H \text{ (kcal/g-atom)} = -23.07\, Z\, (X_A - X_B)^2$$

- Others – to be decided