

MSE 3001 Syllabus

Chemical Thermodynamics of Materials

Fall Semester 2026
Prof. Robert F. Speyer
Robert.Speyer@mse.gatech.edu

Course Description

Chemical Thermodynamics is foundational to the discipline of Materials Engineering. Concepts based on the first and second laws build one upon another, to provide computational tools as well as an intuition into reaction and phase equilibria as well as the thermodynamics of surfaces and interfaces.

Course Learning Objectives

Upon successful completion of this course, you should be able to:

- Understand the origins of the first (energy conservation) and second (spontaneity) laws of thermodynamics.
- Correlate extensive and intensive functions to equilibrium conditions, and be able to manipulate them in computations consistent with experimental observation.
- Utilize thermodynamic data along with concepts of reaction equilibria to predict flame temperatures and extent of reaction, as examples, to industrial materials processing such as steel manufacture.
- Use solution theory as the basis for developing phase diagrams which accurately describe phase formation processes as a function of temperature.
- Use the phase rule combined with analytical geometry to generate and analyze ternary phase equilibria.
- Develop concepts of surface energy/tension and show its applications in capillarity, colloidal behavior, and solid-state microstructural processes.

Required Course Materials

Printed chapters from the textbook *Applied Chemical Thermodynamics*¹ will be provided. This is the only required resource for the class.

Policies and Etiquette

- All lectures will be live during the class hour, and not recorded. Students are encouraged to email the professor with questions; video conferencing or in-person meetings with individuals and study groups are encouraged and may be set up by appointment. Missed classes or exams may be excused (at the Professor's discretion) for reasons of health, professional or sports travel, so long as requested by email in advance.
- Homework from previous semesters are posted on Canvas as a resource. Matlab programming primers are also posted on Canvas. It is expected that Matlab programming will be done using only the more generic commands enumerated in the primers unless otherwise specified in the assignment.
- It is hoped that the classroom environment is one of learning and interaction. There will be certain pause points during the lecture in which questions are invited, which include requests to repeat portions of the lecture. All students should feel welcome to raise questions during the lecture, preferably with no students remaining silent for the entirety of the semester and no students who overwhelmingly dominate the discourse.

¹Robert F. Speyer, *Applied Chemical Thermodynamics*, 1st Ed., Midtown Scientific Publishing, 2026.

Grading Policy

Grading will be based on attendance (10%), homework (30%) and exams (60%). All grades will be based on a 90 and above is an A, 80-89 is a B,... scale, after a curve is applied.

Description of Graded Components

Attendance: The lecture hour will consist of presentation of the content to be covered that day, answers to student questions, and students answering the Professor's questions to review and refine understanding of the lecture. To be marked as present, students are expected to be attentive (no distractions such as texting), sit in designated seating, actively participate, and make a good-faith effort to answer questions. All electronic devices need to be put away; however, students may audio record the lectures using their phones or other audio devices. Students who are more than five minutes late to class will be counted as absent. Grading: 0-2 missed classes = 100, 3 missed class = 90, 4 missed classes = 80, ...

Homework: Homework is due at the beginning of the class hour (paper copy) on dates indicated in the course calendar (Table 1). Matlab code written for homework must also be emailed to the grader's email address: MSE3001thermo@gmail.com. Students are welcome to collaborate with each other on homework so long as what is turned in is the student's own work. Questions to the Professor are also welcomed regarding the homework (hints but not answers will likely be provided). Students are asked to not submit homework questions to websites such as Chegg. Questions that have been found to have been submitted to such websites may be eliminated from the point total for the homework for the entire class. Further, answers to questions that the graders reasonably believe came from AI sources such as ChatGPT may not be awarded credit. Late homework will receive at most only partial credit, at the discretion of the graders. Homework will not be accepted after graded homework has been handed back.

Exams: Exams will be on the dates indicated on the course calendar (Table 1). They will be 55 minutes long, and open notes (notes that were provided by the Professor). The seventh exam is also 55 minutes long, and will take place during the final exam period (there is no comprehensive final exam). No other resources (additional notes, homework, books, internet access, etc.) are permitted during exams. Additional information may be hand-written into the notes, but not additional pages, notes outside the content tested on that exam, post-it notes, or index tabs. The exam questions may ask students to refer to the notes by a specified page or figure number as part of a question. Answers are to be hand-written into provided blue-books. If calculators and/or rulers are needed, they will be provided. The blue books and the exam question sheets must be submitted together at the end of the exam. Students may appeal the grading of exams and homework. if it is believed a mistake in grading has occurred, or more explanation is requested as to why more credit was not given. The student should email their concerns to the graders at MSE3001thermo@gmail.com. They will respond with either corrected grading or a further explanation for why the requested credit was not awarded. Students should not interact directly with the graders.

Course Topics

1. Gases

- (a) The Ideal Gas Law
- (b) Pressure
- (c) Gas Velocity and Energy
- (d) Gas Pressure Measurement
- (e) Temperature
- (f) Real Gases: A. Condensation; B. Law of Corresponding States; C. Empirical Equations of State for Pure Gases; D. Gaseous Mixtures.

Table 1: Course Calendar

August 24	Ch 1: Gases
August 26	Ch 1: Gases
August 28	Ch 2: First Law
August 31	Ch 2: First Law, Ch 3 Second Law, HW 1 Due
September 2	Ch 3: Second Law
September 4	Exam 1
September 9	Ch 3: Second Law, Ch4: Statistical View of Entropy
September 11	Ch 4: Statistical View of Entropy
September 14	Ch 5: Fundamental Equations
September 16	Ch 5: Fundamental Equations, HW2 Due
September 18	Ch 6: Chemical Thermodynamics
September 21	Exam 2
September 23	Ch 6: Chemical Thermodynamics
September 25	Ch 6: Chemical Thermodynamics, Ch7: Thermodynamic Data
September 28	Ch 7: Thermodynamic Data
September 30	Ch 8: Gaseous Reactions, HW 3 Due
October 2	Ch 8: Gaseous Reactions
October 7	Exam 3
October 9	Ch 8: Gaseous Reactions, Ch 9: Gases and Pure Cond. Phases
October 12	Ch 9: Gases and Pure Cond. Phases
October 14	Ch 10: Raoultian Solutions and Gases
October 16	Ch 11: Condensed Raoultian Solutions, HW 4 Due
October 19	Ch 11: Condensed Raoultian Solutions
October 21	Exam 4
October 23	Ch 11: Condensed Raoultian Solutions
October 26	Ch 12: Immiscibility
October 28	Ch 12: Immiscibility
October 30	Ch 13: Binary Systems and Phase Rule, HW 5 Due
November 2	Ch 14: Ternary Phase Equilibria
November 4	Exam 5
November 6	Ch 14: Ternary Phase Equilibria
November 9	Ch 14: Ternary Phase Equilibria
November 11	Ch 15: Surface Energy
November 13	Ch 15: Surface Energy, HW 6 Due
November 16	Ch 15: Surface Energy
November 18	Exam 6
November 20	Ch 16: Colloidal Effects
November 23	Ch 16: Colloidal Effects, Ch 17: Condensed Phase Interfaces
November 30	Ch 17: Condensed Phase Interfaces
December 2	Ch 17: Condensed Phase Interfaces, HW 7 Due
December 4	Ch 17: Condensed Phase Interfaces
TBD	Final Exam

2. First Law
 - (a) Work
 - (b) Cycles
 - (c) The First Law
 - (d) Restrictive Conditions: A. Constant Volume; B. Constant Temperature; C. Adiabatic.
3. Second Law
 - (a) The Carnot Cycle
 - (b) The Thermodynamic Temperature Scale: A. Cycle Efficiency Based on Reservoir Temperatures; B. Thermodynamic Requirements for Temperature.
 - (c) Entropy
 - (d) The Clausius Inequality
 - (e) Entropy as an Indicator of Spontaneity
 - (f) Applied Cycles: A. Otto and Diesel Cycles; B. Rankine Cycle; C. Refrigeration and Heat Pumps.
4. Statistical View of Entropy
 - (a) Binary Systems
 - (b) Equilibrium Among Interacting Subsystems
 - (c) Multiplicity and Entropy
 - (d) Spontaneous Subsystem Changes
 - (e) Thermal Entropy in States of Matter
 - (f) Configurational Entropy: A. Effect of Volume; B. Homogenization of a Mixture; C. Entropy of Mixing; D. Gas Diffusion; E. Entropy Springs.
 - (g) Thermal and Configurational Entropy
5. The Fundamental Equations
 - (a) Enthalpy
 - (b) First Law with Entropy
 - (c) Spontaneous Heat Transfer: A. Between Reservoirs; B. Quenching into a Reservoir; C. Between Subsystems of Finite Extent; D. Reversible Cooling.
 - (d) Maxwell Relations
 - (e) Conversion of Thermodynamic Derivatives
 - (f) Isothermal Internal Energy Changes in Real Gases
 - (g) Heat Capacity: A. Debye Model for Solids; B. Ideal Gases.
 - (h) Joule-Thomson Throttling
 - (i) Cryogenic Liquids
6. Chemical Thermodynamics
 - (a) Phase Transformations: A. Equilibrium among Condensed Phases; B. Condensed Phase-Vapor Equilibrium; C. Vaporization in Open Systems.
 - (b) Intensive and Extensive Properties
 - (c) Equilibria in Multiphase Systems
 - (d) Spontaneity and Equilibrium for Isothermal Processes: A. Helmholtz and Gibbs Energies; B. Intensive Variables.

- (e) Entropy-Energy Competition: A. Vapor Pressure; B. Solubility.
 - (f) Thermodynamics of Vacancy Formation
 - (g) Unary Phase Equilibria: A. Chemical Potential of a Single-Component System; B. Coexistence Curves; C. Interpretation of the Phase Diagram; D. Supercritical Fluids.
 - (h) Climate
 - (i) Vapor Pressures with a Foreign Gas: A. Chemical Potentials Across a Semipermeable Membrane; B. Enhanced Ideal Gas Vapor Pressure; C. Enhanced Vapor Pressures of Real Gases.
 - (j) Le Châtelier's Principle
7. Thermodynamic Data
- (a) Temperature Dependence
 - (b) Temperature Trends of Heat Capacity
 - (c) Formation Reactions
 - (d) Calorimetry: A. Drop Calorimetry; B. Adiabatic Calorimetry; C. Bomb Calorimetry; D. Solution Calorimetry; E. Continuous Flow Calorimetry.
 - (e) Thermodynamic Approximations
8. Gaseous Reactions
- (a) Combustion: A. Heat of Reaction; B. Flames; C. Adiabatic Flame Temperature
 - (b) Combustion Calculations
 - (c) True Adiabatic Flame Temperatures
 - (d) The Equilibrium Constant
 - (e) Trends in $\Delta G_{\text{rxn}}^{\circ}$ with Temperature
 - (f) Predominance of Reactants or Products
 - (g) Coupled Equilibria
 - (h) Pressure Effects Equilibrium
 - (i) Fugacity: A. Definition; B. Relation to the Pressure of a Single-Component Gas; C. Lewis and Randall Rule; D. Applied to Ammonia Formation.
9. Gases and Pure Condensed Phases
- (a) Equilibrium Constant with Condensed Phases
 - (b) Controlling Low Levels of Oxygen Partial Pressure
 - (c) Equilibria among $\text{C}_{(s)}$, $\text{CO}_{(g)}$, $\text{CO}_{2(g)}$ and $\text{O}_{2(g)}$
 - (d) Reduction of Oxides
 - (e) The Gibbs-Helmholtz Relation
 - (f) Predominance Area Diagrams
 - (g) Metallurgy: A. Mineral Origins; B. Commercially Important Deposits; C. Extraction and Beneficiation; C. Iron Production; D. Steel Production; E. Copper Smelting.
10. Raoultian Solutions and their Vapors
- (a) Raoult's and Henry's Laws
 - (b) Measurement of Vapor Pressure
 - (c) Phase Diagrams of Raoultian Liquids and their Vapors: A. Fixed Volume; B. Fixed Total Pressure; C. Fixed Temperature.
 - (d) Fractional Distillation

11. Condensed Raoultian Solutions
 - (a) Chemical Equilibrium Revisited: A. Mathematical Approach; B. Chemical Potentials in Multi-component Equilibria.
 - (b) Partial Molar Gibbs Energy of Mixing
 - (c) Condensed Solutions and a Reactive Gas
 - (d) Osmotic Pressure
 - (e) The Gibbs-Duhem Equation
 - (f) The Tangent Rule: A. Integral Molar Gibbs Energy of Mixing; B. Graphical Construction.
 - (g) Raoultian Solid and Liquid Solutions: A. The Silicon-Germanium Phase Diagram; B. Activities in the Ge-Si Binary System; C. Interpreting the Phase Diagram.
12. Immiscibility
 - (a) Integration of the Gibbs-Duhem Equation
 - (b) Regular Solutions: A. Atomistic Formulation; B. Condensed Conjugate Phases; C. Activities of Regular Solutions; D. Sub-Regular Solutions; E. Azeotropes.
 - (c) Extent of Solid Immiscibility
 - (d) Raoultian Liquid Conjugate with a Pure Solid: A. Liquidus Curves; B. Freezing Point Depression.
 - (e) Binary Phase Diagrams of Regular Solutions
13. Binary Systems and the Phase Rule
 - (a) Intermediate Compounds
 - (b) Experimental Methods for Phase Diagrams
 - (c) The Gibbs Phase Rule: A. Formulation; B. Phases and Components; C. Applications of the Phase Rule.
14. Ternary Phase Equilibria
 - (a) Compositions within the Gibbs Triangle: A. Single-Phase Composition; B. Tie Lines for a Conjugate Phase Pair; C. Tie Triangles for Three Conjugate Phases.
 - (b) Ternary Phase Diagrams with Immiscible Solids: A. Thermodynamic Basis; B. A Hypothetical Ternary System; C. The CaO-Al₂O₃-SiO₂ System.
 - (c) Ternary Systems with Solid Solution: A. Thermodynamic Basis; B. Isothermal Sections.
 - (d) The MgO-FeO-SiO₂ System
15. Surface Energy
 - (a) Surface Energy and Surface Tension
 - (b) Young-Laplace Equation: A. Spherical Interface; B. Non-Spherical Interface.
 - (c) Capillary Action
 - (d) Measurement of Liquid Surface Energy: A. Capillary Rise with a Spherical Cap Meniscus; B. Capillary Rise with a Non-spherical Meniscus; C. Wilhelmy Plate.
 - (e) Trends in Liquid Surface Energies: A. Bond Strength; B. Temperature.
 - (f) Applied Capillarity: A. Familiar Examples; B. Capillarity in Materials Processing; C. Capillarity in Materials Characterization.
 - (g) Equilibrium Shapes of Crystals
16. Colloidal Effects and Surface Segregation

- (a) The Kelvin Equation: A. Thermodynamic Formulation; B. Applications; C. Experimental Verification.
 - (b) Effect of Colloid Size: A. Melting Temperature; B. Liquid Solubility.
 - (c) Gibbs Dividing Surface: A. Thermodynamic Formulation; B. Examples.
 - (d) Surfactants: A. Surfactant Molecules and Micelles; B. Detergents and Emulsions; C. Foams; D. Froth Flotation.
17. Condensed Phase Interfaces
- (a) Young Dupré Equation: A. Derivation; B. Interpretation
 - (b) Measurement of Contact Angle
 - (c) Solid Surface Irregularities: A. Wenzel Surfaces; B. Contact Angle Hysteresis; C. Cassie Surfaces; D. Superhydrophobic Surfaces.
 - (d) Interfaces of Insoluble Liquids
 - (e) Grain Boundaries: A. Origins; B. Dihedral Angles.
 - (f) Measurement of Solid Surface Energies
 - (g) Solid State Sintering: A. Initial Stage; B. Intermediate and Final States; C. Grain Growth and Pore Coarsening; D. Sintering Toward Theoretical Density.

Additional References²

1. D. R. Gaskell, *Introduction to the Thermodynamics of Materials*, 5th Ed., Taylor and Francis, Washington, DC, 2008.
2. W. J. Moore, *Physical Chemistry*, 4th Ed., Prentice Hall, Englewood Cliffs, NJ, 1972.
3. G. W. Castellan, *Physical Chemistry*, 3rd Ed., Addison-Wesley, Reading, MA, 1983.
4. K. Denbigh, *The Principles of Chemical Equilibrium*, 4th Ed., Cambridge University Press, Cambridge, UK, 1981.
5. C. G. Bergeron and S. H. Risbud, *Introduction to Phase Equilibria in Ceramics*, American Ceramic Soc., Westerville, OH, 1984.
6. F. N. Rhines, *Phase Diagrams in Metallurgy, Their Development and Application*, McGraw-Hill, New York, 1956.
7. H. B. Callen, *Thermodynamics and an Introduction to Thermostatistics*, 2nd Ed., John Wiley and Sons, New York, 1985.
8. O. Kubaschewski, C. B. Alcock, and P. J. Spencer, *Materials Thermochemistry*, 6th Ed., Pergamon Press, New York, 1993.
9. C. Kittel and H. Kroemer, *Thermal Physics*, 2nd Ed., W. H. Freeman and Company, San Francisco, CA, 1980.
10. R. E. Reed-Hill, *Physical Metallurgy Principles*, 2nd Ed., Brooks Cole Engineering Division, Monterey, CA, 1973.
11. T. Rosenqvist, *Principles of Extractive Metallurgy*, McGraw Hill, New York, 1974.
12. A. Prince, *Alloy Phase Equilibria*, Elsevier Publishing Company, New York, 1966.
13. M. W. Zemansky and R. H. Dittman, *Heat and Thermodynamics*, 6th Ed., McGraw Hill Book Company, New York, 1981.

²Available at the Georgia Tech Library.

14. P. G. Shewmon, *Diffusion in Solids*, J. Williams Book Company, Jenks, OK, 1983.
15. D. V. Ragone, *Thermodynamics of Materials*, Volume 1, John Wiley and Sons, New York, 1995.
16. F. W. Sears, M. W. Zemansky, and H. D. Young, *University Physics*, 5th Edition, Addison-Wesley, Reading, MA, 1976.
17. R. J. Reed, *North American Combustion Handbook*, Volume 1, 3rd Edition, North American Manufacturing Company, New York, NY, 1985.
18. D. A. McQuarrie and J. D. Simon, *Physical Chemistry, A Molecular Approach*, University Science Books, Hendron, VA, 1997.
19. F. T. Wall, *Chemical Thermodynamics*, 3rd Ed., W. H. Freeman and Company, San Francisco, CA, 1974.
20. I. M. Klotz and R. M. Rosenberg, *Chemical Thermodynamics*, 6th Ed., John Wiley and Sons, New York, 2000.
21. R. DeHoff, *Thermodynamics in Materials Science*, 2nd Ed., Taylor and Francis, Boca Raton, FL, 2006.
22. T. Engel and P. Reid, *Thermodynamics, Statistical Thermodynamics, and Kinetics*, 4th Ed., Pearson Education, Upper Saddle River, NJ, 2019.
23. Y. A. Cengel and M. A. Boles, *Thermodynamics, and Engineering Approach*, 4th Ed., McGraw Hill, Boston, MA., 2002.
24. C. H. P. Lupis, *Chemical Thermodynamics of Materials*, Prentice-Hall, Englewood Cliffs, NJ, 1983.
25. W. Z. Black, and J. G. Hartley, *Thermodynamics*, 3rd Ed., HarperCollins, New York, 1996.
26. A. W. Adamson and A. P. Gast, *Physical Chemistry of Surfaces*, 6th Ed., John Wiley and Sons, New York, 1997.
27. H. Butt, K. Graf, and M. Kappl, *Physics and Chemistry of Interfaces*, 3rd Ed., Wiley-VCH, Weinheim, Germany, 2013.
28. G. H. Meier, *Thermodynamics of Surfaces and Interfaces*, Cambridge University Press, Cambridge, UK, 2014.

Academic Integrity

Georgia Tech aims to cultivate a community based on trust, academic integrity, and honor. Students are expected to act according to the highest ethical standards. Review Georgia Tech's Honor Code and the student Code of Conduct.

Any student suspected of cheating or plagiarism on a quiz, exam, or assignment will be reported to the Office of Student Integrity, who will investigate the incident and identify the appropriate penalty for violations.

Accommodations for Students with Disabilities

If you are a student with learning needs that require special accommodation, contact the Office of Disability Services (404-894-2563) as soon as possible to make an appointment to discuss your special needs and to obtain an accommodations letter. Please also e-mail me as soon as possible in order to set up a time to discuss your learning needs.

Student-Faculty Expectations Agreement

At Georgia Tech, we believe that it is important to strive for an atmosphere of mutual respect, acknowledgment, and responsibility between faculty members and the student body. The Student-Faculty Expectations articulate some basic expectations that you can have of me and that I have of you. In the end, simple respect for knowledge, hard work, and cordial interactions will help build the environment we seek. Therefore, I encourage you to remain committed to the ideals of Georgia Tech while in this class.