Materials Science and Engineering 422
Thermodynamics

Instructor: Dr. Bill Fahrenholtz
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Time: MWF 9:00 to 9:50 am, 201 Engineering Management

Office Hours: Drop by anytime. If you can't find me, make an appointment by email. Email is also an excellent way to get questions answered.

Course Objective: The goal of this course to develop critical thinking and analytical problem solving skills related to macroscopic thermodynamics

Required Text: D.R. Gaskell, Introduction to the Thermodynamics of Materials, 5th Edition

Supplemental Texts D.V. Ragone, Thermodynamics of Materials, Vol 1 and 2
C.H.P. Lupis, Chemical Thermodynamics of Materials

Lectures: The lectures will discuss fundamental phenomena that control the behavior of materials. Students are expected to contribute to the discussions of each lecture topic and class participation will be a significant part of the grade.

Reading/Quizzes: It is the student's responsibility to keep up with the reading. Assigned readings from the required text are listed in the syllabus. A quiz over the reading will be given on the first day of each of the five sections of the course. Unannounced quizzes may also be given periodically through the semester.

Group Projects: Each of the sections of the course will culminate with a discussion session. The discussions will focus on the critical evaluation of a paper from the recent technical literature. A group will be assigned to lead the discussion of each paper. Details are provided on the "Group Projects" sheet that follows.

Individual Projects Each individual will complete a semester project for this course. The project will include an oral presentation and a written report.

Final Exam: The written report and the oral presentation for the individual project will serve as the final exam for this class.

Grading:

Individual project	40%
Group project	20%
Quizzes	10%
Class participation	10%
Homework	20%

$A \geq 90 > B \geq 80 > C \geq 70 > D \geq 60 > F$

Cheating: The Missouri S&T policy on academic dishonesty (e.g. cheating, plagiarism) allows the instructor to make a judgment about the student's grade on the work in question and requires that alleged cases of academic dishonesty be reported to the Primary Administrative Officer.

Class	Date	Lecture Topic	Assignment
1	8/22	Course overview, project assignments	
2	8/24	Nomenclature, review of undergraduate material	Review Gaskell, Ch 1-9
3	8/26	G and activity	Gaskell, Ch. 10
4	8/29	Regular solutions	
5	8/31	Standard states	
6	9/2	G and phase diagrams	
	9/5	**No class, Labor Day Holiday**	
7	9/7	Binary isoplethal analysis	
8	9/9	**Critical Analysis 1: Binary phase equilibria**	Paper 1
9	9/12	Reaction equilibria in gas mixtures	Gaskell, Ch. 11
10	9/14	Effects of T and P on equilibria	
11	9/16	pO_2 control in practical systems	Project title due
12	9/19	**Critical Analysis 2: Gaseous equilibria**	Paper 2
13	9/21	Gas-solid reactions	Gaskell, Ch. 12
14	9/23	The effect of temperature on equilibrium	
15	9/26	Phase stability diagrams	
16	9/28	Ellingham diagrams	
17	9/30	Passive and active oxidation	
18	10/3	Volatility diagrams	
19	10/5	**Critical Analysis 3: Gas-solid reactions**	Paper 3
20	10/7	Criteria for equilibria	Gaskell, Ch. 13.1-13.6
21	10/10	Binary solutions and Gibbs' phase rule	
22	10/12	Compound formation	
23	10/14	**Critical Analysis 4: Binary solution equilibria**	Paper 4
24	10/17	**No Class: MS&T Houston**	
25	10/19	**No Class: MS&T Houston**	
26	10/21	Solubility of gases in metals	Gaskell, Ch. 13.7-13.11
27	10/24	Activity in solution with several dissolved species	Project abstract due
28	10/26	Models for activity in solution	
29	10/28	Interaction coefficients	
30	10/31	**No Class: Composites at Lake Louise Conference**	
31	11/2	**No Class: Composites at Lake Louise Conference**	
32	11/4	**No Class: Composites at Lake Louise Conference**	
33	11/7	**Critical Analysis 5: Complex solution behavior**	Paper 5
34	11/9	Ternary Introduction	No reading/no quiz
35	11/11	Cooling path analysis	Project outline due
36	11/14	Ternary Isoplethal Analysis	
37	11/16	Solution systems	
38	11/18	Case study: Liquid phase sintering	
	11/21	**No Class, Thanksgiving Break**	
	11/23	**No Class, Thanksgiving Break**	
	11/25	**No Class, Thanksgiving Break**	
39	11/28	**Critical Analysis: Complex Solution Behavior**	Paper 6
40	11/30	**No Class: SERDP Symposium**	
41	12/2	**Student project presentations**	Draft paper due
42	12/5	**Student project presentations**	
43	12/7	**Student project presentations**	
44	12/9	**Student project presentations**	
	12/13	**Student project presentations 10:30 am-12:30 pm**	Final paper due 5:00 pm

Review Materials

Some review materials are available on Blackboard. The posted resources include example problems, homework problems and solutions from a prior course (Met 478), and notes from a former version of the undergraduate thermo course that I teach (Cer 259). If you need additional help with the basic concepts, please see me outside of class to discuss an appropriate course of action.

Group Projects

Each section of the course will include a group project. Project groups will be assigned in class. The group projects will focus on the critical evaluation of papers from the recent technical literature. For this assignment, you want to take the position that the group is acting as one of the reviewers who will make a recommendation to an editor as to whether the paper should be published in the journal (pretend it has just been submitted, not published). The papers will be selected based on their relevance to the course topics. The groups are expected to prepare an analysis of the paper that focuses on the value of the contribution to the field. The groups will also search the technical literature to collect several (3 to 5) related papers that they will use in their analysis. After analyzing the assigned paper, the groups will make a presentation (~15 min) that gives a short overview (the class has read the paper, so be brief) of the assigned paper, analyzes its strengths and weaknesses, presents corroborating or competing theories from the literature, raises questions for discussion, and then makes a recommendation for or against publication. Following the presentation, the entire of the class is expected to participate in a discussion of the paper. Evaluation of the presentation by your peers in the class and the instructor will determine the grade for the group projects. At the option of the instructor, within group peer evaluations may also be used as part of the evaluation.

Some of the factors that you want to consider in your analysis of your manuscript include: 1) the fit of the paper with the scope and aims of the journal in which it was published; 2) the quality of the new insight into behavior provided by the paper; 3) the thoroughness of the literature review; 4) any potential controversy regarding the analysis or conclusions of the paper; and 5) the potential impact of the manuscript. To do this properly, you will need to do some research on the journal in which the paper was published in addition to finding other papers on similar topics. As an example of what reviewers are asked to do, information from the Journal of the American Ceramic Society is included.

Instructor and Peer Evaluation of Presentation

Style/Format (30%)		**Max**	**Grade**
Time	15 ± 2 min = 10 pts; subtract 2 pts for each minute outside range	10	
Style	Layout, effective color usage, clarity of tables/graphs	10	
Delivery	Clear voice, no annoying mannerisms, eye contact, etc.	10	
Substance (70%)			
Overview	Summarized scope/aim of journal & important parts of the paper	15	
Strengths	Identified strengths, pointed out new insight gained from paper	10	
Weaknesses	Identified shortcomings, mistakes, errors in logic, etc.	10	
Other papers	Reviewed the relevant technical literature	10	
Recommendation	Was the paper suitable for publication in this journal?	10	
Discussion points	Suggested appropriate discussion topics	15	
	Total	**100**	

Example Review Criteria for a Peer-Reviewed Technical Journal

REVIEW CRITERIA: Articles published in the Journal of the American Ceramic Society must:

- Fit within the scope of the Journal and be of interest to its readers.
- Report original research and contain substantially new and interesting results that are of sufficient importance to justify publication
- Be written using proper English style and grammar.
- Be well organized with an abstract that concisely conveys the contribution of the manuscript to the technical literature (purpose, approach, results and consequences). In addition, the introduction should describe the reason for the study and describe how the present study differs from past studies.
- Include a thorough literature review with an appropriate list of references from relevant studies or other sources.
- For experimental studies, include a methodology or experimental procedure that is well conducted, designed, and described. This should include the number of tests performed, the number of specimens used, their dimensions, etc. The use of standard experimental procedures is encouraged. If appropriate, the authors should also perform suitable statistical tests to justify their conclusions. Provide enough experimental details that the work can be reproduced. For theoretical work or simulations, the procedure should be verifiable and with appropriate checks for accuracy.
- Clearly display the information in the micrographs and figures, including scale markers and captions that clearly convey their intended message.
- Contain only the number of figures and tables that are necessary to describe the technical content.
- Logically discuss the results in way that leads to a set of sound conclusions.

Content Questions: If you answer "no" to either of the following 2 questions, indicate specific reasons and recommend rejection

1. Does the paper fit within the scope of the journal and is it of interest to Journal readers?
2. Does the paper contain new and interesting results?

Language

1. Are the English style and grammar satisfactory?

Structure

1. Is the title satisfactory? If not, please suggest an alternative title in your written comments.
2. Is the paper well organized and does the abstract concisely convey the contribution of the manuscript to the technical literature (purpose, approach, results and consequences)? Does the manuscript contain original research that is of enduring value and add significantly new and fundamental advances to the ceramic science field? If no, please explain in your written comments.
3. Is the literature review adequate, such that it identifies the appropriate background for the paper? (If not, it would be useful if you could give references or author names).
4. For experimental studies, is the experimental procedure well conducted, designed, and described? Are the numbers of specimens, specimen dimensions, number of tests, etc., clearly indicated? Where Applicable, did the authors perform suitable statistical tests to justify their conclusions? Did the authors provide enough experimental details that the work can be reproduced? For theoretical work, is the procedure verifiable and include appropriate checks for accuracy?
5. Do micrographs clearly display the information the authors wish to show? Are the magnifications clearly displayed with scale markers? Do the figures and their captions convey the intended message clearly? (If no, please specify your concerns.)
6. Are all the text, figures, or tables necessary in describing the technical content? (If no, please indicate items you think should be omitted or shortened in your written remarks.
7. Are the conclusions logical and justified? (If no, please explain why you disagree).

Quality and Impact

1. Please rank the overall scientific quality of this paper (high, good, average, below average, poor).
2. Please rank the expected impact of this paper to the materials science community (high, good, average, below average, poor).

Recommendation

Accept, minor revision, major revision, or reject. Support your recommendation with your comments.

Comments

In this section, you should identify the main strengths and weaknesses of the article plus address any concerns that you have identified above. Note that most journals have blind reviews so the authors do not know the identity of the reviewers.

Individual Projects

Each student will complete an individual project during the semester. The project format is designed to be similar to what is expected for the contribution of a presentation and a peer-reviewed proceedings paper to a technical conference. The focus of the project will be an original thermodynamic calculation; several possible topics are listed on the next page. Ideally, each student will select a problem that is relevant to his/her thesis research focus. However, since the course is taken during the first semester of graduate school for many students, this will not be possible in all cases. The major milestones for the project are: 1) topic selection; 2) abstract preparation; 3) outline; 4) paper draft for peer review; 5) presentation; and 6) final paper submission. Instructor and/or peer feedback will be provided at steps 1, 2, 3, and 4. You may also submit a preview copy of your presentation for comments prior to your scheduled presentation. Grades will only be assigned for steps 5 and 6, although the instructor may use participation credit to penalize students who do not meet the deadlines.

Topic Selection

Students can select any appropriate topic that involves a detailed, original thermodynamic calculation. A list of some suggested topics is provided on the next page. **Topics should be selected no later than 5:00 pm on September 16**. You may discuss potential topics with the instructor anytime up to the deadline. Topics should be submitted by email to the instructor. It may be acceptable to change your topic after it is selected, if you discuss it with the instructor.

Abstract

After the topic is selected, each student will prepare a 150 to 200 word abstract. The abstract should describe the focus of the project, the methods that will be used to achieve the goal, and the significant results that are anticipated. The abstract should be double spaced, 12 point, times new roman font with one inch margins. The file should include the title of the talk/paper, the author's name, and the author's affiliation in addition to the abstract. **The abstract is due no later than 5:00 pm on October 24.** Abstracts should be submitted as a MS Word document attached to an email to the instructor. As with a technical conference, it is a good idea to validate the approach that you intend to use for your project and even have some preliminary results prior to submission of your abstract

Outline

A detailed outline is due no later than 5:00 pm on November 11. The outline should be attached to an email to the instructor. The document should be a MS Word file up to 5 pages long (12 point font, double spaced, 1 inch margins). You should include a list of two or three critical references and an example calculation. Some students may also wish to include a figure or two to demonstrate the validity of their approach. The outline should describe the major parts of your talk and provide some details about preliminary results along with expected outcomes.

Peer Review of Draft Paper

Draft manuscripts are due in class on Friday, December 2. Each student should bring two hard copies of his/her paper to class. The draft paper should be complete in that it should include all of the figures, calculations, tables, literature review, and analysis that you intend to include in your final version. At this stage, papers should be **DOUBLE-SPACED** and **DO NOT** have to conform to the formatting requirements for the final paper. Each student will be given one paper in class and will be expected to review the paper by Monday, December 5. The instructor will complete a second evaluation of each paper. Critiqued papers will be returned to the authors on Monday, December 5.

Presentation

Each individual will present his/her results to the class. The presentation should be 12 ± 1 minutes in length. The presentations should include background information regarding the problem, details of the methods used to attack the problem, graphical and tabulated results, analysis of results, and conclusions. The presenters should be prepared to answer questions from the instructor and the class following the presentation. Presentations will be graded using the sheet that follows. Presentations will be made in class on the dates listed on the syllabus. The exact dates of the presentations will be assigned by the instructor around the end of November.

Final Paper

The final paper is due on Tuesday, December 13 no later than 5:00 pm. The final version should be a PDF file that is emailed as an attachment to the instructor. The formatting requirements and page limitations are given in a separate section below. The format is based on that used for submissions to proceedings of American Ceramic Society conferences. The papers will be graded based on format and content, with emphasis placed on the clarity of the argument and the depth of the analysis.

Potential Project Topics

Graphical Representation of Information

1. Calculated phase diagrams
2. Phase stability diagrams
3. E-pH diagrams
4. Ellingham diagrams
5. Volatility diagrams

Description of Physical Phenomena

1. Calculation of driving forces (e.g., densification, solubility, phase changes) as a function of process parameters (e.g., temperature, pressure, particle size, electric field, magnetic field, applied stress).
2. Evaluation of the inter-relationships among properties (e.g., Heckman diagrams, adiabatic thermo-elastic effect, piezoelectric coupling coefficients).
3. Description of why high temperature phases tend to have higher symmetry than lower temperature phases
4. The use of advanced materials for membranes and separation
5. Thermodynamic analysis of common objects (e.g., lightbulb filaments, vapor lamps, fireworks, combustion of fossil fuels, or other topics)

Corrosion and Gas Phase Reactions

1. Conditions for stability and attack in aqueous environments, Pourbaix/E-pH diagrams
2. The effect of atmosphere on stoichiometry, volatilization
3. Active/passive corrosion, application of volatility diagrams to gaseous corrosion
4. The use of Ellingham diagrams in mineral processing
5. Sensors

Phase Equilibria

1. Activity coefficients in metal or ceramic systems
2. Control of microstructure by understanding and controlling solid solution
3. Comparison of calculated and experimental phase relations

Presentation Grading Sheet for Individual Project

Style (30%)		**Max**	**Grade**
Time	10 to 12 = 10 pts; subtract 2 pts for each minute outside range	10	
Format	Layout, effective color usage, clarity of tables/graphs	10	
Delivery	Clear voice, no annoying mannerisms, eye contact, etc.	10	
Substance (70%)			
Background information	Problem was defined, literature reviewed, objective stated	15	
Procedure	Details of the calculation method, any experimental details	15	
Presentation of data	Appropriate graphs, figures, and tables were included	10	
Analysis of results	Results were discussed and placed into context	20	
Conclusions	Effectively summarized the effort	10	
	Total	**100**	

Paper Grading Sheet for Individual Project

Style (30%)		**Max**	**Grade**
Length	The target page limit was met	10	
Format	The layout met the formatting requirements	10	
Grammar/usage	The writing was appropriate for a technical paper.	10	
Substance (70%)			
Background information	Problem was defined, literature reviewed, objective stated	15	
Procedure	Details of the calculation method, any experimental details	15	
Presentation of data	Appropriate graphs, figures, and tables were included	10	
Analysis of results	Results were discussed and placed into context	25	
Conclusions	Effectively summarized the effort	5	
	Total	**100**	

PLEASE REPLACE THIS TEXT WITH THE TITLE OF YOUR PAPER. ALIGN FLUSH LEFT, ALL CAPS, DO NOT BOLD, 12 PT FONT

Author Name
Affiliation
Address
City, State, Zip

ABSTRACT

Limit your abstract to 200 words or less. Use single spacing and indent the first line of each paragraph by one tab. Your paper should be no more than 8 pages.

INTRODUCTION

The text should be justified, Times New Roman font, 12 point. Use single spacing and indent the first paragraph by one tab (0.5 inches). Do not insert a space between paragraphs within each section.

The word "INTRODUCTION" above is an example of the main heading style. Do not number or letter your headings. Insert one space between the heading and the body of the last line of text from the previous section. Your paper should be divided into several distinct sections such as INTRODUCTION, CALCULATIONS, RESULTS AND DISCUSSION, CONCLUSIONS, and REFERENCES.

The page dimensions should be US Style, 8.5 by 11 inches. Margins should be 1 inch at the top, bottom, right and left. Papers should be no more than 8 pages total, which includes text, figures, tables, and references.

Center graphs, figures, tables and equations within the text as soon as possible after they are mentioned. Number tables with Roman numerals (I, II, III, etc.) followed by the table title and place above the table. Figure captions should be placed below the figures. Figures should each be numbered consecutively with numerals (1, 2, 3, etc.). Number equations consecutively in parentheses at the right-hand margin, in line with the last line of the equation. Equations, tables, and figures should be separated from the text by one blank line above and below.

REFERENCES

Place references at the end of your paper. Use the following format:

1. E. Traversa, S. Villanti, G. Gusmano, H. Aono, and Y. Sadaoka, "Design of Ceramic Materials for Chemical Sensors: $SmFeO_3$ Thick-Films Sensitive to NO_2," Journal of the American Ceramic Society, 82(9) 2442-2450 (1999).
2. D.R. Gaskell, Introduction to the Thermodynamics of Materials, 4th Edition, Taylor and Francis, New York (2003).
3. R.A. Cutler, "Engineering Properties of Borides," pp. 787-803 in Ceramics and Glass: Engineered Materials Handbook Vol. 4, ed. by S.J. Schneider, Jr., ASM International, Materials Park, OH (1991).

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* These instructions are based on the format requirements for the Ceramic Engineering and Science Proceedings series papers published by the American Ceramic Society.