STATISTICAL THERMODYNAMICS & MECHANICS OF MATERIALS

MSE 500 **Fall 2017**

Instructor : Professor Ken Schweizer
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MWF, 9-10:50 am, Ceramics 218 **TA: none**

TIMES: The class is formally scheduled to meet from 9 – 10:50 am. The reasons are: (i) the course is based on regular 75-80 minute classes, and (ii) to allow flexibility in making up canceled classes due to my possible travel. ***Typically, we will meet for ~ 75 minutes, so 9 -> 10:15 am.*** When/ if I need time for makeups, class may go an extra 15-20 minutes.

ROOM: The course is highly quantitative, with derivations and mathematical analysis playing a key role. The material is largely delivered the "old fashioned" way --- by writing on the blackboard. ***Thus, I insist that all students sit as close to the blackboard as possible, NOT in the last 2-3 rows of this rather large classroom.*** I will endeavor to write large enough to be visible to all; if I fail to do this, just shout out and tell me!

OFFICE HOURS: Flexible, since the class is large, with students from diverse departments (typically 5 different ones) it is too hard to set just one time. Please send me an email when you want to meet. I typically respond quickly. Please do not hesitate to come see me with questions about the class lectures or homework. ***I very much welcome this.***

HOMEWORK: No TA, so not collected/graded. I will give you the answers.

EXAMS: Two in class midterms (90 minutes) cover parts I & II, respectively.

First exam : **(tentative) Wednesday, October 11**

Second exam : **(tentative) Monday or Wednesday, November 13 or 15**

Final Exam: Comprehensive, 3 hour exam but will strongly emphasize part III.

ALL Exams are CLOSED book. You can bring one sheet (ONE side) of formulas/information you think important. Putting such a sheet together is a good review experience of identifying what is really important.

Grading :

Homework will be given essentially every week and is a large ***key to learning***. I suggest you first work hard on it ***alone***. If you have difficulties, then discuss the problems with each other. STUDENTS WHO HAVE TROUBLE WITH THE COURSE ALMOST ALWAYS MAKE THE INITIAL MISTAKE OF NOT FIRST WORKING HARD BY THEMSELVES ON THE HOMEWORK. YOU LEARN NOTHING BY LOOKING AT ANSWERS IF YOU HAVE NOT ALREADY ATTEMPTED THE PROBLEMS YOURSELF. Homework will not be collected, but I will pass out an answer key. It is your job to carefully study this, and see what you did not get correct. If you then have any questions, please come see me!

Final course grade determined ROUGHLY as follows.

Exam 1: 20-30%　　　Exam 2: 20-30 %　　　Final: 40-60 %

I determine the weighting factor for the mid-terms versus the final in a manner that optimizes your composite exam average.

****REQUIRED TEXT**

KD: Ken A. Dill and Sarina Bromberg, *Molecular Driving Forces – Statistical Thermodynamics in Chemistry and Biology*, Garland Science, Taylor & Francis Group, New York and London, ***2nd edition.*** This book, and its 1st edition, are on reserve in the Grainger Library.

RECOMMENDED BOOKS on reserve in Grainger Engineering Library

DC : David Chandler, *Introduction to Modern Statistical Mechanics*, 1987.

McQ : Donald A. McQuarrie, *Statistical Mechanics*, 2000.

TLH : T.L.Hill, *Introduction to Statistical Thermodynamics*, 1960.

NG : N.Goldenfeld, *Lectures on Phase Transitions & Renormalization Group.*

PM : P.M. Morse, *Thermal Physics*, second edition, 1969.

Book abbreviations employed in the suggested reading for each topic in the course outline given below.

LECTURES and ADVICE :

It is ***very important*** to regularly attend class, ***take good notes***, and ***ask questions. Please feel free to shout out if you have a question in case I do not see your hand up. Do not be shy...all questions are good questions!***

I urge you to not fall behind since this is a fundamental science course that continuously builds on prior material, and integrates the concepts and methods throughout the semester. It is not easy to recover from a "bad start". For MSE PhD grad students this is especially important since you must receive a "B" or higher so that it counts towards passing the qualifying exam. Unfortunately, every year a few students receive a course grade below "B". But there is no mandate this must happen, and it can be avoided by good study habits and effort. I strongly suggest you review your notes after every class, and also supplement them as needed with the suggested reading of books on the recommended list.

For some topics I will follow the Dill book. For ***many*** others I will not. For a few topics there is ***nothing*** in the textbook. Even if I follow Dill, I may sometimes/often do things in a different order or manner for clarity. In all cases I strive to provide additional explanation not in any texts. More reason to take good notes.

FRIENDLY WARNING:

Statistical thermodynamics and mechanics is a quantitative science that requires mathematics. If your math skills are rusty then I urge you to brush up on basic calculus of one and many variables, differentiation, integration, etc. Note the Dill book has nice review material on the math tools. I will NOT cover these in class, but read these chapters if needed. ***This includes the elementary probability and statistics of Dill chapter 1 which I will only briefly cover in the first lecture.***

OUTLINE (2017)

The estimated number of lectures for each topic is indicated. Relevant reference material is indicated using the abbreviations for books defined above.

I think that the references in ITALICS are the best to read.

** PART I : Fundamentals and Elementary Applications (14)

I. Brief Introduction to Probability and Statistics (1)

***Read ALL of KD Ch.1 ;* not all will be covered in class

II. Thermodynamics, Entropy, First & Second Laws (6)

A. Extremum Principles
KD, Ch.2

B. Heat, Work, Energy and the First Law
KD, Ch.3; DC, Ch. 1.1

C. Boltzmann Entropy and Introductory Statistical Thermodynamics
K2, Ch.5

D. Free Energies, Temperature, Equilibrium and Ideal Gas
KD, Ch. 7, Ch.8 ; DC, Ch. 1.2,1-1.4 ; PM, Ch.17

III. Statistical Mechanics and Elementary Applications (7)

A. Boltzmann Distribution Law, Partition Function, Ensembles
Ensembles, Heat Capacity, Energy Fluctuations
KD, Ch.10 ; Ch.12, p.230-232; DC, Ch.3.1-3.4 ; PM, Ch.18,19

B. Discrete Systems
flexible molecules, paramagnetism via Boltzman & "order parameter" approaches
KD, Ch.10, p.184-188

C. Continuum Systems
Ideal atomic gas, Classical vs. Quantum, Particle-in-a-Box model
Vibrations, Harmonic Oscillators, Einstein model of solids
Molecules, degrees of freedom, and Partition function factorization
KD, Ch.11 and Ch. 12, p228-232 ; PM, Ch.18,21,22

** PART II: Liquids, Mixtures, Phase Behavior & Surfaces (12)

IV. Phase Equilibria & Thermodynamics of 1-Component Fluids (5)

A. Interactions & Generic Phase Equilibria
KD, Ch.24, p.471-479 *KD, Ch. 14, 1st two sections; Ch.25*

C. Classic Van der Waals Model
Equation-of-State, Virial expansion, Liquid-Vapor phase transition, Isothermal compressibility, Law of corresponding states
KD, Ch.24 , p.479-483 NG, Ch 4.1-4.4

C. Microscopic Lattice Fluid Model
Partition function, athermal limit, mean field approximation, attractions, connection to van der Waals model
DC, Ch.5.2 ; KD, Ch.24, p.485-486

V. Continuum Fluids : Thermodynamics, Structure and Freezing (3)

*(*Note: Dill book has virtually nothing for this Section*)*

A. Hard Sphere Fluids (relevant to atoms, molecules, colloids)

1-dimensional Tonks model, comparison to lattice fluid model

B. Correlation functions, Radial Distribution function g(r)

DC, Ch. 7.2, 7.3, 7.5 ; McQ, Ch. 13.1-13.3 *KD, Ch.24, p.483-485*

C. Thermodynamic properties, Structure and Crystallization

3-dimensional packing effects, repulsive vs. attractive forces

DC, Ch. 7.4 ; McQ , Ch.2.1-12.3, 13.9, 14.3

VI. Two Component Liquid Solutions and Solid Alloys (3)

Phase Diagrams & mean field theory for Liquid-Liquid phase separation

KD, Ch. 15 and 25 TLH, Ch.14.4, 20.1

VII. Surfaces (1)

Physical Adsorption, Monolayers and Langmuir Isotherm

KD, Ch.27, p.541-546 TLH, Ch 7.1+14.1

**PART III: Solids, Magnets, Biopolymers and Quantum Statistics (12)

VIII. Thermal Properties of Crystals (1)

Collective phonons, vibrational properties, heat capacity, Debye model, comparison of Debye and Einstein models, characteristic temperatures

McQ Ch. 11.1-11.3 + 11.6 DC, Ch.4.3 ; PM, Ch.20

IX. Cooperative Phenomena (8 or 9)

A. Order Parameters, Critical Phenomena, Broken Symmetry

General concepts, Landau approach

KD, Ch 26

B. Spatial Correlations and Susceptibility

Spin correlation functions, density fluctuations, Correlation length

C. Ising Model, Spins, Magnets

1-d Ising model, Curie-Weiss Mean Field theory, Fluctuation effects and energy-entropy competition; Effect of dimension; External fields

DC, 5.1, 5.3,5.4 ; NG, Ch. 3.7, 4.5 *KD, p.525-527*

D. Order-Disorder Phase Transitions in Solids

Description of ordered state (e.g. Cu-Zn alloy), Mean Field theory

Handout

E. Helix-Coil Conformational Transition in Biopolymers

Polypeptides, Conformation, Hydrogen-bonding, Entropy vs. Energy

KD, Ch.26, p.527-535

X. Quantum Electronic Phenomena (3 or 2)

Topics in this section not covered at all in the Dill book

A. Quantum Statistics

Non-interacting systems, Fermi-Dirac statistics, Fermi level

DC, Ch. 4.3, 4.4 ; McQ, Ch.4.2 ; PM, Ch 24

B. Electron Gas and Metals

Weakly and strongly degenerate Fermi gas, Electronic heat capacity

DC, Ch.4.5 ; McQ , Ch. 10.1,10.2 ; PM, Ch.26