STATISTICAL THERMODYNAMICS & MECHANICS OF MATERIALS

MSE 500 **Fall 2021**

Instructor: Professor Ken Schweizer 206 MSEB 333-6440 kschweiz@illinois.edu

MWF 8:30-9:50 am (sometimes ends earlier)

2017 ECEB (Electrical & Computer Engineering Building)
north of Springfield Avenue, on north quad, on the left just before getting to the Beckman Institute
Room location: enter from atrium stairs to 2nd floor, turn left, at the end of the hall turn right

Overall LOGISTICS
In the pre-covid era, the course was delivered on the blackboard with students taking notes. That was not possible last fall, and I developed a full set of lecture notes and visual aids ("Vugraphs" in pre-covid days) organized in PDFs which mimic how the lectures were previously given. *This fall I will lecture using these PDFs.* So, you really do not need to take notes, *so please ask more questions*. I will use the blackboard mainly to answer specific student questions (if needed), or occasionally further elaborate on a specific topic. ***I will send you** the PDF lecture notes in packets of roughly 3 as we go through the material. I will send you the full packet of Vugraph slides for each of the 3 parts of the course in one document each.*

If you are on campus, I urge you to regularly attend in person and ask questions.
The lectures will be recorded using the Echo360 automated system https://echo360.org. This will be available to both students formally taking the remote section and those taking the in person section. Login with your Illinois email address. You will be prompted to authenticate using the Active Directory (AD) password. Once that is done, you can see the dashboard page displaying content for which you are enrolled as a student. Student Echo360 user accounts are auto-generated based on enrollment rosters within 24 hours. For further information see: https://answers.uillinois.edu/illinois.engineering/page?id=81743 .
***I have no control over any of this**, and cannot answer your questions nor do anything about your access.*

If you have a question not asked during class, first try emailing me. Students have effectively done this in the past. If more in depth questions arise, we can arrange a 1 on 1 meeting in person or via Zoom.

All homework sets and answers and any other course materials will be sent to you directly by email. I do upload anything on a course website; I prefer direct communication with students.

Office Hours: The class is rather large and it is not practical to set one time. Just email me and we can arrange a meeting. I also can almost always stay after class and answer questions.

Homework: No TA, so ***not*** collected/graded. I will give you the answers. ***It is your job to carefully study this***, and see what you did not get correct. If you then have any questions, please contact me.

Homework will be given every week and is a ***key to learning***. I suggest you first work hard on it ***alone***. If you have difficulties, then discuss the problems with each other. If you look at the answers before working hard on problems yourself then you will learn nothing. ***Students who have trouble with the course almost always make the mistake of not first working hard by themselves on the problems, and/or are fall behind a lot early in the course and do not promptly resolve things they do not understand.***

EXAMS: Two midterms covering parts I and II of outline.

First exam: **mid-October**
Second exam: **mid-November**
Final Exam: Comprehensive, but will strongly emphasize part III.

Exams will be taken in class. Mid-terms are 80 minutes. Final exam is 3 hours. The precise dates will be determined later. All exams are *closed book and notes*. You are allowed to create one sheet (1 side) of formulas/information to allow you to avoid having to memorize formulas and such. Putting it together is a good experience to identify what is really important.

Final Course Grading: Exam 1: 20 or 30% Exam 2: 20 or 30 % Final: 40 or 60 %
I determine the weighting factors in a manner that optimizes your composite exam average.

***REQUIRED TEXT**:

KD: Ken A. Dill & Sarina Bromberg, *Molecular Driving Forces – Statistical Thermodynamics in Chemistry & Biology*, Garland Science, Taylor & Francis Group, NY and London, ***2nd edition***.

For some topics I will follow the Dill book. For ***many*** others I will not. For a few topics there is ***nothing*** in the book. Even if I follow Dill, I often do things differently for better clarity. In all cases I strive to provide additional explanation not in any texts.

RECOMMENDED BOOKS ***on reserve in Grainger Engineering Library for fall 2021.***

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.

****Friendly Advice****

I urge you to not fall behind since this is a fundamental science course that continuously builds on prior material, and integrates 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. Typically one or a couple of students receive a course grade below "B". But there is ***no*** mandate this must happen, it can be avoided by good study habits and effort.

Statistical thermodynamics and mechanics is a quantitative science that requires mathematics. ***If your math skills are rusty, I urge you to brush up on basic calculus.*** The Dill book has nice review material on 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 briefly cover a little of in mainly the first lecture.* The course outline is given below. On the copies of my lecture PDF slides (my transcribed notes) you will see a **Lecture #** is indicated for each class. I will sometimes switch back and forth to the **"Vugraph" file** during the lecture. It has extra information, illustrates specific points, show graphs and data, etc. Each vugraph slide is numbered as **VG#**. I refer to them on the lecture notes slides.

OUTLINE (2021)

The estimated number of lectures for each topic is indicated. Relevant reference material available from the Dill textbook (KD) and other books is indicated using their abbreviations. The references in ITALICS are the best to read if you want extra information or explanations beyond what I present.

** 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*
- **B. 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)

** 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, Chapters 15 and 25 TLH, Ch.14.4, 20.1

VII. Surfaces (1*)*

Physical Adsorption, Monolayers & 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 (handout) 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 (2 or 3) **topics not covered 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