STATISTICAL THERMODYNAMICS & MECHANICS OF MATERIALS

MSE 500 **Fall 2020**

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MWF, 9-10:20 am (or shorter), ***synchronous lectures via Zoom*** **TA: none**

On Line / Pandemic Adjustments

The lectures will be delivered MWF using UIUC Zoom in real time starting at 9 am CST. They will last (including questions) of order 50-75 minutes.

I will create a Zoom link and email it to every registered student the day before each class. You can log on up to ~10 minutes before 9 am. When you do, you will hopefully be muted; *turn off* your video and audio if it is not already off.

The lectures (and questions during) will be recorded. My plan is to upload it immediately after the lecture is done on UIUC Media Space (mediaspace.illinois.edu). Then I will send the class an email with the link to the lecture. Click on it and follow directions. This will allow you to view the lectures any time you wish. *How to access:* after clicking on the link I send you should have direct access to lecture (after signing in with your UIUC account). All lectures should be on the same website in chronological order. I will label them as : MSE500lecture##. *If you encounter technical problems I likely cannot help much since I know none of the technical details and have never done any of this before. All I likely can fix is if for some reason the lecture is not uploaded due to my mistake.*

I will be using a PDF of my lecture notes to deliver the material in a style that is the same as when I teach using a blackboard or whiteboard. It will be supplemented sometimes with other visuals from another file that is called the vugraph file. My plan is to send you the lecture notes in packets of 3 (1 week's worth), shortly before the beginning of a new week. I will send you the full packet of vugraph slides for each of the 3 parts of the course.

Logistics for Questions *during* class: about every 2 slides, I will stop and ask if anyone has a question. Doing so is highly encouraged. Please ask by "unmuting" your audio on Zoom. When our discussion of the question is done, re-mute yourself. In the past I sometimes answered questions not just with words but by writing on the blackboard in real time; I will not have that option.

At the very end of a lecture, I again will ask if there are any questions on the material of the day.

If you have a question that was not asked during class, I suggest you first try emailing me directly. Students have effectively done this in the past. If more in depth and/or many questions arise, e.g., before an exam, I can arrange a 1 on 1 discussion via Zoom at a mutually agreed upon time.

All homework sets and answers and any other course materials will be sent to you directly by email attachment. Homework is not graded (no TA). I do not plan uploading anything on the course website; I prefer direct communication with students.

Exams will be taken virtually on specific days in a logistical way I will determine and explain later. *For students on campus, the exam time will be the class time.* For students not on campus, I will work with you to arrange something that can work for you and me. However, the goal will always be that exams are taken by all students on essentially the same day, to within variations of national and global time zones differences.

TIMES and FORMAT: In the pre-pandemic days, the class was taught using a huge blackboard filled up from left to right with students required to take notes. Each class ran roughly 75 minutes. Now I will be teaching by projecting a hand written multi-color version of my notes on Zoom. The amount of material presented will be the same as in a real class before. As I speak, I will use my computer mouse pointer to lead you through the material on each slide. At present, I cannot know precisely how long each lecture will take in this format, but I will strive to control pace and deliver material slowly. However, things will likely go faster since I am not writing on a board in real time. The "good news" is you now have my notes electronically. Every slide I show will be numbered to facilitate cross referencing. Hence, except for perhaps writing down a few things I say that are not on the slides which you feel are important, you do not need to take notes. ***I am hoping this will allow the class to ask even more questions than usual.*** My plan is to stop roughly every 2 slides on Zoom and ask if there are questions. **Questions other times during the lecture do not seem a good idea to me logistically, but we can revisit this later in the semester after we all get acclimated to this new world.**

OFFICE HOURS: Since the class is rather large, with students from diverse departments (typically 4-5), it is not practical to set one time. Just send me an email. We could then set up a Zoom meeting. Alternatively, as I stated above, I suggest you firs ask questions by email, which students did a fair amount in the past, and alot more than direct meetings. This seems the ***best first approach*** to asking questions, especially since you writing down the question and me writing down the answer may help of us better understand each other.

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

EXAMS: Two midterms cover parts I and II of outline, respectively.

First exam:	**mid-October**
Second exam:	**mid-November**

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

The precise dates and how exams will be given will be determined later. No matter what, one lecture class will not be held the week of the exams.

All exams are CLOSED book and notes. You are allowed to create one sheet (1 side) of formulas/information. Putting it together is a good experience to identify what is really important.

Grading: 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 HOMEWORK.*** 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 contact 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 exam 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 should be on reserve in the Grainger Library, but not clear you can access it this year.
***You should get/buy this book*. I am told it can be ordered through the University bookstore, and you already have been informed about the logistics of how to do that**.

RECOMMENDED BOOKS on reserve in Grainger Engineering Library

(in pre-pandemic days….likely not accessible in the present world, and this is not at all critical)

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 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. 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. The good news is that the pandemic has forced me to write up my notes and you have them.

FRIENDLY WARNING:
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 in mainly the first lecture.**

Other Pandemic LECTURE LOGISTICS:

The course outline is given below. It is the same as in prior recent years. On the copies of my lecture PDF slides (my transcribed notes) you will have is indicated a **Lecture #** for each class.

I will send you 1 week of notes (typically 3 lectures) a few days ahead of time. I will sometimes switch back and forth to the **"Vugraph" file** while I lecture. It has extra information to explain material, illustrate points, show graphs and data, etc. Each vugraph slide is numbered as **VG#**. I refer to them on the lecture notes you will have. When I lecture, I will switch to this file in real time on Zoom.

OUTLINE (2020)

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 in my notes.

** 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 (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