STATISTICAL THERMODYNAMICS & MECHANICS OF MATERIALS

MSE 500 **Fall 2023**

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MWF 9-10:20 am (sometimes ends earlier) **218 Ceramics Bldg**

LOGISTICS

In the pre-covid era, the course was delivered on the blackboard with students furiously taking notes. During fall 2020 on Zoom, I developed a full set of lecture notes and visual aids (called "vugraphs" in pre-covid days) organized in PDFs which mimic how the lectures were previously given. This fall I will again lecture using these PDFs with computer projection. So, you really do not need to take notes, ***hence please ask more questions, they benefit everyone.*** I will use the blackboard mainly to answer specific student questions or occasionally further elaborate on a specific topic. *I will send you the PDF lecture notes by email 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.*

I cannot force you, but I urge everyone to regularly attend class. Unfortunately, attendance in this class, and essentially all other MSE courses post-covid, has dropped a lot. That is not good. MSE500 is a rather demanding graduate course, and falling behind generally has serious consequences. Moreover, learning the material solely by reading lecture notes alone is not a good idea, and it also conflicts with the goal of building community in the classroom. Everyone learns from students asking questions in class. *****The lectures will NOT be recorded*****

If you have a question not asked during class, you can ask me right after the lecture, or email me. If more in depth questions arise, I am happy to arrange a 1 on 1 meeting in person or via Zoom.

All homework sets and answers and all other course materials will be sent to you directly by email. I do not upload anything on a course website (none exists).

Office Hours: The class is large, and with students from different departments. So it is not practical to set one time. Email me and we can arrange a meeting.

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

Problem sets will be given every week and are 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 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 and a final exam.

First exam:	Wednesday October 11 on part I
Second exam:	mid-November on part II
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. All exams are *closed book and notes*. You can 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 maximizes your composite exam average.

My Travel.

At the moment, I know that will be out of town Wednesday October 11 (exam will be proctored by a postdoc in my group), and Friday October 27 and there will not be an in class meeting that day. Class on Monday October 9 is canceled, as is standard practice to allow you more time to study for the 1st exam.

***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 kind of "follow" Dill to some extent, I often do things differently for clarity and a different perspective with the goal to provide additional explanation not in any texts which deepens understanding.

SUPPLEMENTAL 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.

Friendly Advice

I urge you to not fall behind, especially since this is a fundamental physics-based 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 graduate students, this is especially important since you must receive a "B" or higher so that it counts towards passing the qualifying exam. Typically a few students receive a course grade below "B". But there is ***NO*** mandate or qouta this must happen, and 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 in mainly the first lecture.*

NOTE: The course outline is given below. On the copies of my lecture PDF slides 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 experimental data, etc. Each vugraph slide is numbered as **VG #**. I refer to them on the lecture notes slides.

OUTLINE

The estimated number of lectures for each topic is indicated. Relevant reference material available from the Dill textbook (KD) and other supplementary books is indicated using their abbreviations. The references in ITALICS are best to read if you want extra information/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, and Boltzmann Law Concepts (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: Gases, Fluids, 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: Crystals, 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 spatial 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

Ideal Fermi gas of electrons, Electronic heat capacity

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