STATISTICAL THERMODYNAMICS & MECHANICS OF MATERIALS

MSE 500 **Fall 2024**

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MWF 9-10:20 am (often ends earlier) **101 Transportation Bldg**

LOGISTICS

In the pre-covid era, the course was delivered on the blackboard with students furiously taking notes. During fall 2020 the course was taught on Zoom, and 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 lecture using these PDFs with computer projection. ***So, you really do not need to take notes, hence please ask 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. So do check your email regularly.*

I urge everyone to regularly attend class. Unfortunately, attendance in this class, and many 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, trying to learn the material solely by reading lecture slides is a *bad* idea. I say and explain a lot more than are on the slides. Not attending class also conflicts with the goal of building community in the classroom, and everyone learns when students ask questions in real time. *****Lectures will NOT be recorded*****

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

All homework sets and answers (and all other course materials per above) 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, with students from different departments with many different schedules. It is not practical to set one time. Please 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 on parts I and II plus a final exam. Precise dates to be determined.

First exam on Part I: very likely week of October 14
Second exam on Part II: mid/late November
Final Exam: comprehensive, but strongly emphasizes Part III. The time and date are set by the university: 8 am, Monday, December 16. Last class is Wednesday, December 11.

Exams are in class. Mid-terms are 80 minutes. The 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: Exams 1 and 2: 20 or 30% each 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 I will be out of the country at an international meeting the entire week of September 30-October 4. Per all prior years, one of the lectures in this time period will be canceled to allow you time to "catch up" and begin to prepare for the first exam which is a stressful event for many students. Likely October 4. The other 2 lectures with be recorded and the link sent to you. I also will be out of town Wednesday November 20, and the lecture for that day will be recorded.

***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 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 to some extent, I almost always do things differently both for further clarity and in order to give you an additional perspective not in any text which helps deepen 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 nor quota 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.*

COURSE OUTLINE

NOTE #1: *The estimated number of lectures for each topic is indicated in parentheses. Relevant reference material available from the Dill textbook (KD) and other supplementary books is indicated using their abbreviations. Reading this material is optional. By far the most important thing is to deeply understand what is presented in the class lectures. The references in ITALICS are best to read if you want extra information/explanations beyond what I present. You will need to decide if it is helpful.*

NOTE #2: *On the copies of the PDF lecture slides you will see a **Lecture #** is indicated for each class. I will sometimes switch back and forth to the **"Vugraph" file** during class. 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.*

NOTE #3: *This course is not about classical macroscopic thermodynamics. That is a pre-requisite. I will review the key aspect of thermodynamics as needed as we go through different topics.*

PART I: Fundamentals and Elementary Applications (16)

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 (7)

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 (8)

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 (3 or 2) **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

There are a total of 43 classes scheduled in the semester from August 26 thru December 11.

Total number of lecture classes is estimated to be 40 (including the 3 in recorded mode).

One class will be canceled before the first exam. Two classes will be exams. This adds up to 43.