STATISTICAL THERMODYNAMICS & MECHANICS OF MATERIALS

MSE 500 **Fall 2025**

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MWF 9-10:20 am (often ends earlier) **4039 CIF Bldg (Campus Instructional Facility)**

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 to answer specific questions or occasionally further elaborate on a 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 course parts 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 significantly dropped. **That is not good**. MSE500 is a demanding graduate course, and **falling behind generally has serious consequences**. Trying to learn the material solely by reading lecture slides is a ***bad*** idea. I say a lot more than are on the slides. Not attending class also conflicts with the goal of building community, and everyone learns when students ask questions.

*****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) are 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 with many different schedules and also from different departments. 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 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.

First exam on Part I (expect material covered ends October 1 or 3)**:** **exam** likely October 20
Second exam on Part II (expect material covered ends November 5)**:** **exam** likely November 19
Final Exam: comprehensive, but ***strongly*** emphasizes Part III. The time and date are set by the university: **8 am, Monday, December 15**. Last class is Wednesday, December 10.

Exams are in class. Mid-terms are 80 minutes. The final exam is 3 hours. All exams are *closed book and notes*. You are allowed to create one sheet (1 side) of formulas/information in order to avoid having to memorize. Putting it together is a good experience to identify what is really important. But do not overemphasize its importance. Exams are meant to test you understanding and critical thinking ability, not deliver facts.

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.

I know for sure I will be out of town: Weds September 24, Monday October 20, Weds October 22, and Weds November 19. **Per above, I expect in class midterm exams will be given on Oct. 20 and Nov. 19** which will be administered by one of my postdocs. For the other 2 dates, there will be no in person class. I will send you a link to a recorded lecture.

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 do 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 immediately if needed. *This includes the elementary probability and statistics of Dill chapter 1 which is briefly covered in mainly the first lecture.*

COURSE OUTLINE 2025

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 given above.* ***Reading this material is optional. By far the most important thing is to deeply understand what is presented in the class lectures/notes.*** *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 I distribute 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 #**. They are referred to on the lecture notes slides.*

NOTE #3: *This course is **not** about classical macroscopic thermodynamics. That is an undergrad pre-requisite. I will briefly review key aspects 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 on 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 (11)

Last class is Weds Dec. 10 and you are responsible for the lecture material that day

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 (7 or 8 ; may skip section E this year)

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