MATE 664 Lecture 01

Thermodynamics and Kinetics

Dr. Tian Tian

2026-01-05

Land Acknowledgement

The University of Alberta acknowledges that we are located on Treaty 6 territory, and respects the histories, languages, and cultures of the First Nations, Métis, Inuit, and all First Peoples of Canada, whose presence continues to enrich our vibrant community.

Learning Outcomes

After today's lecture, you will be able to:

- **Identify** the key components of the course syllabus, content and grading schemes.
- **Recall** common interaction methods and resources available in the course.
- **Recall** basic concepts in thermodynamics and kinetics
- **State** assumptions of equilibrium
- **Describe** the influence of entropy in kinetic systems

Course Information

- **Course:** MAT E 664 – Kinetics of Materials
- **Term:** Winter 2026
- **Lectures:** Mon & Wed
- **Time:** 14:00 – 15:20
- **Location:** HC 2-14

Meet the Instructor

- **Office**: DICE 12-245
- **Email**: tian.tian@ualberta.ca
- **Office hour**: by appointment
- I joined CME in 2025 as assistant professor.
- Research fields: machine learning, multiscale materials simulations, computational tools
- Let's enjoy learning together!

TAs & Seminar Sessions

- **Teaching Assistant**
  - Hanlin Wang — hanlin7@ualberta.ca
- **Course & Assignment Questions**
  - No formal seminar or lab sessions
  - Questions related to course content or assignments
  - Please book an appointment with the TA (and instructor) as needed
- **Support Format**
  - One-on-one or small-group discussions
  - Concept clarification and guidance

Course Grading

- **Assignments:** 25%
  - 4 assignments (best 3 counted)
  - Submission via Canvas
- **Final Project:** 30%
  - Research-related topic
  - In-class oral presentation
- **Final Exam:** 45%
  - In person, open book
  - **Apr 20, 2026 · 1:00 p.m.**

Details please see the course syllabus

Textbook and References

Our primary textbooks for this course are:

- **Kinetics of Materials** by R.W. Balluffi, S.M. Allen, and W.C. Carter.
- **Materials Kinetics: Transport and Rate Phenomena** by John C. Mauro.

What Will We Learn in MAT E 664 (1)?

Theory: irreversible thermodynamics & driving forces

$$\text{Flux} = \text{Kinetic coefficients} \times \text{Driving Force}$$

What Will We Learn in MAT E 664 (2)?

Mass transport on solid material interfaces: $v_{step} = \beta(c - c_{eq})$

[1]

What Will We Learn in MAT E 664 (3)?

Nucleation theory: $r_c = -\dfrac{2\gamma}{\Delta G_v}$

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[1] *Image credit: A.R. Verma*

[2] *Image credit: crystalverse.com*

What Will We Learn in MAT E 664 (4)?

Spinodal Decomposition (Pattern Formation)

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(M \nabla \left[\frac{\partial f(c)}{\partial c} - \kappa \nabla^2 c \right] \right)$$

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Interaction Time!

We will use Wooclap in this course for real-time interactions.

Participation link https://app.wooclap.com/664L01?from=instruction-slide

Results to be published after the class

Thermodynamics vs. Kinetics

Feature	Thermodynamics	Kinetics
Greek Name	*Therme* (heat) + *dynamis* (power)	*Kinetikos* (of motion)
Focus	**Eventually**: Predicts the final state	**Rate**: How fast a process occurs
General Form	Free energy change (ΔG)	Reaction rates, flux, activation energy
Condition	Equilibrium	Non-equilibrium

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[3] *Image credit: Mathis Plapp, École Polytechnique (FR)*

The True Meaning of Equilibrium

Equilibrium is a balance of time scales:

$$\tau_{\text{observation}} \gg \tau_{\text{process}}$$

- **Thermodynamic descriptions** are relevant when the observation time scale is much larger than the time scale of the processes reaching equilibrium.
- It's about **specific processes** reaching a steady state, not necessarily the entire system.

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Kinetic Processes

Kinetic processes are distinct from thermodynamic equilibrium:

1. **Conditions:** Occur away from equilibrium.
2. **Cause** Require a thermodynamic **driving force**.
3. **Rate:** Coupled with a **rate parameter** or **coefficient**.

Irreversible Thermodynamics is key to understanding these processes (Lecture 2).

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Classical Thermodynamics Revisited

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Thermodynamic Interplay Between H and S

Whether a process from A → B is **spontaneous** or **non-spontaneous** depends on the sign of free energy difference, $\Delta G = G_B - G_A$.

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- What is ΔG for a reversible process at equilibrium?: $\Delta G = 0$,
- How can we check the stability of a certain material at P, T?: Use the phase diagram!

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[4] *Image credit: John C. Mauro*

[5] *Image credit: John C. Mauro*

[6] *Image credit: John C. Mauro*

How Stable Is Diamond?

- Which phase is the most stable at r.t. & 1 atm?
- Should we worry our diamond rings turn into pencil?

Two-State model of Thermodynamics vs Kinetics

- ΔG^0: Free energy of **reaction** → will reaction happen? (**Thermodynamics**)
- ΔG^*: Free energy of **activation** → how likely / fast? (**Kinetics**)

Arrhenius Plot Demo

Where Does Entropy S Come From?

- Claussius (1865) **Classical thermodynamics**.
  - Entropy is a state variable of internal energy.
  - $dU(S, V) = TdS - pdV$
- Boltzmann (1877) **Statistical mechanics**.
  - Entropy is a measure of accessible microstates (atoms + probability!)
  - $S = k_B \log(\Omega)$

Why The Logarithm?

- S as an **extensive** quantity → **Additive** $S_T = S_1 + S_2$
- Ω as microstates is **multiplicative** → $\Omega_T = \Omega_1 \cdot \Omega_2$
- If $S = f(\Omega)$, then $S_T = f(\Omega_T) = f(\Omega_1 \cdot \Omega_2) \rightarrow f(\Omega_1 \cdot \Omega_2) = f(\Omega_1) + f(\Omega_2)$
- $f(x) = C\log(x)$ is the unique solution using Cauchy's functional equation results

Entropy *IS NOT* Disorder!

- Common statement of entropy is measure of *disorder*
- Boltzmann equation measures **how many possibilities** of arrangement
- Disorder is not uniquely linked to number of microstates!

Entropy *IS NOT* Disorder – II!

- **High entropy alloys (HEAs)**: Example of high configurational entropy material
- Many HEAs have much more ordered lattice than binary alloys

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What Should We Really Think of Entropy

- **Arrow of time**: mixed cream and coffee cannot be demixed
  - Newtonian dynamics is time-reversible
  - We cannot rewind to low entropy state from Newtonian dynamics!
- **Loss of information**:
  - **Shannon entropy**: $S_{info} = -k_B \sum_i p_i \log(p_i)$
  - Shannon entropy **can be measured** on the exact state!
- **Uncertainty**:
  - Link to Heisenberg's principle $\Delta x \Delta p \leq \hbar/2$
  - See Hirschman *Am. J. Math.*, **1957** 79, 152

Where Can We Go From Here?

- **Irreversible thermodynamics**

  Real processes occur away from equilibrium, where entropy is **produced**.
- **Entropy generation as a driving force**

  Gradients in temperature, concentration, and chemical potential drive fluxes by increasing total entropy.
- **From equilibrium to dynamics**

  Entropy provides the unifying language for diffusion, heat flow, chemical reactions, and transport phenomena.

Stay Tuned!

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[7] *Small* **2024**, 20, 2311929

Brief Introduction to Course AI Helper

- A Socratic Gemini chatbot aiming to help course learning and key concepts
- **Access the AI helper here:** https://gemini.google.com/gem/1c118102b2d1

Summary

What we learned today:

- Syllabus / course contents of MATE 664
- Kinetic rate and equilibrium
- Concept of entropy revisited
- Laws of thermodynamics revisited

See you next time!