

VK330 Thermodynamics of materials

Fall 2021

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Office Hours:	Mon 2:00pm-3:00pm (Tentative)
Classroom:	E1-204 (on-line if necessary: Feishu)
Time:	Mon/Wed 8:00am-9:40am, Fri 8:00am-9:40am (even weeks)
TA:	None

Course Description:

The course introduces fundamental concepts and principles of thermodynamics, with their applications in explaining and predicting important materials phenomena, such as behaviors of gases and solutions, and phase equilibria of one-component and binary systems.

Credits: 4

Prerequisites: Vp140/Vp145/Vp150/Vp160, Vc210/Vc209

Course Objectives:

- 1. To teach the relationship between heat and work and the first law of thermodynamics.
- 2. To teach the types of thermodynamic processes and the second law of thermodynamics.
- 3. To introduce the concept of entropy and the third law of thermodynamics.
- 4. To explain fundamental thermodynamic properties and the relationships among them.
- 5. To discuss the microscopic interpretations of thermodynamic properties
- 6. To teach the laws and relationships that govern the behavior of ideal and non-ideal gases.
- 7. To discuss the properties of ideal and non-ideal solutions from the free energy point of view.

- 8. To discuss the phase equilibria of matter and their graphical representation.
- 9. To provide an overview of common types of phase diagrams.
- 10. To teach the methods for interpreting and constructing a phase diagram based on free energy.

Course Outcomes:

After completing VK330, students should be able to:

- 1. Calculate the work done during one thermodynamic process.
- 2. Predict the direction and reversibility of a process.
- 3. Quantify the degree of disorder of a system.
- 4. Solve the fundamental equations for predicting thermodynamic properties at a given system state.
- 5. Demonstrate the connections among the fundamental thermodynamic properties.
- 6. Explain the connections between macroscopic thermodynamics and statistical thermodynamics.
- 7. Analyze the processes involving ideal gases.
- 8. Explain the formation of solution and calculate its solubility and activity.
- 9. Construct P-T and P-V phase diagrams.
- 10. Predict equilibrium phase of matter under a given condition.
- 11. Identify different types of binary phase diagrams.
- 12. Predict phase stability and equilibrium composition based on phase diagram.
- 13. Construct binary phase diagram from free energy data.
- 14. Apply thermodynamics principles and theories to practical materials science problems.

Textbook/Required Material:

- 1. Slides used in the lectures.
- 2. David R. Gaskell & David E. Laughlin, *Introduction to the Thermodynamics of Materials*, 6th ed., CRC press, 2017. (Suggested reading)

Week	Dates	Topics
1	9/13	Course introduction and basic thermodynamic concepts and
		definitions
	9/15	Work, energy and the 1st law of thermodynamics
	9/18	Reversible and irreversible processes, determination of the
		direction of a process (Make-up lecture)
2	9/22	Entropy and the 2nd law of thermodynamics (HW1 assigned)
	9/24	Heat engine and maximum work
3	9/27	Statistical and microscopic interpretation of entropy (HW1 due
		and HW2 assigned)
	9/29	Energy, enthalpy, free energy and chemical potential

4	10/4	- (National holiday)	
	10/6	- (National holiday)	
	10/8	Free energy in statistical mechanics	
	10/9	(Potential make-up lecture)	
5	10/11	Fundamental equations in a thermodynamic system	
		(HW2 due and HW3 assigned)	
	10/13	The Maxwell's relations and the Gibbs-Helmholtz equation	
	10/18	Theoretical calculations of heat capacity and the 3rd law of	
		thermodynamics (HW3 due and HW4 assigned)	
6	10/20	Applications of fundamental equations in MSE	
	10/22	Midterm review	
7	10/25	Midterm (in class)	
1	10/27	Mixing of gases	
	11/1	Treatment of non-ideal gases (HW4 due and HW5 assigned)	
8	11/3	Ideal solutions in the dilute limit	
	11/5	Non-ideal solutions and models of solutions	
	11/8	Basic concepts of phases and phase transitions (HW5 due and	
9		HW6 assigned)	
	11/10	One-component phase diagram	
10	11/15	Binary phase diagram I, free energy and diagram construction (HW6 due and HW7 assigned, Project assigned)	
10	11/17	Binary phase diagram II, types of common phase diagrams	
	11/19	Binary phase diagram III, phase stability	
11	11/22	Ternary phase diagram (HW7 due and HW8 assigned)	
11	11/24	Applications of thermodynamics: reactions involving gases	
12	11/29	Applications of thermodynamics: reactions in condensed solutions	
	12/1	Applications of thermodynamics: solidification	
	12/3	Applications of thermodynamics: electrochemistry	
13	12/6	Project presentations (HW8 due)	
	12/8	Final review and Q&A	
14	12/13	Final exam (in class)	
	12/15	-	
	12/17	-	

Course Policies:

- Honor Code: All students in the class are bound by the Honor Code of the Joint Institute (https://www.ji.sjtu.edu.cn/academics/academic-integrity/honor-code/) as well as the Addendum to the Honor Code for Online Teaching. You may not seek to gain an unfair advantage over your fellow students; you may not consult, look at, or possess the unpublished work of another without their permission; and you must appropriately acknowledge your use of another's work.
- <u>Attendance</u>: Attendance to the lectures is strongly encouraged. On-line attendance is acceptable under the conditions when difficulties exist for in-person attendance. Reasonable explanations need to be given for continuous absence for more than *one week*.
- <u>Participation</u>: Active participation is highly expected for all students, including interactive activities during the lecture, attendance of instructor's office hours, inperson and on-line discussions with instructor and other students in a proper way, etc.
- <u>Assignments</u>: Unless specified, all the assignments are *individual* assignments, and all submissions must represent the student's own work. Duplicated submission is not allowed and will trigger an honor code violation investigation. However, students are encouraged to discuss course topics and help each other to understand the problems.
- <u>Submission</u>: All assignments should be submitted electronically on Canvas before the specific deadline.
- <u>Exams</u>: Exams will be conducted following all the standard regulations of JI and SJTU. If needed, additional procedures will be announced prior to the exams. Anyone who fail to follow the procedures will be given an 'F' for the exam.

Addendum to the Honor Code for Online Teaching

- The Honor Code in the Context of Online Courses The JI Honor Code applies to courses taught in an online fashion in the same way that it does to all courses. It is worth repeating the central tenets here:
 - Engineers must possess personal integrity as students and as professionals. They must honorably ensure safety, health, fairness, and the proper use of available resources in their undertakings.
 - Members of JI are honorable and trustworthy persons.
 - The students, faculty members, and staff members of JI trust each other to uphold the principles of the Honor Code. They are jointly responsible for precautions against violations of its policies.

 It is dishonorable for students to receive credit for work that is not the result of their own efforts.

In particular, the parts of the Honor Code regarding conduct during in-class examinations, for coursework, projects etc. apply correspondingly for such work conducted in courses taught online. Additional rules adapted to remote examinations, coursework etc. may be imposed as necessary.

In addition, students are required to abide by following rules specific to online teaching. These requirements are provisionally considered part of the Honor Code for the current teaching term.

Due to the new types of interaction and the new forms of learning activities there may be further issues that are not covered below. Students should not hesitate to contact their instructor, the Honor Council (jihonor@sjtu.edu.cn) or the FCD (jifcd@sjtu.edu.cn) if they have any questions.

• Online Presence and Activities

The Joint Institute imposes a "real name" policy for all online activities organized by JI instructors. This policy applies to groups or communication by E-Mail, Canvas, Piazza, Feishu, WeChat and all other platforms where groups are set up by JI or by individual instructors for students attending JI courses, events or other activities.

Students are required to use their actual name (in Pinyin) as part of their online presence for such groups and when communicating online. Individual instructors may also require students to add their name in Chinese characters (if applicable) and/or their Student ID.

Unless otherwise noted, such online activities are intended for the exclusive participation of JI students. Account names, meeting IDs, passwords and other information intended to protect the exclusivity of such activities may not be shared with anyone who is not part of the course or activity.

For example, it is not permissible to give a Feishu meeting ID of a given course to any person who is not enrolled in that course, whether or not the person is a JI student.

• Online Etiquette

When communicating or otherwise using online groups, students should follow the regulations set down by instructors concerning the use of online tools. Vandalism,

spam messages, verbal and other forms of abuse, violation of English-only policies (as detailed by instructors) and disturbance of the learning experience of other students are not permitted.

• Teaching and Learning Materials

Teaching and learning materials, such as lecture slides, assignments, quizzes, videos etc. are copyrighted and may not be passed on to others without the express permission of the course instructor. This applies in particular to recordings of Zoom lectures and other videos created by instructors.

In particular, it is not permissible to upload videos to sharing platforms (such as Youku or YouTube) or to post lecture slides, assignment questions, project descriptions etc. on public sites such as SlideShare.

Course Assessment Methods:

Homework:

Homework problems are designed such that the students can apply and exercise the knowledge taught in the lectures. Through solving these problems, the students are expected to digest the knowledge better and turn it into their own scientific understandings and skills, for applying thermodynamic theories to practical materials science problems.

Project:

Individual project is assigned to each student with its topic closely combining the course content with practical problems. These problems usually cover several knowledge points of the course with moderate extensions. Thus, the project provides an opportunity for the students to integrate the knowledge they learn from the class, and it serves as a motivation for them to learn outside the class. The project may also provide them an experience of independently solving research problems.

Examination:

Examinations (midterm & final) are means to comprehensively measure the students' level of achievement of the Course Outcomes. The typical types of exam problems include T/F and multiple-choice questions, proofs, derivations, calculations, sketches, and etc. If the form of the examinations is determined to be on-line, then the submission is expected to be via Canvas and handing in the exam papers in person is not accepted.

Grading Policy:

Homework	30%
Midterm Exam	20%
Project	20%
Final Exam	30%
Total	100%