MSE 1053: Structure of Crystals and Diffraction

Fall 2022

Instructor:	Shan Gong	**Time:**	Wednesdays 8:15am – 11:00am
Email:	shan.gong@scupi.cn	**Place:**	Room 4-216
Office:	Room 4-221		

Course Pages

- https://pibb.scu.edu.cn
- We will post lecture notes, assignments, projects, announcements and your grades on it.

Office Hours

- Mondays & Wednesdays: 1:00PM – 4:00 PM
- By appointment via Email
- Online via QQ Group: 1130692671

Teaching Assistant

- Weiyi Zhao
- Contact: florencezwy@163.com
- If you have any question regarding to homework grading, please contact TA **within one week** after the homework is returned to you.

Course Description

Basic crystallography of materials; symmetry; point groups and space groups; tensor properties of crystals; diffraction methods in materials science; atomic packing and structures; glassy state, polycrystalline aggregates; grain boundaries and interfaces in materials; textures; multiphase materials; quantitative stereology and microstructural characterization. (3 credits)

Prerequisites

- Materials Structure and Properties (Or equivalent, or consent of instructor)
- MSE 1052–Manufacturing Processes and Analysis (recommended, not required)
- It is assumed that students have a basic knowledge of:
  - **Phase diagrams:** reading and understanding the diagrams, identifying phases and eutectics, solubility and relative composition of phases
  - **Basic kinetics:** equilibrium cooling (i.e., through a phase boundary) and time-temperature-transformation diagrams.
  - **Microstructure:** phases, eutectics, lamellae, connection to phase diagrams and kinetics.
- If these terms are fuzzy to you, review your course notes. Some of these concepts and phenomena will be briefly reviewed during class.

Course Objectives

After this course the students will be able to:

1. List the four states of matter and different structural states of condensed phases.
2. Discuss examples of how structure in addition to chemical composition of an engineered material affects properties and performance in applications.
3. Differentiate between long range and short range order as it relates to the description of the structure of materials.
4. Define the differences between non-crystalline and crystalline materials in terms of suitable descriptors.
5. List symmetry properties and use of them to describe structure of crystals.
6. List several basic descriptors suitable for discussion of the structure of materials.

Textbook

- M. De Graef and M.E. McHenry, "Structure of Materials", Cambridge University Press, 2nd edition (2012)

Reference Books

- C. Hammond, The Basics of Crystallography and Diffraction, Oxford University Press, 2nd edition (2000) and reprinted 2003. (**Key Reference**)
- Kelly and G.W. Groves, Crystallography and Crystal Defects, Addison-Wesley (1970).
- Kelly, G.W. Groves and P. Kidd, Crystallography and Crystal Defects, John Wiley & Sons (2000).
- M.J. Buerger, Elementary Crystallography, Wiley (1963).
- B.D. Cullity, Elements of X-Ray Diffraction, Addison-Wesley (1978).
- B.D. Cullity and S.R. Stock, Elements of X-Ray Diffraction, 3rd Edition Prentice Hall (2001).
- K.J. Kurdzydlowski and B. Ralph, The Quantitative Description of the Microstructure of Materials, CRC (1995).
- D.M. Adams, Inorganic Solids, Wiley (1974).
- V. Randle, Microstructure Determination and its Applications, Inst. Of Materials, London (1992).
- V. Randle, The Role of Coincidence Site Lattice in Grain Boundary Engineering, Inst. Of Materials, London (1996).
- C.S. Barrett and T.B. Massalski, Structure of Metals, McGraw-Hill, 3rd ed. (1966).
- R. Tiley, Crystals and Crystal Structures, Wiley (2006).
- S.M. Allen and E.L. Thomas, "Structure of Materials", Wiley, 1999.

Assessments

Homework:	30%
Midterm Examination:	30%
Final Examination:	40%
	100%

Grade

90.00 – 100.00	A	85.00 – 89.99	A-	80.00 – 84.99	B+	76.00 – 79.99	B	73.00 – 75.99	B-
70.00 – 72.99	C+	66.00 – 69.99	C	63.00 – 65.99	C-	60.00 – 62.99	D	0.00 – 59.99	F

Class Policy

- Regular attendance is essential and expected.
- Important dates and plans will be announced during class.

Homework and Other Assignments

Homework problems and other assignments will be assigned periodically and are due as stated in the assigned paper. All work will be submitted electronically through the Blackboard system. Late submission **WILL NOT** be accepted. It is **your duty** to make sure that submission through Blackboard has been properly processed. **Unless specifically requested, emailed homework will not be accepted.**

All of the homework scores will be used in your grade computation. Unless otherwise indicated, you can work with your fellow classmates in the class, but you must submit a distinct and independent write-up to receive credit. **If plagiarism is caught, zero score for all homeworks.** If you have a compelling emergency that prevents you from turning in the homework on time, email Dr. Shan Gong (shan.gong@scupi.cn).

If you believe an error has been made in the grading of an assignment, bring it to the attention of your TA **within ONE WEEK** from its return. Please adhere to these **homework guidelines:**

- Put your name, ID number (last four digits), and class section at the top of the first page.
- All work must be shown for each solution to receive full credit. Present your solution in a logical fashion, showing and explaining all steps in detail.
- Obtaining the correct answer includes getting the correct quantity, **number of significant digits**, sign, and **unit**.

Exams

There will be two exams (one Midterm and one Final), all are **CLOSED-BOOK**. Students can bring **one** A4 page note and it must be **hand-written** on **two sides** of the paper. It cannot be a photocopy. All midterm and final exams are mandatory. If you must miss an exam, you **MUST** make alternative arrangements with the instructor before the exam is given. If you missed an exam without prior notification, you will receive a score of **ZERO** for that exam except under extenuating circumstances. If you missed the midterm or final, a make-up exam may be given if the student has the approval from the instructor or emergencies and health issues **with a valid proof**. I will not accept the student deceleration for absence form for the final exam. Students who have not taken either the midterm or the final exams are **NOT**

eligible to take th make-up exam if he/she failed the course. Students taking make-up exams can only attain at most a **D** grade if he/she failed the course.

Academic Integrity

At Sichuan University, we are guided in all of our work by the values of academic integrity: honesty, trust, fairness, responsibility and respect (The Center for Academic Integrity, Duke University, 1999). As a student, you are required to demonstrate these values in all of the work you do.

Unacknowledged direct copying from the work of another person, or the close paraphrasing of somebody else's work, is called **plagiarism** and is a serious offense, equated with cheating in examinations. This applies to copying both from other students' work and from published sources such as books, reports or journal articles.

Paraphrasing, when the original statement is still identifiable and has also no acknowledgement, is plagiarism. A close paraphrase of another person's work must have an acknowledgement to the source. It is not acceptable for you to put together Unacknowledged passages from the same or from different sources linking these together with a few words or sentences of your own and changing a few words from the original text: this is regarded as over-dependence on other sources, which is a form of plagiarism.

Everyone at SCUPI is expected to treat others with dignity and respect. The Code of Student Conduct allows Sichuan University to take disciplinary action if students don't follow this community expectation.

Course Content

A schedule in detail will not be available as the pace of the course will highly be determined by students' reception of the content.

1. Crystal structure
    - Two-dimensional symmetry and lattices
    - Bravais lattices and crystal system
2. Crystal symmetry
    - Symmetry operations
    - Point groups
    - Space groups
3. Lattice directions and planes
    - Miller indices, Miller-Bravais indices
    - Zones axes
4. Reciprocal lattice
5. X-ray diffraction
    - Diffraction geometry
    - Diffraction intensities
    - Diffraction of polycrystal
6. Electron diffraction