MSE 1053: Structure of Crystals and Diffraction

FALL, 2026

NOTE: This syllabus may be adjusted to match class progress. Official announcements on Blackboard take precedence.

INSTRUCTOR: Shan Gong

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OFFICE HOURS: Tuesdays and Thursdays, 14:00-17:00

LECTURES: Tuesdays, 08:15-11:00, SCUPI Building N208. Materials and announcements: https://pibb.scu.edu.cn.

RECITATION: No separate recitation; problem solving and formative activities are integrated into lectures.

TEXTBOOK: Primary: Marc De Graef and Michael E. McHenry, Structure of Materials: An Introduction to Crystallography, Diffraction and Symmetry, 2nd ed.
Reference: C. Hammond, The Basics of Crystallography and Diffraction, 4th ed.

TEACHING ASSISTANT: Yuehan Luo, 2023141520072@stu.scu.edu.cn, homework grading.

PREREQUISITE: Introductory physics, general chemistry, or an introductory materials science course. Familiarity with vectors, dot and cross products, matrix multiplication, and basic trigonometry is expected. Essential linear algebra and wave concepts will be reviewed when needed.

DESCRIPTION: Crystallography of materials; Bravais lattices, crystal systems, and crystal structures. Diffraction methods; X-ray, electron, and neutron scattering; atomic scattering factor; structure factor; powder techniques; Laue method; reciprocal lattice; electron diffraction; amorphous materials; thermodynamics of crystals and crystal defects; polymorphism; order-disorder phenomena.

COURSE OBJECTIVES: The course builds quantitative fluency in crystallographic description and calculation, connects real-space structure and symmetry to reciprocal-space diffraction, and develops the ability to test a simple structure model using geometry, symmetry, intensity, chemistry, thermodynamic stability, and property evidence.

LEARNING OUTCOMES FOR THIS COURSE:
By the end of the course, students will be able to:

1. Describe crystal structures using lattices, motifs, unit cells, fractional coordinates, crystal systems, and Bravais lattices.
2. Calculate crystal directions, Miller indices, distances, angles, interplanar spacings, densities, and simple coordination environments.
3. Interpret symmetry operations, crystallographic point groups, space-group symbols, equivalent positions, and Wyckoff sites at an introductory level.
4. Explain the relationship among reciprocal lattices, Bragg's law, the Ewald sphere, and diffraction geometry; interpret powder-diffraction peak positions and the basic Laue method.

5. Use structure factors and reflection conditions to decide which reflections are present, absent, or relatively strong.
6. Compare X-ray, neutron, and electron diffraction in terms of geometry, scattering contrast, and the structural questions they can answer.
7. Distinguish crystalline, amorphous, polymorphic, and ordered/disordered structures using structural and diffraction evidence.
8. Use elementary free-energy and defect-equilibrium relationships to explain structural stability and point-defect populations and relate site occupancy or disorder to diffraction features.

GRADE DETERMINATION:

Component	**Weight**	**Description**
Homework	30%	Problem sets aligned with the required weekly content.
Quizzes and in-class activities	10%	Combined points from short quizzes and submitted in-class activities; no separate subjective participation score.
Midterm examination	30%	Semi-open-book; tentatively scheduled for Week 9.
Final examination	30%	Semi-open-book; tentatively scheduled for Week 18.

EXAMS: There will be two examinations, one midterm and one final, both semi-open-book. The midterm is tentatively scheduled for Week 9, and the final examination is tentatively scheduled for Week 18. The exact final-examination time and location will follow the university examination timetable and Blackboard announcement. For each examination, students may bring one A4 sheet of handwritten notes; both sides may be used. Printed, photocopied, or digitally reproduced notes are not permitted. Attendance at both examinations is mandatory. Examination absences and make-up arrangements are governed by the MAKE-UP POLICY below.

QUIZZES AND IN-CLASS ACTIVITIES: This 10% category is calculated from the combined points earned on short quizzes and submitted in-class activities; there is no separate subjective participation score. A quiz missed because of an ordinary absence cannot be made up. For a documented, unavoidable absence, the instructor may excuse the missed item or assign equivalent work, and the category grade will be adjusted accordingly.

GRADE REBUTTAL: Questions about grading should be raised promptly with the instructor and supported by the original graded work. The instructor will communicate the formal review procedure and deadlines. Questions about homework grading must be submitted to the responsible grader within one week after work is returned. Include MSE 1053, item number, and supporting work.

HOMEWORK: Submit an individual solution through Blackboard by the stated deadline. Group discussion is encouraged, but copied work is not acceptable. Late work is not accepted unless an extension is approved in advance or a documented emergency prevents timely submission. Show the reasoning, units, and final answer, and include your name, student ID, and section.

ATTENDANCE: Regular attendance and active participation are expected because calculation workshops, model reading, and pattern discussions are integral to the course. Students are responsible for announcements, examples, and formative activities completed during class. Students should follow SCUPI procedures for documented absences.

MAKE-UP POLICY: If an unavoidable circumstance prevents attendance at an examination, notify the instructor before the examination begins whenever practicable. A make-up examination may be granted only with the instructor's approval and valid documentation. Except in documented extenuating circumstances, missing an examination without prior notice will result in a score of zero. Arrangements follow SCUPI policy and the instructor's announced procedures.

MATERIAL COVERED: Chapters 1-14 of De Graef and McHenry provide the principal crystallographic and diffraction framework. Required concepts from the approved catalog description are embedded in the weekly sequence. Unless identified as an APPLICATION EXAMPLE or OPTIONAL ENRICHMENT, the topics listed in the weekly schedule form the assessable core of the course.

Week	Contents	Descriptions
1	Course Orientation and Ch1: Materials and Material Properties	Syllabus; structure-property thinking; length scales; anisotropy; symmetry and diffraction preview. REQUIRED: crystalline versus amorphous order, short- and long-range order, and their diffraction signatures. APPLICATION EXAMPLE: selected metallic-glass examples.
2	Ch2: Periodic Table and Interatomic Bonds	Atoms, periodic trends, ionic, covalent, metallic, and weak bonding. REQUIRED: cohesive energy, elementary free-energy concepts, and structural stability. APPLICATION EXAMPLE: atomic size and alloy bonding, ionic radii and packing rules, and silicate networks.
3	Ch3: What Is a Crystal Structure?	Periodic arrangements; lattice plus motif; unit cells; crystal systems; the 14 Bravais lattices. REQUIRED: polymorphism and allotropy - the same composition with different structures and properties. APPLICATION EXAMPLE: parent metallic structures and selected polymorph examples.
4	Ch4: Crystallographic Computations	Fractional coordinates, directions, metric tensor, distances, angles, volume, density, and calculation workflow.
5	Ch5: Lattice Planes	Miller indices, plane and direction families, hexagonal notation, and crystal forms. APPLICATION EXAMPLE: close-packed metallic planes and planes in simple ionic structures.
6	Ch6: Reciprocal Space	Reciprocal basis and metric; reciprocal vectors, plane normals, angles, and interplanar spacing. REQUIRED: reciprocal-space signatures of crystalline and amorphous order. APPLICATION EXAMPLE: qualitative superlattice and quasicrystal comparisons. *Subject to the University's National Day teaching adjustment notice*
7	Ch7: Additional Crystallographic Computations	Zones, zone axes, direct-reciprocal relations, coordinate transformations, and selected stereographic concepts.

Week	Contents	Descriptions
8	Ch8: Symmetry in Crystallography	Symmetry elements and operations; rotation, reflection, inversion, translation, screw axes, glide planes, and point symmetry. APPLICATION EXAMPLE: symmetry operations in selected metallic and ceramic structures. A brief integration of Weeks 1-8 supports preparation for the midterm.
9	Midterm Examination	Examination only. Required scope: all required content taught in Weeks 1-8. No lecture, review, transition, or new content. Tentative schedule, subject to change.
10	Ch9: Point Groups	Group idea; crystallographic point-group families; Hermann-Mauguin symbols; property constraints. APPLICATION EXAMPLE: fivefold quasicrystal symmetry as a contrast to crystallographic restriction.
11	Ch10: Plane Groups and Space Groups	Translations plus point symmetry; plane and space groups; symmorphic and non-symmorphic operations; International Tables; equivalent and Wyckoff positions.
12	Ch11: X-ray Diffraction - Geometry	X-ray generation and wavelength selection; Bragg's law in direct and reciprocal space; Ewald construction. REQUIRED: powder diffraction and the basic Laue method using a fixed crystal and polychromatic beam, including transmission and reflection geometry.
13	Ch12: X-ray Diffraction - Intensities	Electron scattering and atomic scattering factors; structure factors; lattice centering; symmetry and systematic absences; measured-intensity context. REQUIRED: site occupancy, order-disorder, ordering-sensitive superlattice reflections, and their intensities. APPLICATION EXAMPLE: Cu_3Au and other ordered alloys.
14	Ch13: Other Diffraction Techniques	Introductory electron diffraction, including basic diffraction geometry and reciprocal-space interpretation; conceptual comparison of X-ray, neutron, electron, and synchrotron diffraction in terms of scattering contrast and the structural questions each method can answer. REQUIRED: point defects, charge compensation, simple equilibrium defect populations, site occupancy, and diffraction signatures. APPLICATION EXAMPLE: YSZ oxygen vacancies and probe selection for local order and functional ceramics.
15	Ch14: Crystal Structures and Diffraction Patterns	Space-group and graphical structure descriptions; forward and inverse links between structure and powder pattern; Ni and NaCl core examples. REQUIRED: distinguishing polymorphs from powder patterns and recognizing defect or disorder effects on intensity and peak shape. APPLICATION EXAMPLE: selected metallic, ceramic, and mineral cases.
16	Integrated Structure Analysis: From Diffraction Evidence to a Defensible Model	Formal lecture and guided case analysis. Connect peak positions, systematic absences, relative intensities, density, chemistry, and complementary scattering to test competing structure models; interpret whole-pattern agreement and uncertainty. No new textbook chapter.
17	Comprehensive Review	Comprehensive review and integration of all required course content, including crystallography, symmetry, reciprocal space, diffraction, and structure-to-pattern reasoning. No new content.

Week	Contents	Descriptions
18	Final Examination	Cumulative examination only. Covers all required instructional content taught through Week 16. No review or instruction. Tentative schedule, subject to change.