

MSE 6402 – Structure and Defects

School of Materials Science and Engineering
Georgia Institute of Technology

Spring Semester 2024

Course Objective	To impart students with a fundamental understanding of the structural features of crystalline materials, including point and space groups, representative crystal structures, point and linear defects, and the effect of symmetry and defects on material properties.
Mode of Instruction	This course will be delivered in the residential mode. Lectures may be recorded for students who are unable to attend the class, but arrangements must be made in advance.
Lecture	3:30 - 4:45pm W F, Instruction Center 209
Instructors	Meilin Liu
Office	Love 258
Phone	404-406-2207
E-mail	meilin.liu@mse.gatech.edu
Office Hour	W F 5 - 6:30 pm or by appointment, call or e-mail
TA	Michael Rademacher: mrademacher@gatech.edu
Office Hour	11-12:00 Tuesdays in Love 183; 2:30-3:30 Wednesdays in MRDC 3403
Homework	Homework problems will be assigned periodically, and solutions will be provided at a later time. While homework may be collected, it will not be graded.
Exam/grading	Exam 1 – Structure & symmetry of materials Exam 2 – Structure-property relationships Exam 3 – Point and linear defects
Grading Basis	>90% A guaranteed >80% B guaranteed >70% C guaranteed >60% D guaranteed
Learning Accommodations:	Kindly inform me if you have a documented disability or specific needs requiring accommodation. We will ensure appropriate accommodations in accordance with the Office of Disability Services (https://disabilityservices.gatech.edu). However, this must be arranged in advance (within the first two weeks).

Learning Objectives:	<p>Upon completion of this course, students will be able to:</p> <ul style="list-style-type: none"> • Deduce the point groups of simple structures and geometric figures. • Understand space group notations and all symmetry elements associated with each space group. • Become familiar with structural features of crystalline materials. • Understand point defects and linear defects in crystalline solids. • Understand the inherent correlation between crystal structure, defects, and properties of materials.
Academic Integrity	<p>Students are reminded of the obligations and expectations associated with the Georgia Tech Academic Honor Code and Student Code of Conduct, available online at www.honor.gatech.edu. Academic dishonesty will not be tolerated, including cheating, lying about course matters, plagiarism, or helping others commit a violation of the Honor Code. Academic misconduct refers to any act that may improperly distort student grades or other student academic records. Such acts include but are not limited to the following:</p> <ul style="list-style-type: none"> • Possessing, using or exchanging improperly acquired written or verbal information in the preparation of exams or assignment • Submission of material that is wholly or substantially identical to that created or published by another person or persons, without adequate credit notations indicating authorship (plagiarism); • Obtaining details/help on tests and assignments from students previously enrolled in the course • Scholastic dishonesty by a few is unfair to the students who are honest. Please help us keep the grading fair and the learning opportunity in this course as equitable as possible.
Electronic Devices	<p>During class, be sure to turn off and put away all electronic devices, including cell phones, smartphones, laptops, tablets and similar devices) that can be used to view Internet web pages, or to communicate voice, data, text or graphic messages.</p> <p>During an exam, the only electronic device that you may have out and available for use is a commercially available calculator.</p>

References

1. **Lecture notes** – to be posted on **Canvas**
2. **Structure of Materials: An Introduction to Crystallography, Diffraction and Symmetry**, 2nd Edition, M. De Graef and M. E. McHenry, 2012, Cambridge University Press. (Chapters 3, 9, 10, 17)
https://gatech-primo.hosted.exlibrisgroup.com/permalink/f/1vgrnp4/01GALI_GIT_ALMA51247241770002947
3. **Physical Ceramics**, Y. M. Chiang, D. Birnie, and W. D. Kingery, Wiley, 1997.
4. **Crystallography – An Introduction**, 3rd ed., Walter Borchardt-Ott, Springer-Verlag, 2012
https://gatech-primo.hosted.exlibrisgroup.com/permalink/f/1vgrnp4/01GALI_GIT_ALMA51158461550002
5. **Physical Properties of Crystals: Their Representation by Tensors and Matrices**, 3rd Edition, J.F. Nye, Oxford, 2001.
6. **Defects in Solids**, R.J.D. Tilley, Wiley, 2008, QD921.T53
7. **Introduction of Dislocations**, 4th Edition, D. Hull and D.J. Bacon, Pergamon Press
8. **Elementary Dislocation Theory**, 1992 Edition, Johannes Weertman and Julia R. Weertman, Oxford University Press

Canvas

Lecture notes, assignments of homework problems, homework solutions, announcements and other materials relevant to the course will be posted on Canvas. It is the student's responsibility to check their e-mail and Canvas on a regular basis.

Attendance and Tardiness

While there is no formal attendance policy, it is hoped that you feel attending class is important to your learning and for success in this class. Even for an excused absence, it is your responsibility to find out what was missed. There may be test questions based on material that is exclusively covered in class; thus, missing class could have some effect on your grade in the course.

It is disruptive to the class when someone arrives late (or leave early). Try to come to class on time or a few minutes early to get prepared for class.

Institute Absence Policy

<https://catalog.gatech.edu/rules/4/>

Seeking Assistance

I would be more than happy to meet with students to provide assistance with course material and/or other school and career related issues. Please feel free to stop by during my office hours or email me to arrange a time to meet. While I can usually be flexible on arranging a meeting time, I may be unavailable to meet with students without an appointment.

Please give yourself sufficient time to study for exams. If you have a specific question or need clarification of a topic, please discuss it with me at least one day before the scheduled exam.

Questions regarding test material will NOT be answered or discussed on the day of the exam.

MSE 6402: Topical Outline

# of Lectures	Date	Topics	Ref
		Crystal Structure and Symmetry	1,2,3,4
9	Jan-10 to Feb-7	<p>Overview of the course; Geometric principles: Representative structures of important materials: metals, alloys, semiconductors, and ceramics (AX, AX₂, ABX₃, AB₂X₄ compounds: Fluorite, Perovskite, Spinel, Garnet, etc.); Pauling rules</p> <p>Crystal Symmetry: Symmetry operations;</p> <p>Crystallographic point groups; Magnetic (color) point groups; Space groups</p>	
	Feb-14	Exam 1: Crystal Structure and Symmetry (100 pts)	
		Structure-property relationships	1,2,5
8	Feb-9 to Mar-8	<p>Non-crystallographic point groups: Curie (limiting) groups (symmetry of force fields and physical properties)</p> <p>Introduction to anisotropy and tensors</p> <p>Effect of crystal symmetry on properties of materials: Neumann's principles; Formulation of physical interactions</p> <p>Number of independent components of tensor properties in different crystals;</p> <p>Ferro-electricity, Ferrimagnetism, and other physical interactions</p>	
	Mar 15	Exam 2: Structure-property relationships (100 pts)	
		Point and Linear Defects	1,3,6,7
9	Mar 13 to Apr 19	<p>Defect Notations</p> <p>Equilibrium Defect Concentrations</p> <p>Defect Reactions</p> <p>Mass-Action Law/Electroneutrality approximation</p> <p>Ionic and Electronic Disorders in materials</p> <p>Brouwer's Approximation</p> <p>Non-stoichiometry: Solid-Gas Interactions</p> <p>Effect of Doping: Donors and acceptors</p> <p>Temperature Effect</p> <p>Line Defects and their Characteristics</p> <p>Charged Surfaces & Space Charge Region, Complex Defects</p>	
Final Period	Apr 26	Exam 3: Defects (100 pts); 2:40 – 4:30 PM	

MSE Diversity, Equity, and Inclusion

Georgia Tech values diversity and inclusion; we are committed to a climate of mutual respect and full participation. Our goal is to create learning environments that are usable, equitable, inclusive, and welcoming. If there are aspects of the instruction or design of this course that result in barriers to your inclusion or accurate assessment or achievement, please notify the instructor as soon as possible. Students with disabilities should contact the Office of Disability Services to discuss options of removing barriers in this course, including accommodations. ODS can be reached at 404.894.2563, dsinfor@gatech.edu or disabilityservices.gatech.edu.

Website: For more information about MSE DEI initiatives, please click the link:

<https://www.mse.gatech.edu/values/diversity>

CRSH (Create Resistance to Sexual Harassment): <https://www.mse.gatech.edu/values/crsh>

MSE is committed to a community that actively resists sexual and gender harassment. If you see or experience any of the following: sexual harassment, domestic and dating violence, sexual assault and stalking, resources are available:

- **Confidential VOICE Advocates** (www.voice.gatech.edu) can provide support 24/7 and explore resources and options. If after hours, call GTPD dispatcher at 404-894-2500 and ask to speak to the On-Call VOICE Advocate. You do not need to make a report nor provide any information other than your phone number for a VOICE advocate to contact you.
- Sexual violence or harassment can be reported directly to Georgia Tech's **Title IX Coordinator**, James Newsome, (404) 385-5583 burnsnewsome@gatech.edu.

Faculty, Staff and TAs are mandatory reporters and are required to inform the Title IX Coordinator should they become aware that you or any student has experienced sexual violence or sexual harassment.

Website: For more information about MSE CRSH, click the link:

<https://www.mse.gatech.edu/values/crsh>