

MSE 6402 – Structure and Defects

School of Materials Science and Engineering
Georgia Institute of Technology

Spring Semester 2023

Course Objective	To provide students with a fundamental understanding of 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 materials properties
Mode of Instruction	This course will be delivered in the residential mode. Most lectures may be recorded in case some students may be unable to make it to the class.
Lecture	3:30 - 4:45pm W F, Instruction Center 209
Instructors	Meilin Liu
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Phone	894-6114
E-mail	meilin.liu@mse.gatech.edu
Office Hour	W F 5 - 6:30 pm or by appointment, also call or e-mail
Teaching Assistant and Office Hour	Weining Wang: office hour time/location/e-mail/phone TBD
Homework	Problems will be assigned periodically and solutions will be posted later. Homework may be collected but will not be graded.
Exam/grading	3 Exams Exam 1 – Structure & symmetry of materials Exam 2 – Structure-property relationships Exam 3 – Point and linear defects
Grading Basis	Scale >90% A guaranteed >80% B guaranteed >70% C guaranteed >60% D guaranteed

Learning Objectives:	<p>Upon completion of this course, students will be able to:</p> <ol style="list-style-type: none"> 1. Deduce point groups of simple crystal structures and geometric figures. 2. Understand space group notations and all symmetry elements associated with each space group. 3. Become familiar with structural features of crystalline materials. 4. Understand point defects and linear defects in crystalline solids. 5. 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.</p>
Learning Accommodations:	<p>For students with documented disabilities, we will make classroom accommodations in accordance with the ADAPTS office (http://www.adapts.gatech.edu). However, this must be arranged in advance.</p>
Electronic Devices	<p>Silence all electronic devices (cell phones, smart watches, etc.) during class.</p> <p>The only electronic device that you may have out and available for use during an exam 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

MSE 6402: Topical Outline

# of Lectures	Date	Topics	Ref
		Crystal Structure and Symmetry	1,2,3,4
9	Jan-11 to Feb-8	<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-15	Exam 1: Crystal Structure and Symmetry (100 pts)	
		Structure-property relationships	1,2,5
8	Feb-10 to Mar-10	<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 17	Exam 2: Structure-property relationships (100 pts)	
		Point and Linear Defects	1,3,6,7
9	Mar 15 to Apr 21	<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	May 3	Exam 3: Defects (100 pts); 2:40 – 4:30 PM	