MSE 6402 - Structure and Defects

School of Materials Science and Engineering Georgia Institute of Technology

Fall Semester 2012

Course Objective	To provide students with a fundamental understanding of crystal structures, symmetry, defects, and microstructure in crystalline materials, and their influence on materials properties.			
Lecture	10-11 M W F in Love	299		
Instructor Office Phone E-mail Office Hour	Meilin Liu Love 258 894-6114 meilin.liu@mse.gatechedu M W F 3-4	Naresh Thadhani Love 166 894-2651 naresh.thadhani@mse.gatech.edu	Arun Gokhale Love 265 894-2887 arun.gokhale@mse.gatech.edu	
Teaching assistant	TBD			
Homework	Problems will be assigned periodically and solutions will be posted a week later. Homework will not be collected or graded.			
Exam/grading	4 Exams, 25% each			
	Exam 1 – Crystal Structure and Symmetry Exam 2 – Point defects Exam 3 – Dislocations Exam 4 – Surfaces, Interfaces, and Microstructures			

References

- 1. Lecture notes to be posted on T-Square
- 2. Physical Ceramics, Y. M. Chiang, D. Birnie, and W. D. Kinggery, Wiley, 1997.
- 3. Crystallography, Walter Borchardt-Ott, Springer-Verlag, 1993, QD 905.2.B713
- 4. Defects in Solids, R.J.D. Tilley, Wiley, 2008, QD921.T53
- 5. The Chemistry of Imperfect Crystals. Vols. 2&3, F.A. Kroger, North Holland/American Elsevier, 1974, QD478.K76.
- 6. Introduction of Dislocations, 4th Edition, D. Hull and D.J. Bacon, Pergamon Press
- 7. Elementary Dislocation Theory, 1992 Edition, Johannes Weertman and Julia R. Weetman, Oxford University Press

MSE 6402: Topical Outline

11 Aug-20 Geometric principles: Representative structures of important materials: metals, alloys, semiconductors, and ceramics (AX, Sept-14 AX ₃ , ABX ₃ , Compounds: Fluorite, Perovskite, Spinel, Garnet, etc.); Pauling rules Crystal Symmetry of proce fields and properties: Limit groups; Effect of symmetry on properties of materials Sept-17 Exam 1: Crystal Structure and Symmetry (25%) 10 Sept-19 Defect Notations Equilibrium Defect Concentrations Defect Notations Equilibrium Defect Concentrations Defect Reactions Mass-Action Law/Electroneutrality approximation Ionic and Electronic Disorders in materials Brouwer's Approximation Non-stoichiometry: Solid-Gas Interactions Effect of Doping: Donors and acceptors Temperature Effect Charged Surfaces & Space Charge Region, Complex Defects Exam 2: Point Defects (25%) Surfaces, Interfaces, and Microstructures - A. Gokhale 12 Oct 17 Structure of Grain Boundaries and Interfaces Geometric Topological Aspect of Grain Structures Mathematical Correlation of Microstructures in terms of correlation functions, near neighbor distributions, morphological orientation distributions, size and shape distributions, metric and topological attributes, etc. Modeling and simulations of microstructural geometry, solutions to inverse problems Effects of microstructural geometry on important classes of material properties Nov-12 Exam 3: Surfaces, Interfaces, & Microstructures (25%) Dislocations - N. Thadhani 10 Nov-14 Line Defects and their Characteristics Movement of Dislocations Dislocations in FCC Systems Dislocations in FCC Systems Dislocations in FCC Systems Dislocation in FCC Systems Dislocation Arrays and Crystal Boundaries TBD Exam 4: Dislocations (25%)	# of Lectures	Date	Topics	Ref
materials: metals, alloys, semiconductors, and ceramics (AX, AZ ₂ , ABX ₃ , AB ₃ X ₄ compounds: Fluorite, Perovskite, Spinel, Garnet, etc.); Pauling rules Crystal Symmetry: Symmetry operations: Crystallographic point groups; Magnetic (color) point groups; Space groups; Symmetry of force fields and properties: Limit groups; Effect of symmetry on properties of materials Sept-17 Point Defects – M. Liu 10 Sept-19 10 Defect Notations Equilibrium Defect Concentrations Defect Reactions Mass-Action Law/Electroneutrality approximation lonic and Electronic Disorders in materials Brouwer's Approximation Non-stoichiometry: Solid-Gas Interactions Effect of Doping: Donors and acceptors Temperature Effect Charged Surfaces & Space Charge Region, Complex Defects Charged Surfaces, and Microstructures – A. Gokhale 12 Oct 17 Surfaces, Interfaces, and Microstructures – A. Gokhale 1 Structure of Grain Boundaries and Interfaces Geometric Topological Aspect of Grain Structures Nov-9 Nov-9 Mathematical Correlation of Microstructures in terms of correlation functions, near neighbor distributions, morphological orientation distributions, size and shape distributions, metric and topological attributes, etc. Modeling and simulations of microstructural geometry, solutions to inverse problems Effects of microstructural geometry on important classes of material properties Nov-12 Dislocations – N. Thadhani 10 Nov-14 Line Defects and their Characteristics Movement of Dislocations Strain Energy of a Dislocation Forces on Dislocations Dislocations in Other Systems Dislocations in Other Systems Dislocation Arrays and Crystal Boundaries			Crystal Structure and Symmetry – M. Liu	1,2,3
Point Defects – M. Liu 1,2,4,5	11	to Sept-14	materials: metals, alloys, semiconductors, and ceramics (AX, AX ₂ , ABX ₃ , AB ₂ X ₄ compounds: Fluorite, Perovskite, Spinel, Garnet, etc.); Pauling rules Crystal Symmetry: Symmetry operations; Crystallographic point groups; Magnetic (color) point groups; Space groups; Symmetry of force fields and properties: Limit groups; Effect of symmetry on properties of materials	5 6.30 D
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Oct-17 Exam 2: Point Defects (25%) Surfaces, Interfaces, and Microstructures – A. Gokhale 12 Oct 17 Structure of Grain Boundaries and Interfaces Geometric Topological Aspect of Grain Structures Nov-9 Mathematical Correlation of Microstructures in terms of correlation functions, near neighbor distributions, morphological orientation distributions, size and shape distributions, metric and topological attributes, etc. Modeling and simulations of microstructural geometry, solutions to inverse problems Effects of microstructural geometry on important classes of material properties Nov-12 Exam 3: Surfaces, Interfaces, & Microstructures (25%) Dislocations – N. Thadhani 1,6,7 10 Nov-14 Line Defects and their Characteristics Movement of Dislocations Dec-7 Elastic Properties of Dislocations Strain Energy of a Dislocation Forces on Dislocations Dislocations in FCC Systems Dislocations in Other Systems Jogs and Intersection of Dislocations Origin and Multiplication of Dislocations Dislocation Arrays and Crystal Boundaries	10	to	Equilibrium Defect Concentrations Defect Reactions Mass-Action Law/Electroneutrality approximation Ionic and Electronic Disorders in materials Brouwer's Approximation Non-stoichiometry: Solid-Gas Interactions Effect of Doping: Donors and acceptors Temperature Effect	
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TBD Exam 4: Dislocations (25%)	10	to	Movement of Dislocations Elastic Properties of Dislocations Strain Energy of a Dislocation Forces on Dislocations Dislocations in FCC Systems Dislocations in Other Systems Jogs and Intersection of Dislocations Origin and Multiplication of Dislocations	
		TBD		