

MATSE 400 CRYSTAL CHEMISTRY

Course Designation: This is a required course for Ceramic Science and Engineering and Electronic and Photonic Materials. It is an optional course for the other options. It is planned that this course become required for all options.

Catalog Description: Principles of crystal chemistry applied to structures, structural defects and properties of organic, inorganic, intermetallic, and metallic crystals

Course Description: This course is an introduction to the principles of crystal chemistry and its use in describing structure-property relations in solids. The principles that govern assembly of crystal and glass structures are described, models of many of the technologically important crystal structures are built, and the impact of structure on the various fundamental mechanisms responsible for many physical properties are discussed.

Prerequisites: CHEM 013, CHEM 015, MATH 231, MATH 251, PHYS 214

Textbook: Crystal Chemistry and Refractivity by Howard W. Jaffe
Class Notes

Course Objectives:

1. To identify important raw materials and minerals as well as their names and chemical formulae.
2. To describe the crystal structure of important materials and to be able to build their atomic models.
3. To learn the systematics of crystal and glass chemistry.
4. To understand how physical and chemical properties are related to crystal structure and microstructure.
5. To appreciate the engineering significance of these ideas and how they relate to industrial products: past, present, and future.

Topics Covered:

1. Chemical Bonding, electronegativity
2. Fundamentals of crystallography: crystal systems, Miller indices, symmetry elements, bond lengths and radii, theoretical density
3. Crystal and glass structure prediction: Pauling's and Zachariasen's rules
4. Phase Diagrams and crystal chemistry (including solid solutions)
5. Imperfections: (including defect chemistry and line defects)
6. Phase transformations
7. Structure – property relations: Neumann's law: melting point, mechanical properties (hardness, slip, cleavage, elastic moduli), wetting, thermal properties (thermal expansion specific heat, thermal conductivity), diffusion, ionic conductivity, refractive index, absorption, color, dielectrics and ferroelectrics, magnetism
8. Introduction to crystal structures of representative metals, semiconductors, polymers, and ceramics

Class Schedule: 3 credit course offered annually meeting 3 times per week; 2 meetings are 50 minutes long, the laboratory component (3rd meeting) is 115 minutes in length

Course Outcomes:

1. Students should be able to write and balance chemical formulae for commercially important raw and engineered materials.
2. Students should be able to build and describe important crystal structures and understand the impact of bond length, coordination, and symmetry on the resultant physical properties.
3. Students should be able to use various tools of crystallography, including an understanding of symmetry, point groups and space groups, Miller indices, and direction indices.
4. Students should understand the types of bonding in solids, and the impact on properties.
5. Given an initial chemistry, students should be able to apply Pauling's rules to determine anion and cation coordinations, and should be able to make intelligent suppositions about the resulting crystal structure.

Similarly, on the basis of Zachariasen's rules, students should be able to assess the likelihood of easy glass formation in a particular materials system.

6. Students should understand the rules governing the stability of crystal structures as a function of temperature, pressure, and composition changes.
7. Students should understand the basic mechanisms controlling a wide variety of physical properties, and should be able to correlate this information with crystal structures to predict materials properties.
8. Students should be able to describe defects in solids.

Assessment Tools:

1. Midterm and final exams
2. Weekly quizzes in lab class
3. Problem sets utilizing crystallography software, which allow student collaboration.

Professional Component: This class is one of the first that Materials Science and Engineering students take that details crystal structures and structure-property relations. As a result, it serves as the underpinnings for much of their subsequent education in materials. The class draws on concepts learned previously in physics and chemistry classes. This information is coupled with the principles of crystal chemistry and the opportunity to build models of a >30 key structures, in order to guide students to an understanding of the factors that govern many of the fundamental physical properties of materials.

Prepared by: Susan Trolier-McKinstry, February 2002

MAP TO DEPARTMENTAL OUTCOMES (For further detail, see coursebook)											
a	b	c	d	e	f	g	h	i	j	k	l
1	2	2	3	2	3	3	2	3	2	1	1

MAP TO DEPARTMENTAL OBJECTIVES (For further detail, see coursebook)						
(1)	(2)	(3)	(4)	(5)	(6)	(7)
2,3,4	1,2,3,4	2,3,4,5	1,5		2	