DISCIPLINE SPECIFIC COURSES Applicable Specifically for B.Sc. Physical Sciences

DISCIPLINE SPECIFIC ELECTIVE COURSE – 23 PS (DSE-23 PS): Crystalline solids: Properties and Methods of Analysis

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Crystalline Solids: Properties and Methods of Analysis (DSE-23 PS)	04	02	--	02	Class 12th with Physics, Chemistry, Mathematics	--

Course Objectives

The objectives of this course are as follows:

- To analyse different crystal systems and understand their properties.
- To study Curie's and Curie-Weiss law and its application to paramagnetic and ferromagnetic materials, respectively.
- To understand the principles and application of basic instrumentation techniques.

Learning outcomes

By studying this course, the students will be able to:

- Distinguish between lattice, unit cell, and the 14 Bravais lattices, and understand their symmetry and properties.
- Interpret XRD patterns of NaCl, CsCl, and KCl to deduce structural information.
- Understand the Curie-Weiss law and its application to ferromagnetic materials.
- Analyse and interpretation of experimental data obtained through experimental techniques.

Theory:

Unit 1: Crystalline Solids **(9 Hours)**

Classification and characteristics of crystalline solids, seven crystal systems. Fundamentals of lattice, unit cell and fourteen Bravais lattices. Types of closed-packed structures. Elementary idea of symmetry. Crystal's direction and planes, Miller indices.

Unit 2: Diffraction Methods **(9 Hours)**

Bragg's law and Bragg's conditions. X-ray diffraction pattern of simple cubic systems i.e. NaCl, CsCl, and KCl, Laue method, Crystallite size (Scherrer equation) and Williamson-Hall method to determine lattice strains from diffraction patterns. Elementary idea of Thermogravimetric analysis (TGA).

Unit 3: Electronic Properties and Band Theory of Solids **(6 Hours)**

Introduction- metals, insulators, and semiconductors. Electronic structure, k-space and Brillouin zone, band structure of metals, insulators, and semiconductors.

Unit 4: Magnetic Properties **(6 Hours)**

Magnetic moment, Curie law, Curie-Weiss law, magnetic ordering, exchange Interaction, Hysteresis, anisotropy, paramagnetism, ferromagnetism, ferrimagnetism, antiferromagnetism

Practicals: **Credits: 02**

(Laboratory periods:15 classes of 4 hours each)

1. Preparation of semiconducting TiO_2 /ZnO/ CdSe/ ZnSe/ In_2S_3 and metal nanomaterials (Ag/ Cu/ Ni etc.) by any soft chemical approach (emulsion based, co-precipitation etc.). (Minimum two preparations)
2. Analysis of diffraction pattern obtained from Powder X-ray diffractometer. Identifying crystal phase, diffraction peaks with lattice planes for a given compound*.
3. Determination of approximate crystallite size using the given PXRD pattern of a known compound i.e. TiO_2, ZnO etc by employing Scherer equation*.
4. Determination of lattice strain using Williamson-Hall equation and from the measured PXRD pattern of a known inorganic compound for example, TiO_2, ZnO etc.*
5. Determination of band gap of a semiconducting nanoparticle (in solution) using UV-visible spectrophotometer.
6. Thermogravimetric analysis of a known compound*. (Analysis of the thermal decomposition pattern of a hydrated salt like calcium sulfate pentahydrate, magnesium sulfate heptahydrate, etc.)
7. Determination of congruent composition and temperature of a binary system (e.g. diphenylamine-benzophenone/ Urea-resorcinol system).
8. Analysis of p-XRD data of a given set of Metals/ compounds* (Ag/Au/Cu/NaCl/CsCl) and confirmation of the type of the cubic system corresponding to given species.
9. Demonstrate the Principles, experimental setup, and instrumentation of TGA, and Interpretation of the analytical information from TGA curves*.

*[Diffraction patterns of known sample along with Standard JCPDS file (JCPDS: Joint Committee for Powder Diffraction Studies) be provided to students for analysis]

Essential/recommended readings

Theory:

1. Kapoor, K.L. (2015), A Textbook of Physical Chemistry, Vol 1, 5th Edition, Mc Graw Hill Education.
2. Levine I.N. (2009), Physical Chemistry 6th Edition, Mc Graw Hill Education.
3. Pillai S.O., (2022) Solid State Physics 6th Edition, New Age International Publishers.
4. Chakrabarty, (2022) D. K., Solid State Chemistry, 2nd Edition, New Age International Publishers.
5. West, A.R., (2022), Solid State Chemistry and its Applications, 2nd Edition, Wiley Inc.
6. Callister W. D., (2018) Materials Science and Engineering: An Introduction, 10th Edition, Willey Inc.
7. Keer H. V., (Reprint 2005), Principles of the Solid State, New Age International Publishers.

Practical:

1. Cullity, B. D. (2001) *Elements of X-ray Diffraction*, 3rd ed.; Prentice Hall.
2. Hammond, C. (2015) *The Basics of Crystallography and Diffraction*, 4th ed.; Oxford University Press.
3. Snyder, R. L. (1996) Jenkins, R. *Introduction to X-ray Diffractometry*; Wiley: New York.
4. Evans J. S. O., Evans I.R., Structure Analysis from Powder Diffraction Data: Rietveld Refinement in Excel, *J. Chem. Educ.* **2021**, *98, 2, 495-505*.
5. Hulien M.L., Lekse J.W., Rosmus K. A., Devlin K. P., Glenn J.R., Wisneski S. D., Wildfong P., Lake C. H., MacNeil J. H.Aitken J. A., An Inquiry-Based Project Focused on the X-ray Powder Diffraction Analysis of Common Household Solids, *J. Chem. Educ.* **2015**, *92, 12, 2152-2156*.
6. Bentley A. K., Farhoud M, Ellis A. B., Lisensky G.C., Nickel A-Marie L, Crone W. C., Template Synthesis and Magnetic Manipulation of Nickel Nanowires, *J. Chem. Educ.* **2005**, *82, 5, 765-768*.
7. Oliveira M. L., Pagung E., Lorenzini L., Neves T.R., Pereira J.R.P., Ferreira S. A. D., Freitas M. B. J.G. de, Moura P. R.G., Lelis M. F. F., Synthesis of Iron Oxide Nanoparticles and their Application in Photo-Fenton Process: An Undergraduate Experiment in Chemistry, *J. Chem. Educ.* **2025**, *102, 1590-1597*.
8. How to Characterize 4−90nm Size Gold Nanospheres with Experimental and Simulated UV−Vis and a Single SEM Image, *J. Chem. Educ.* **2023**, *100, 1589-1596*.
9. https://www.icdd.com/ (International Centre for Diffraction Data).

Assessment Methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.-