2021-22

Name of the Department/Society: **Department of Physics & Electronics/LUMEN**
Name of Event 4: Winter School 2021-22
Dates of Event: 31st December 2021 to 8th January 2022

Since 1913, when W. L. Bragg solved the structure of NaCl, the structures of many thousands of crystals, organic and inorganic, have been determined using X-ray diffraction tool. This vast body of knowledge is of fundamental importance in such fields as crystal chemistry, solidstate physics, and the biological sciences because, to a large extent, structure determines properties and the properties of a substance are never fully understood until its structure is known. In metallurgy, a knowledge of crystal structure is a necessary prerequisite to any understanding of such phenomena as plastic deformation, alloy formation, or phase transformations. Crystal structure underlies technologically useful effects such as piezoelectricity, and knowledge of it is required for understanding the nature of point and other atomic-scale defects controlling many materials properties.

Winter School was held from 31st December 2021 to 08th January 2022. All the session were conducted in online mode via M S Teams due to on-going situation of Covid-19.

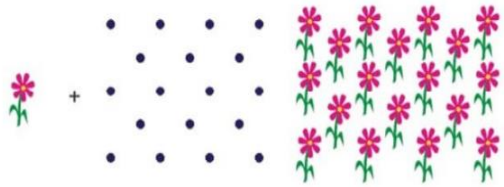
- **Total number of registrations: 66**
- **Total numbers of participant with 60% of overall session were 41 (got Certificate of Participation)**
- **Total numbers of students involved in doing data analysis of x-ray diffraction were 15 (got Certificate of Participation and X-ray Data Analysis)**

Day 1 (31-12-2021): Focus was on basics of crystal structure:

The session was conducted by **Dr. Maya Verma**, Associate Professor, Dept. of Physics and Electronics, Hansraj College. Various aspects of crystal structure was explained to the students such as about Crystalline and Amorphous solids, Lattice, Basis, Crystal, Unit cell, lattice parameters, Types of lattices, Bravais lattices in 2D, Bravais lattices in 3D, Cubic lattices, Miller indices and Interplanar spacing.

Lattice: An array of imaginary points in space such that every point has identical surrounding

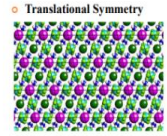
Basis: Group of atoms/ molecules attached to each lattice point

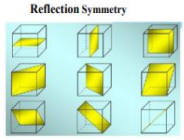


CRYSTAL SYMMETRY

Translational Symmetry

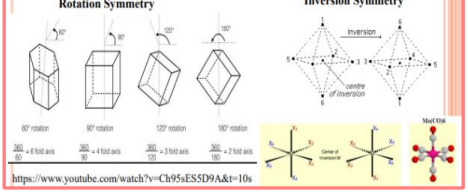
Reflection Symmetry





Rotation Symmetry

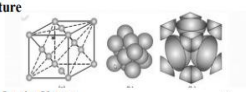
Inversion Symmetry



https://www.youtube.com/watch?v=Ch95sES5D9A&t=10s

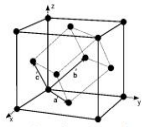
Face Centered Cubic (FCC): -

Structure



Primitive Lattice Vectors

$$a' = \frac{a}{2}(\hat{x} + \hat{y})$$
$$b' = \frac{a}{2}(\hat{y} + \hat{z})$$
$$c' = \frac{a}{2}(\hat{x} + \hat{z})$$



Lattice points per Conventional unit cell: - $\left(\frac{1}{8} \times 8\right) + \left(\frac{1}{2} \times 6\right) = 4$

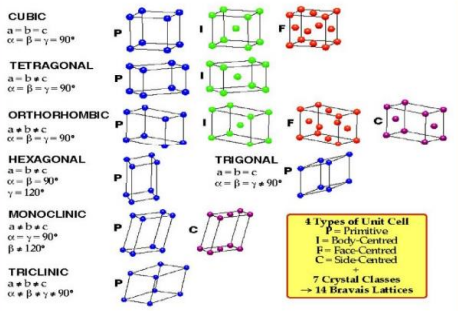
Volume of Conventional unit cell: - $a.(b \times c) = a^2[\hat{x}.(\hat{y} \times \hat{z})] = a^3[\hat{x} \times \hat{x}] = a^3$

Volume of Primitive unit cell: - $a'.(b' \times c') = \frac{a^3}{8}[(\hat{x}+\hat{y}).\{(\hat{y}+\hat{z}) \times (\hat{x}+\hat{z})\}]$

$$= \frac{a^3}{8}[(\hat{x}+\hat{y}).\{(\hat{x}+\hat{y}+\hat{z})\}]$$
$$= \frac{a^3}{8}[1+1] = \frac{a^3}{4}$$

BRAVAIS LATTICES IN 3 D

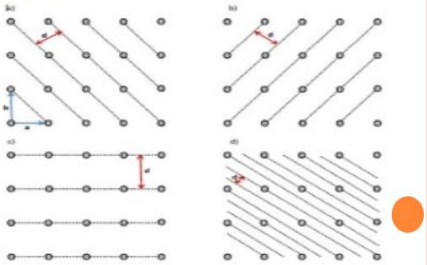
7 crystal systems; 14 Bravais Lattice



7 Crystal Classes with 4 possible unit cell types
Symmetry indicates that only 14 3-D lattice types occur

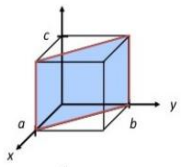
MILLER INDICES (H K L)

The Lattice points forming a space lattice may be thought of as occupying various sets of planes. With reference to axes of 'unit cell', each set of planes has a particular orientation. In order to specify the orientation, Miller Indices is used.
A crystal lattice may be considered as an assembly of a number of equidistant parallel planes passing through the lattice points and are called lattice planes. For a given lattice, these sets of planes can be selected in number of ways. The interplanar spacing for a given set of parallel planes is fixed but for different sets of planes the interplanar spacing vary.

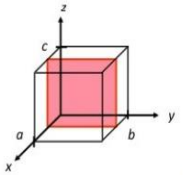


MILLER INDICES IN UNIT CUBE: -

example	a	b	c
1. Intercepts	1	1	∞
2. Reciprocals	1/1	1/1	1/∞
	1	1	0
3. Reduction	1	1	0
4. Miller Indices	(110)		

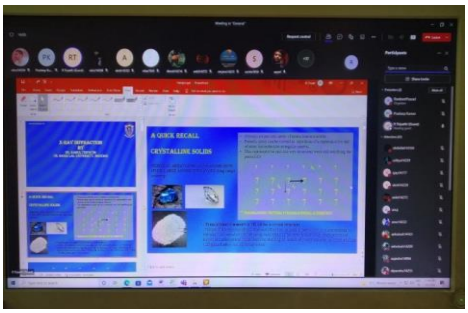


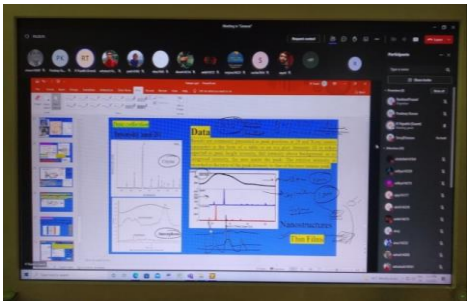
example	a	b	c
1. Intercepts	1/2	∞	∞
2. Reciprocals	1/½	1/∞	1/∞
	2	0	0
3. Reduction	2	0	0
4. Miller Indices	(200)		

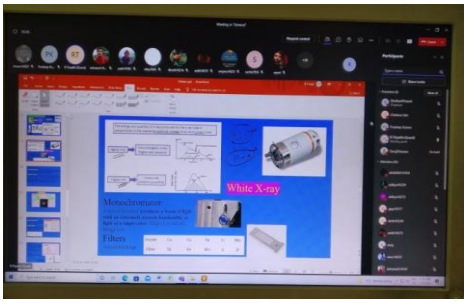


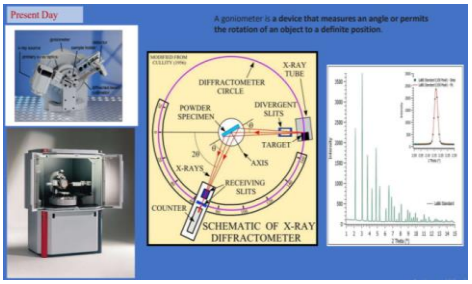
Day 2 (02-01-2022): Focus was on X-Ray Diffractometer:

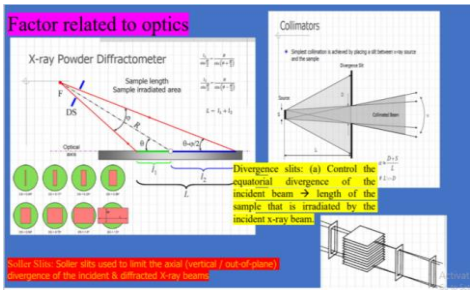
The session was conducted by **Dr. Rahul Tripathi**, Associate Professor, Dept. of Physics, Ch. Bansi Lal University, Bhiwani. Various aspect of X-Ray diffractometer was explained to the students. How the X-Ray are produced, optics for intense beam of X-ray, sample holder, How X-Ray Diffraction is done, various type of X-Ray detectors were also discussed.

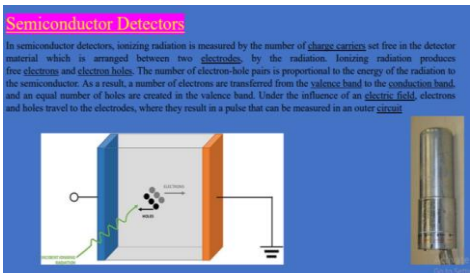


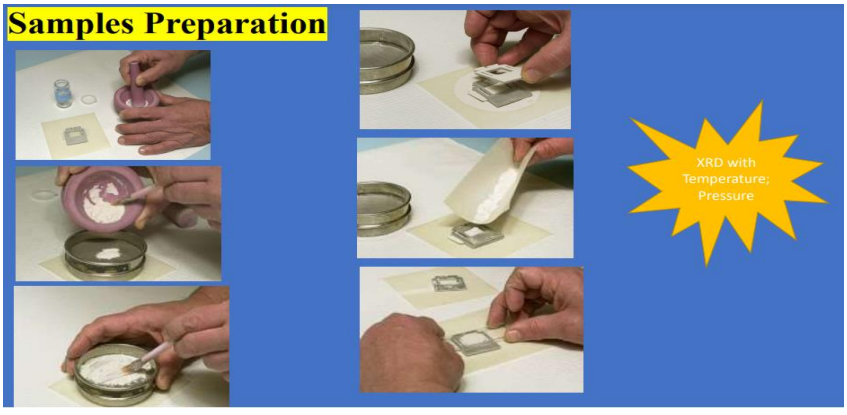






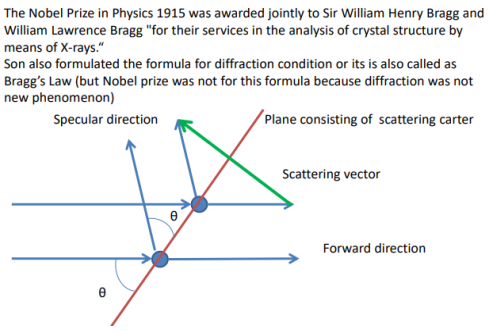


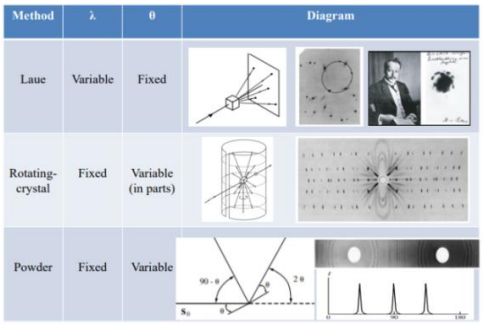


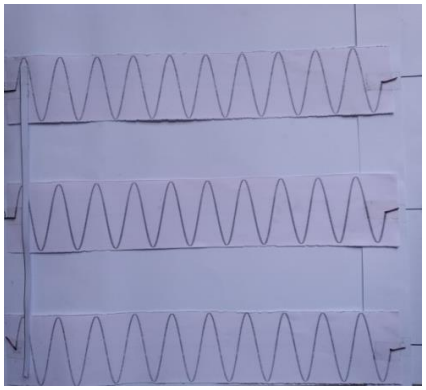


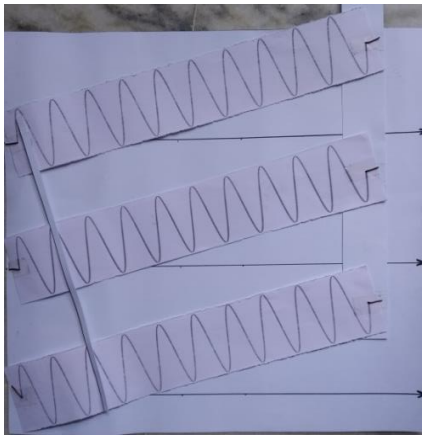
Third Day (03-01-2022): Focus was on Scattering of X-Rays by Crystal Structure:

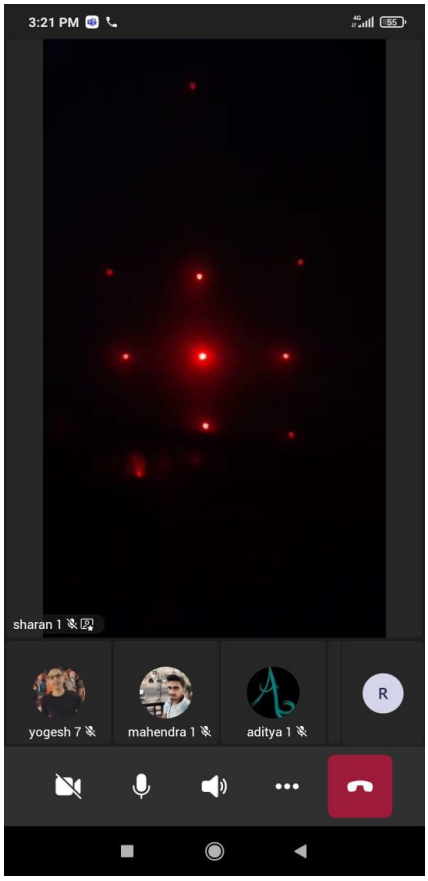
The session was conducted by **Dr. Ravikant Prasad**, Assistant Professor, Dept. of Physics and Electronics, Hansraj College. Various aspect of regarding X-Ray diffraction and intensity calculation was explained to the students such as **Bragg Law, Reciprocal Lattice and Diffraction Directions**. Also scattering by electron, **scattering by An Atom (form factor)**, **scattering by a Unit Cell (structure factor)**, multiplicity factor, Lorentz factor and temperature factor were discussed. Demonstration about how the scattering angle depends on inter-planner spacing and reciprocal lattice requirement was shown by **Wave Machine. 2 D optical diffraction was shown with the help of diffraction grating in P&E Lab 2.**







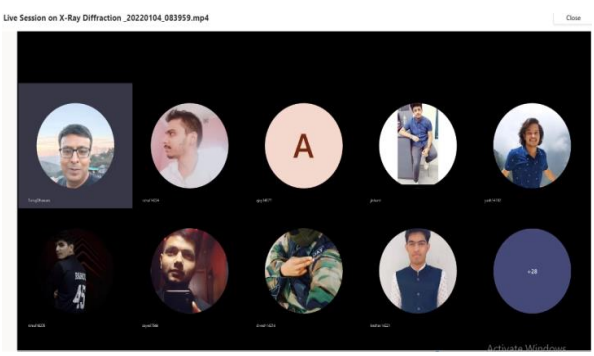




Day 4 (04-01-2022): Focus was on Live Session of X-Ray Diffratometer while performing the diffraction of salts and Data Analysis of X-ray diffraction.

The first session on fourth was of 30 minutes in which the live demo of X-Ray Diffractometer and how we perform the X-Ray diffraction of samples were shown. The session was conducted from central facilities for material characterizations, **Department of Physics and Astrophysics, University of Delhi**. We are very thankful to **Shri. Gauri Shankar**, Engineer at the X-Ray facility, he also explained the working of Ultima IV Regaku X-Ray Diffractometer and helped us to perform the X-Ray Diffraction of our samples.

Later on the fourth day session was conducted by **Dr. Ravikant Prasad** on **Data Analysis of X-ray diffraction via online mode.** In this session it was explained on how we calculate the lattice parameter of any cubic crystal system once we get the data by X-Ray diffraction. Also explained how to index various peaks in diffraction data and identify that sample as SC, BCC or FCC. Later in the evening **X-Ray diffraction data of NaCl, NaI, NaF and KBr are shared** with students to determine the lattice parameters and indexing of peaks. For this purpose, **assignment** was created on MS Teams and 4 days were given for the submission of their result.



Extra session from 05th Jan to 07 Jan 2022 was also conducted by **Dr. Ravikant Prasad** to help students in calculation of lattice parameters as given in the assignment. During these days some software tools were introduced to the students such as Indx and Poudrix which helped them in doing their assignments. The Winter School was concluded on 08-01-2022 with submission of assignments, assessment and certificate distribution.