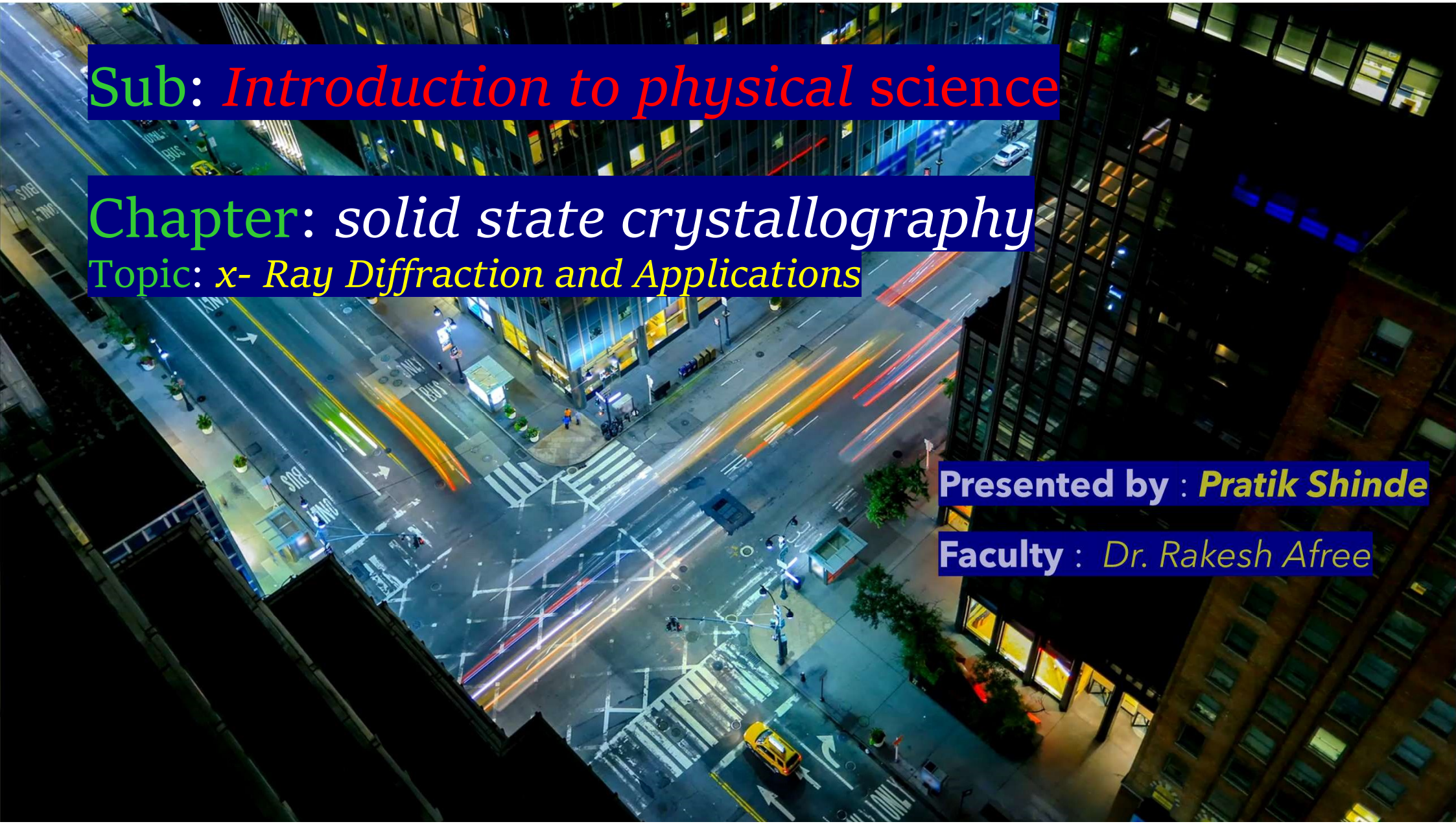

Sub: Introduction to physical science
Chapter: solid state crystallography
Topic: x- Ray Diffraction and Applications
Presented by : Pratik Shinde
Faculty : Dr. Rakesh Afree

CONTENTS

INTRODUCTION

- X-rays were discovered by Wilhelm roentgen who called them x-rays because the nature at first was unknown so x- rays , x-rays are also called roentgen rays. X-ray diffraction in crystals were discovered by max von Laue. The wavelength range is 10^{-7} to about 10^{-15} m

- The penetrating power of x-rays depends on the energy also, there are two types of x-rays
  - Hard x-rays: which have high frequency and have high energy
  - Soft x-rays: which have low penetrating power and have low energy

X-RAYS

- X-rays are short wavelength of electromagnetic radiation produced by the Deceleration of high energy electrons or by electronic transactions of electrons in the inner orbital of atom
- X-ray region :- 0.1 to 100 A
- Analytical purpose:- 0.7 to 2 A

- X-rays are high-frequency, and thus high-energy, electromagnetic radiation. They have wavelengths ranging from 0.01 to 10 nanometres, and thus frequencies from 3×1019 to 3×1016 Hz. They are found to reside between ultraviolet radiation and gamma rays on the electromagnetic spectrum.

PRINCIPLE OF X-RAYS

X-ray diffraction is based on **constructive interference** of monochromatic x-Rays and a crystalline sample. These X-Rays are generated by Cathode ray tube, filtered to produce monochromatic radiations collimated to concentrate and directed towards the sample. The interaction of incident rays with the sample produces constructive interference when conditions satisfies **bragg's law**

BRAGG'S LAW

- Constructive interference of the reflected of the reflected beams emerging from two different planes will take place if the path lengths of two rays is equal to whole number of wavelength.

For constructive interference,

$$n\lambda = 2d\sin\theta$$

this is called as BRAGG'S LAW

INSTRUMENTATION

- Production of x-rays
- Collimator
- Monochromator
  a. Filter
  b. Crystal monochromator
- Detectors
  a. Photographic methods
  b. Counter methods

PRODUCTION OF X-RAY

- X-Rays are generated when high velocity electrons impinge on a metal target
- Approximately 1% of the total energy of the electron beam is converted to x-radiation.
- The reminder being dissipated as heat.
- Many types of X-rays tubes are available which are used for production of X-Rays

X-RAY DIFFRACTION METHOD

These are generally used for investigating the internal structures and crystal structures of various solid compound

They are

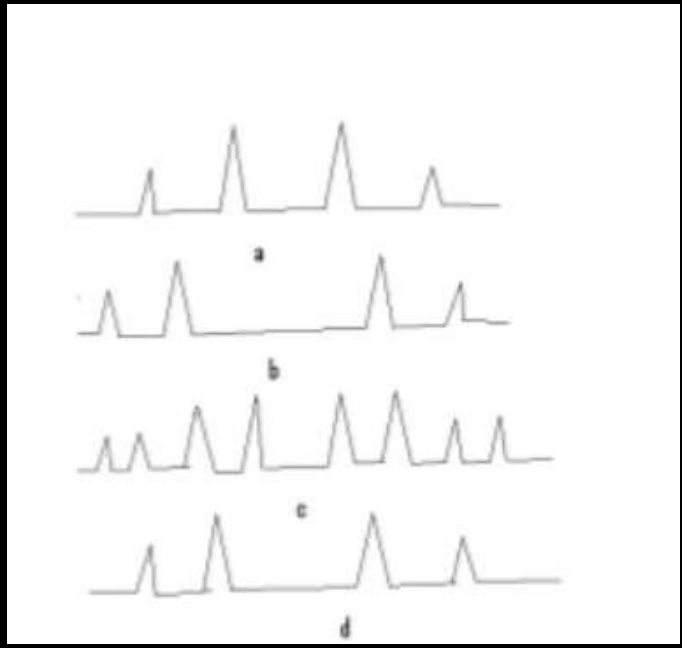
1. Laue's photographic method
    a) Transmission method
    b) Back reflection method
2. Bragg's X-Ray spectrometer method
3. Rotating crystal method
4. Powder method

APPLICATIONS OF XRD

1. Structure of crystal
2. Polymer Characterisation
3. State of anneal in metals
4. Particle size determination
   a) Spot counting method
   b) Broadening of diffraction line.
   c) Low-angle scattering
5. Application of diffraction method to complexes
   a) Determination of cis-trans isomerism
   b) Determination of linkage isomerim
6. Miscellaneous applications

STRUCTURE OF CRYSTAL

a. X ray pattern of salt NaCl
b. x ray pattern of salt KCL
c. x-ray pattern of mixture of NaCl and KCL
d. x-ray pattern of a powder mixed crystal of NaCl and KCL



POLYMER CHARACTERIZATION

- Determine degree of crystallinity
- Non crystalline portions scatters x-ray beam to give a continuous background (amorphous materials)
- Crystalline protein causes diffraction lines that are not continuous. (crystalline materials)

STATE OF ANNEAL METALS:

XRD is used to test the metals without removing the part from its position and without weakening it

PARTICLE SIZE DETERMINATION

Spot counting method:

$v = V.\delta\theta.\cos\theta / 2n$

v = volume of individual crystallite

V = total volume irradiated

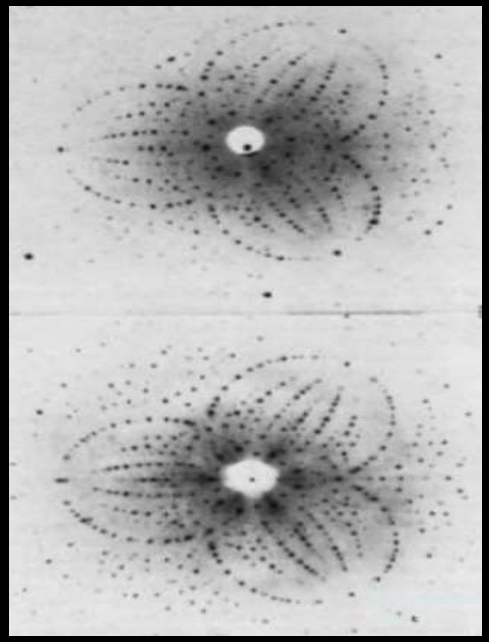
n = number of spots in diffraction ring

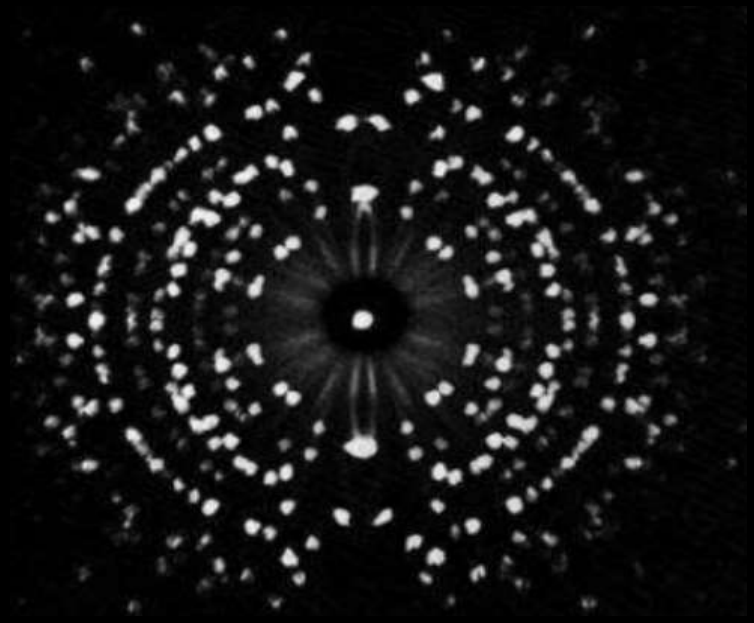
δθ = divergence of X-Ray beam

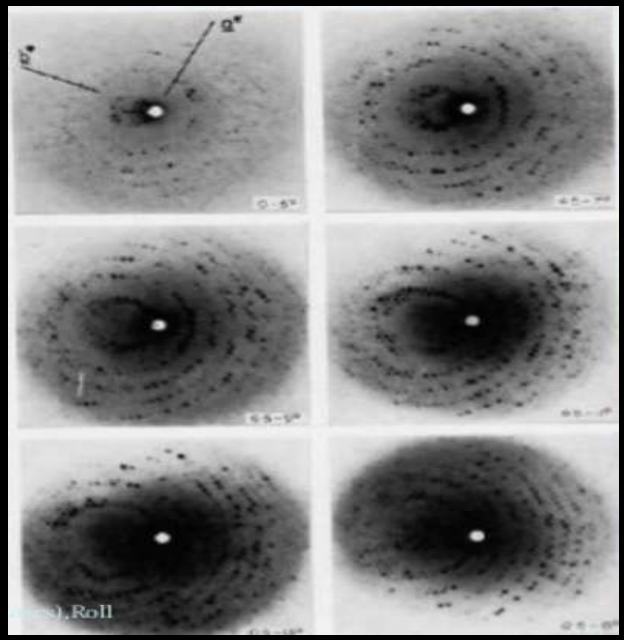
MISCELLANEOUS APPLICATIONS

- Soil classification based on crystallinity
- Analysis of industrial dust
- Assessment of weathering and degradation of minerals and polymers
- Study of corrosion product
- Examination of tooth enamel and dentine
- Examination of bone state and tissue state
- Structure of DNA and RNA
- Treatment of cancer

X-RAY DIFFRACTION PATTERN FOR A SINGLE ATOM CRYSTAL







THANK U