

APPLICATIONS OF XRD

1. Structure of crystals
2. Polymer characterisation
3. State of anneal in metals
4. Particle size determination
 - a) Spot counting method
 - b) Broadening of diffraction lines
 - c) Low-angle scattering
5. Applications of diffraction methods to complexes
 - a) Determination of cis-trans isomerism
 - b) Determination of linkage isomerism
6. Miscellaneous applications

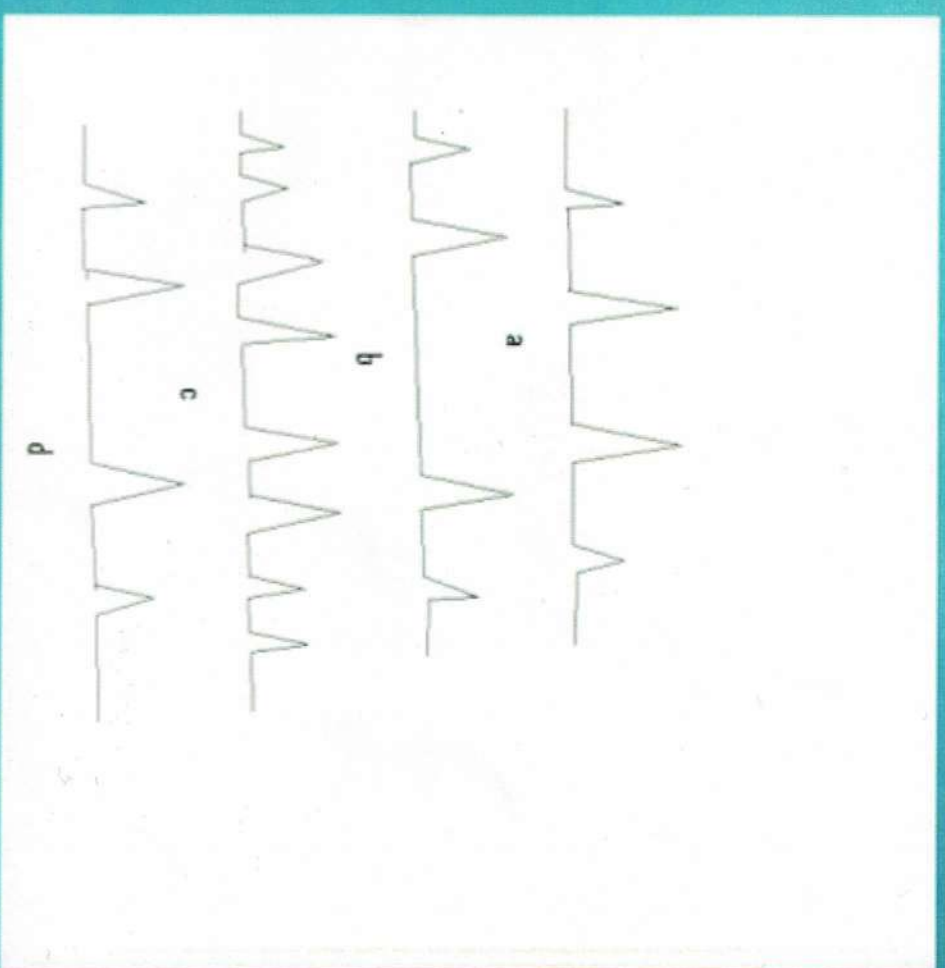
1. STRUCTURE OF CRYSTALS

a-x-ray pattern of salt NaCl

b-x-ray pattern of salt KCl

c-x-ray pattern of mixture of NaCl & KCl

d-x-ray pattern of a powder mixed crystal of NaCl & KCl



2. POLYMER CHARACTERISATION

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

3. State of anneal in metals: XRD is used to test the metals without removing the part from its position and without weakening it.

4. PARTICLE SIZE DETERMINATION

Spot counting method:

$$V = V_0 \cdot \delta\theta \cdot \cos\theta / 2n$$

V_0 = volume of individual crystallite

V = total volume irradiated

n = no. of spots in diffraction ring

$\delta\theta$ = divergence of x-ray beam

MISCELLANEOUS APPLICATIONS

- Soil classification based on crystallinity
- Analysis of industrial dusts
- Assessment of weathering & degradation of minerals & polymers
- Study of corrosion products
- Examination of tooth enamel & dentine
- Examination of bone state & tissue state
- Structure of DNA&RNA

CONCLUSIONS

- For materials including metals, minerals, plastics, pharmaceuticals and semiconductors XRD apparatus provide highly accurate tools for non-destructive analysis.
- The diffraction systems are also supported by an extensive range of application software

4.0 Applications of XRD

- XRD is a nondestructive technique
- To identify crystalline phases and orientation
- To determine structural properties:
Lattice parameters (10^{-4}\AA), strain, grain size, epitaxy, phase composition, preferred orientation (Laue) order-disorder transformation, thermal expansion
- To measure thickness of thin films and multi-layers*
- To determine atomic arrangement
- Detection limits: ~3% in a two phase mixture; can be ~0.1% with synchrotron radiation

Spatial resolution: normally none