University of Basrah
College of Education for Pure Sciences
Department of Chemistry

Ph.D Physical Course
2^{nd} term "2020-2021"

1. **Introduction to X-rays.**
2. **Generation of X-rays.**
3. **Why X-rays?**
4. **Principle of X-rays.**
5. **Instrumentation of X-rays.**
6. **Production of X-rays.**
7. **X-rays diffraction methods.**
8. **Solid state.**
9. **Basics of crystallography.**
10. **Miller indices (hkl).**
11. **Peak position.**
12. **Debye-Scherrer equation.**
13. **Applications of XRD.**

References:

1. **Solid State Physics , J. Moore**
2. **Solid State Chemistry and applications , A. R. West**
3. **Physical Chemistry , Atkins**
4. **Internet.**

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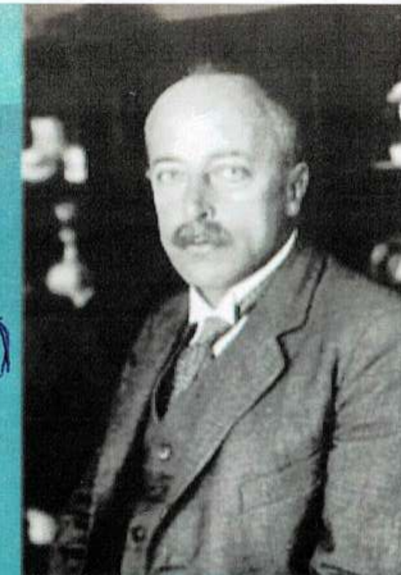
NTRODUCTION:

NOV./1895

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



Max Von Laue

The penetrating power of x-rays depends on energy also, there are two types of x-rays.

i) **Hard x-rays**: which have high frequency and have more energy.

ii) **soft x-rays**: which have less penetrating and have low energy

$1\,\mathring{A} = 1 \times 10^{-10}\,m$

$1m = 1 \times 10^{-9}\,nm$

$1\,\mathring{A} = 0.1\,nm$

X-RAYS

1. X-rays are short wave length electromagnetic radiations produced by the deceleration of high energy electrons or by electronic transitions of electrons in the inner orbital of atoms
2. X-ray region 0.1to100 A°
3. Analytical purpose 0.7 to 2 A°

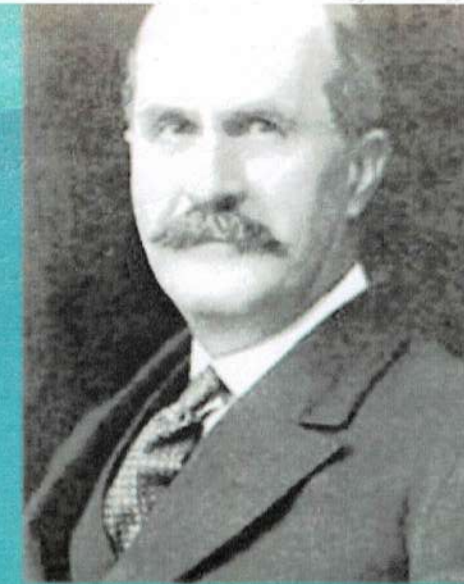
١) هي أشعاعات كهرومغناطيسية ذات طول موجي قصير تنتج عند تباطؤ الالكترونات ذات الطاقة العالية أو عن طريق التحولات الالكترونية للالكترونات في المدارات الداخلية للذرات
٢) منطقة الاشعة السينية تكون من 0.1 - 100 Å.
٣) الغرض التحليلي من 0.7 - 2 Å.

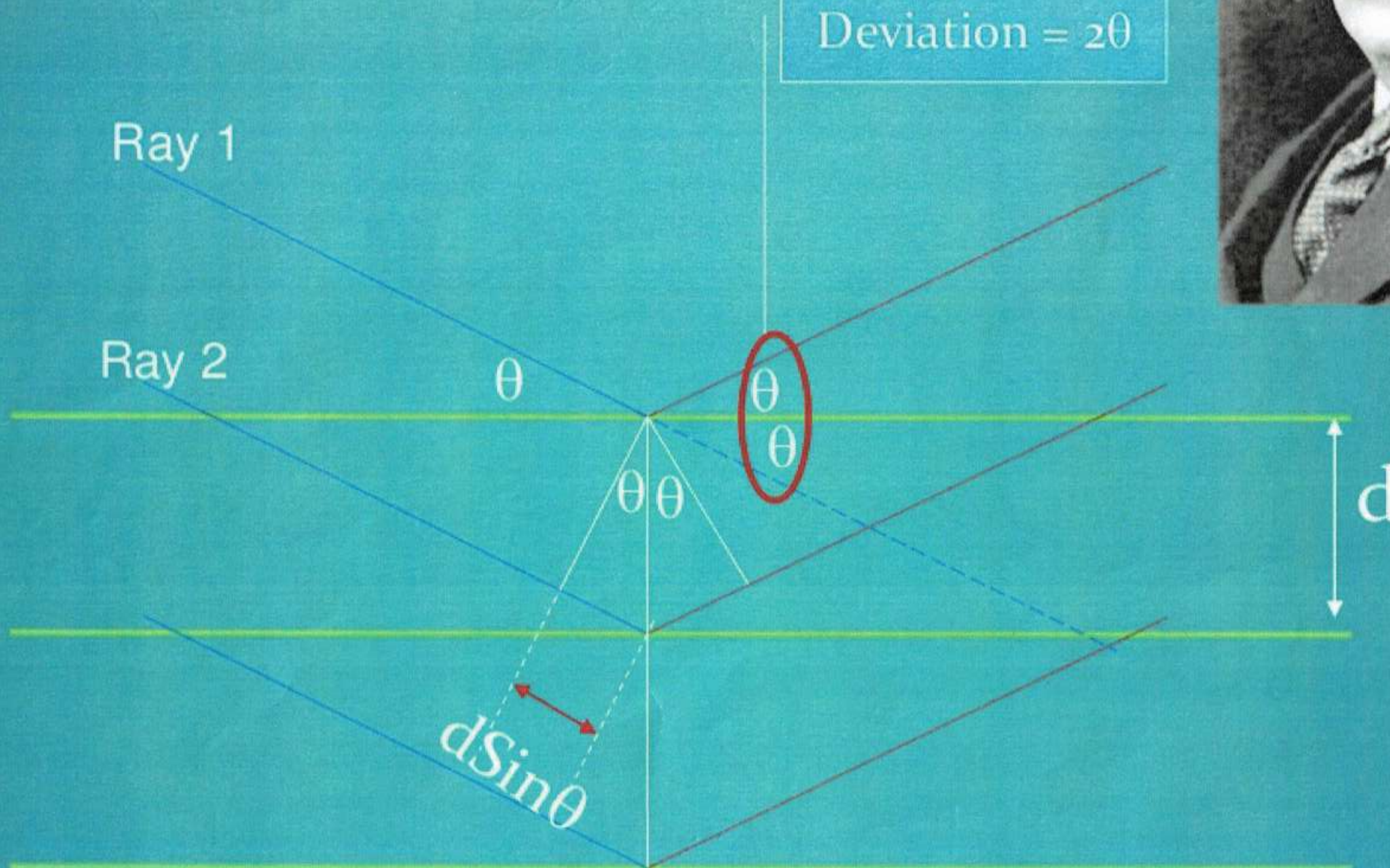
PRINCIPLE

تعتمد حيود الاشعة السينية على التداخل البناء للاشعة السينية احادية اللون
والعينة البلورية، تنشأ هذه الاشعة بواسطة انبوب شعاع الكاثود
الذي يرشح لانتاج شعاع احادي اللون الموازي للتركيز وتوجيهه نحو العينة
وينتج عن تفاعل الاشعة العارضة مع العينة تداخلاً بناءً عندما تلبي
الظروف قانون براغ.

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

BRAGG's EQUATION





The path difference between ray 1 and ray 2 = 2d Sinθ

For constructive interference: $n\lambda = 2d \sin\theta$

onstructive interference of the reflected beams emerging from two different planes will take place if he path lengths of two rays is equal to whole number of wavelengths".

for constructive interference,

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

this is called as BRAGG'S LAW

- يحدث التداخل البناء للحزم المنعكسة الخارجة من مستويين مختلفين ، اذا كانت اطوال مسير الشعاعين تساوي عدداً "كاملاً" من اطوال الموجات بالنسبة للتداخل البناء فهذا يحقق قانون براغ .

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BRAGG'S LAW:

After few months, In 1913, English physicists **Sir William Henry Bragg** and his son **Sir William Lawrence Bragg** developed a relationship to explain why the cleavage faces of crystals appear to reflect X-ray beams at certain angles of incidence (theta, θ).

The variable *d* is the distance between atomic layers in a crystal, and the variable lambda λ is the wavelength of the incident X-ray beam; n is an integer.

Although Bragg's law was used to explain the nterference pattern of X-rays scattered by crystals, iffraction has been developed to study the structure of ll states of matter with any beam.

Bragg carried out a series of experiments, the result of hich he published the Bragg equation –

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

here, assume n = 1 for the first order reflection

= wavelength

= X-ray incidence angle

= distance between atomic layer