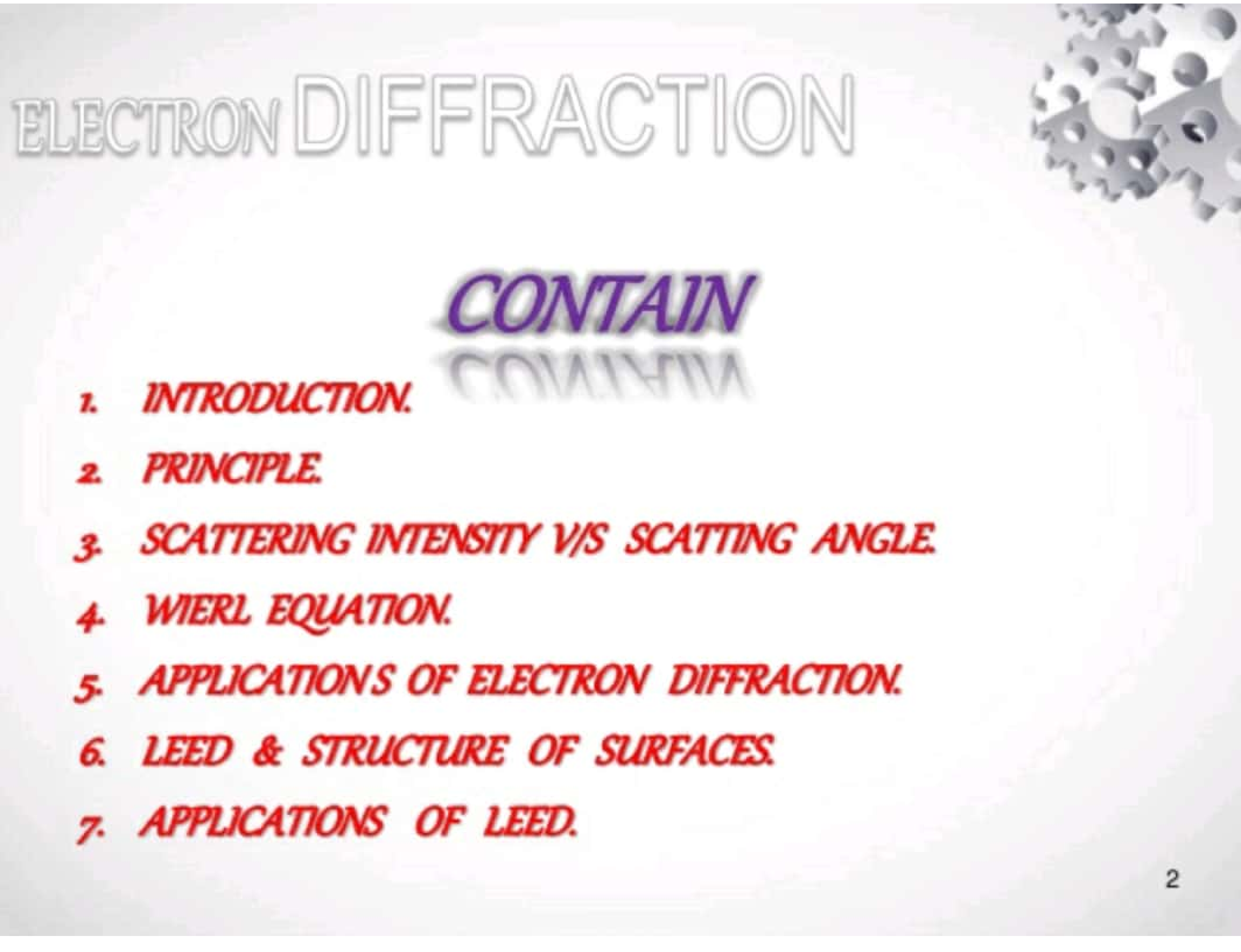


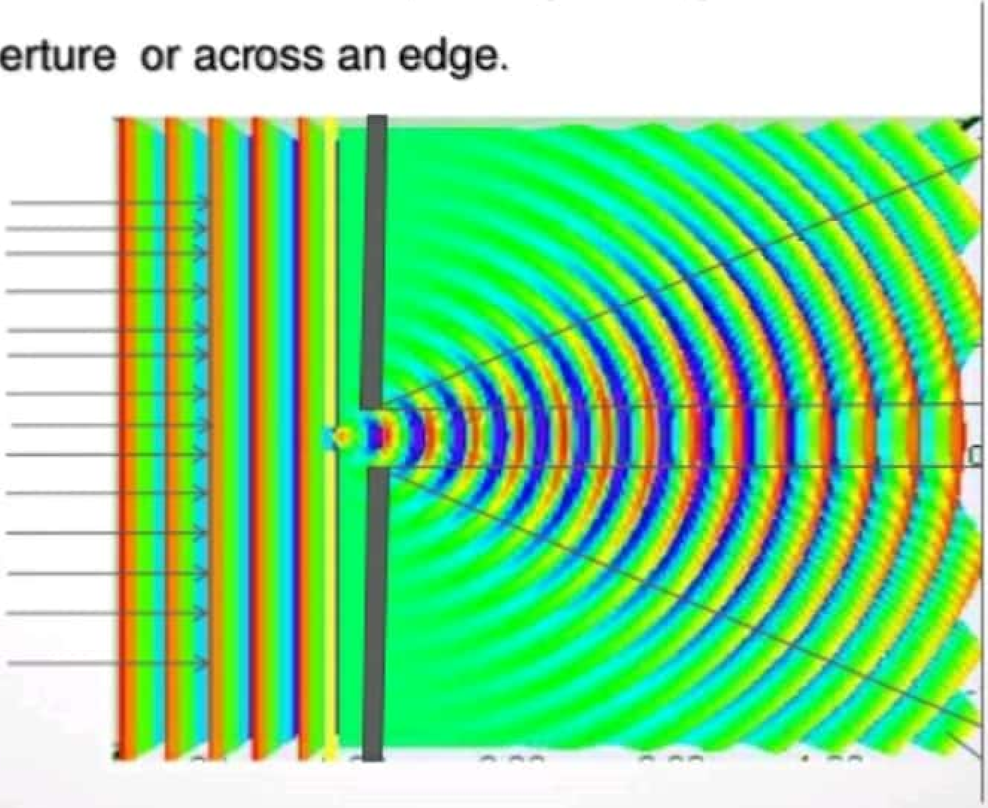
ELECTRON DIFFRACTION

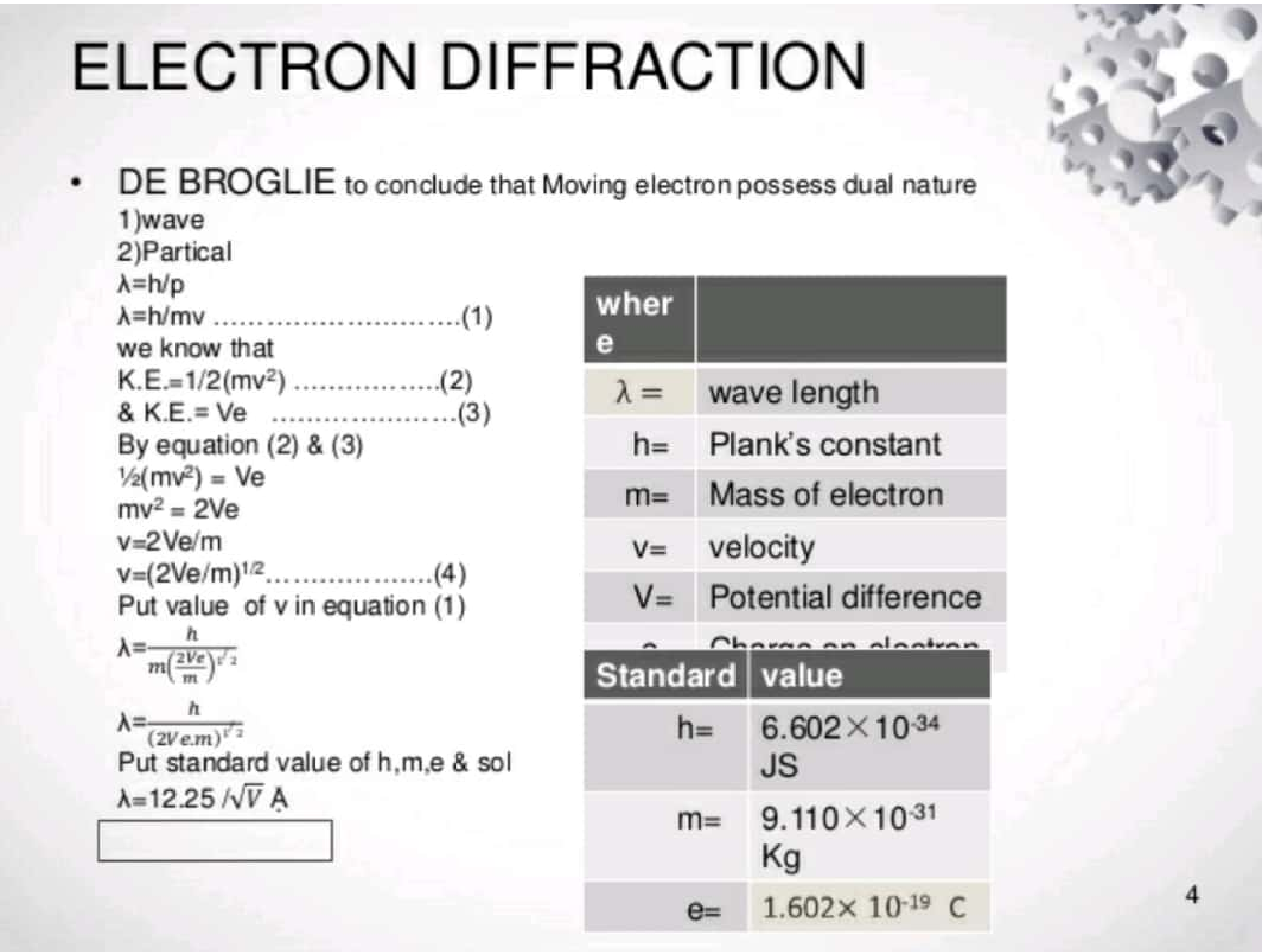
CONTAIN

1. INTRODUCTION.
2. PRINCIPLE.
3. SCATTERING INTENSITY V/S SCATTING ANGLE.
4. WIERL EQUATION.
5. APPLICATIONS OF ELECTRON DIFFRACTION.
6. LEED & STRUCTURE OF SURFACES.
7. APPLICATIONS OF LEED.

ELECTRON DIFFRACTION

1) **INTRODUCTION :-** **a)DIFFRACTION:-**The process by which a beam of light or other system of wave spread out ad result of passing through a narrow aperture or across an edge.





ELECTRON DIFFRACTION

- DE BROGLIE to conclude that Moving electron possess dual nature

  1)wave
  2)Partical
  $\lambda = h/p$
  $\lambda = h/mv$ ……………………….(1)
  we know that
  K.E.$=1/2(mv^2)$ ………………(2)
  & K.E.$=$ Ve …………………(3)
  By equation (2) & (3)
  $½(mv^2) = Ve$
  $mv^2 = 2Ve$
  $v=2Ve/m$
  $v=(2Ve/m)^{1/2}$……………….(4)
  Put value of v in equation (1)
  $\lambda = \frac{h}{m\left(\frac{2Ve}{m}\right)^{1/2}}$
  $\lambda = \frac{h}{(2Ve.m)^{1/2}}$
  Put standard value of h,m,e & sol
  $\lambda = 12.25/\sqrt{V}$ Ȧ

where	
$\lambda =$	wave length
h=	Plank's constant
m=	Mass of electron
v=	velocity
V=	Potential difference
e=	Charge on electron

Standard	value
h=	6.602×10^{-34} JS
m=	9.110×10^{-31} Kg
e=	1.602×10^{-19} C

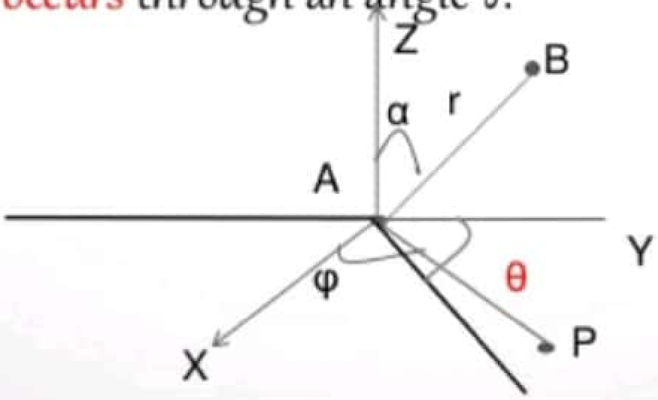
ELECTRON DIFFRACTOIN

- ## 2)PRINCIPL:-

- Electron can be accelerated to precisely controlled energy by applying a known potential difference.
- when **accelerated** through **10 keV** they acquire wave length **12pm** which makes then **suitable** for molecule diffraction.
- Electron diffraction study generally utilized with **energies** of the **order** of **40 keV** .
- Since electron are charged the are scattered strongly by their interaction with electron and nuclei of atom of the sample.
- Hence they cannot be use for studying molecule in gaseous state held on surface and in thin films.(the application to surface which is called LOW ENERGY ELECTRON DIFFRACTION is a major use of the techniqe.)

ELECTRON DIFFRACTION

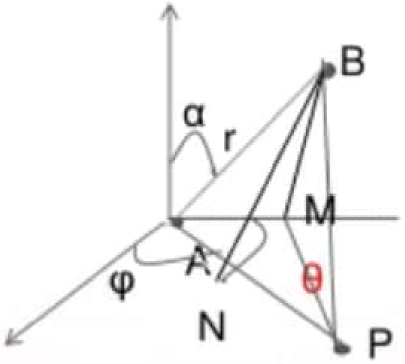
- **3)SCATTERING INTENSITY & SCATTERING ANGLE:-**
- Consider diatomic molecule AB to study electron diffraction theory. The atom A lies at the origin and B at a distance *r* away
- The orientation of molecule AB is specified by angle α and ϕ.
- The indecent electron beam enters parallel to Y-axis and diffraction occurs through an angle ϑ.

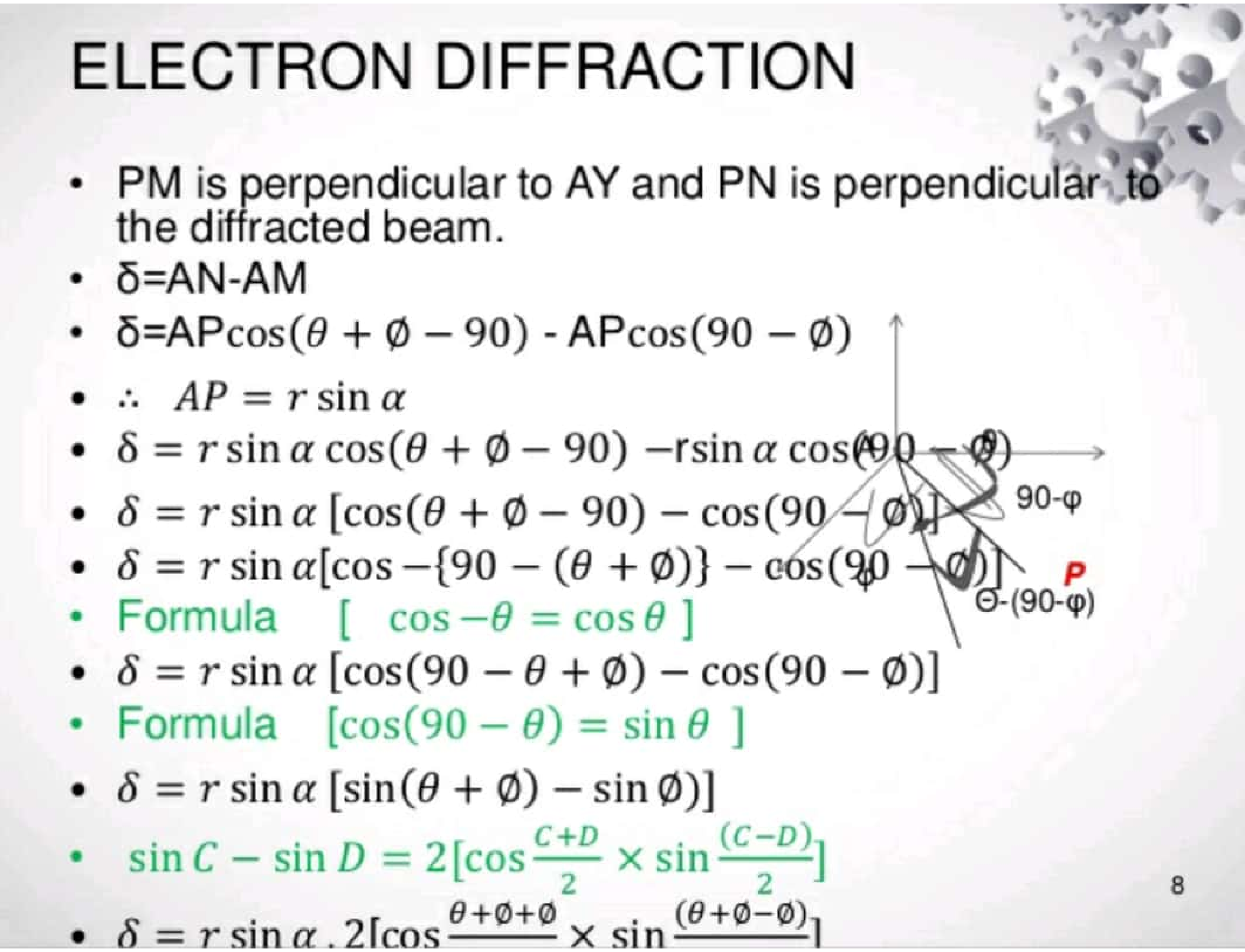


ELECTRON DIFFRACTION

- The interference between the wave scattered A and B depends on the difference between the length of the paths the traverse .
- Draw from B a perpendicular BN on to diffraction direction and a perpendicular BM on to the undiffrected direction to calculate the path difference δ.
- when M and N are in phase the path difference is

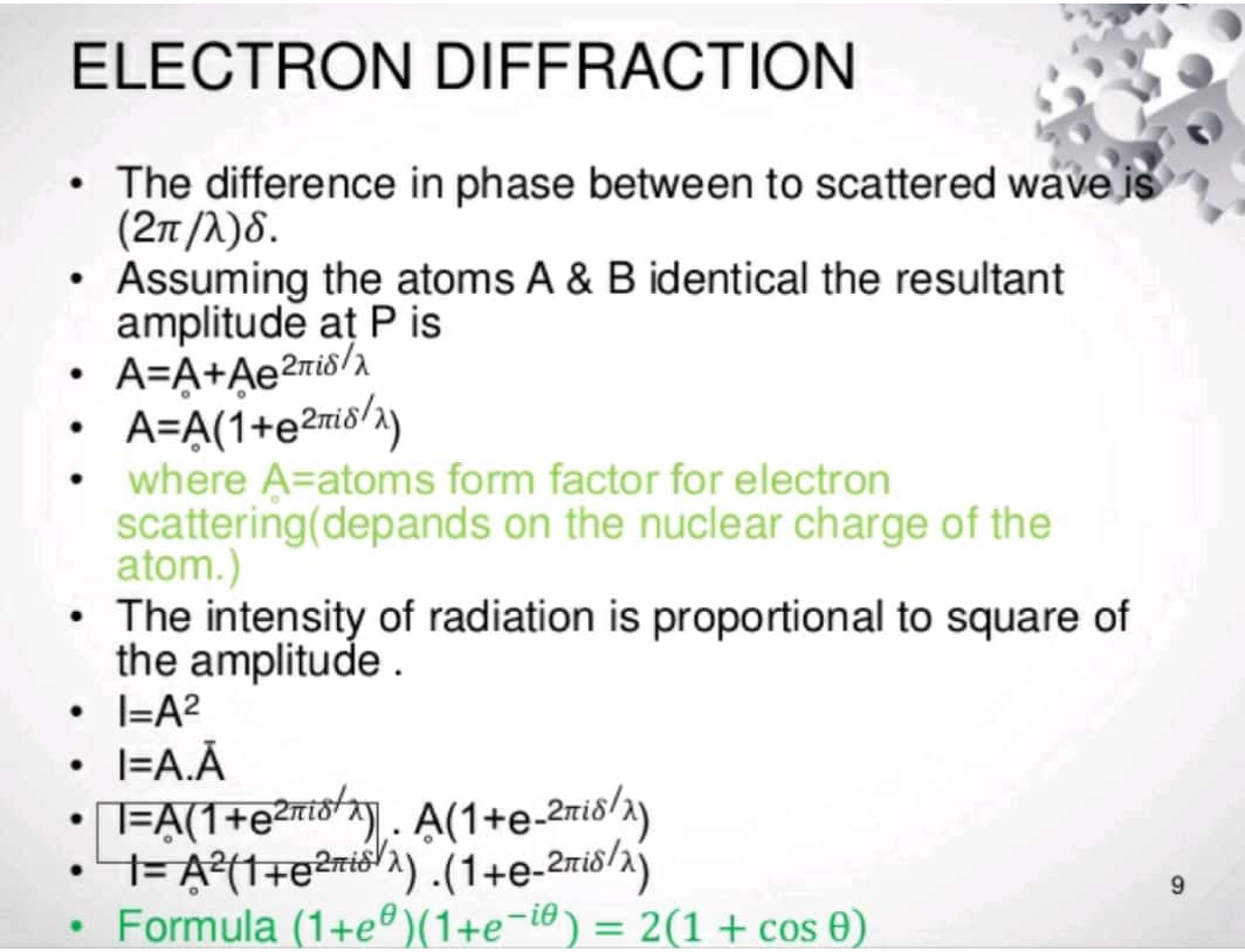
δ=AN-AM





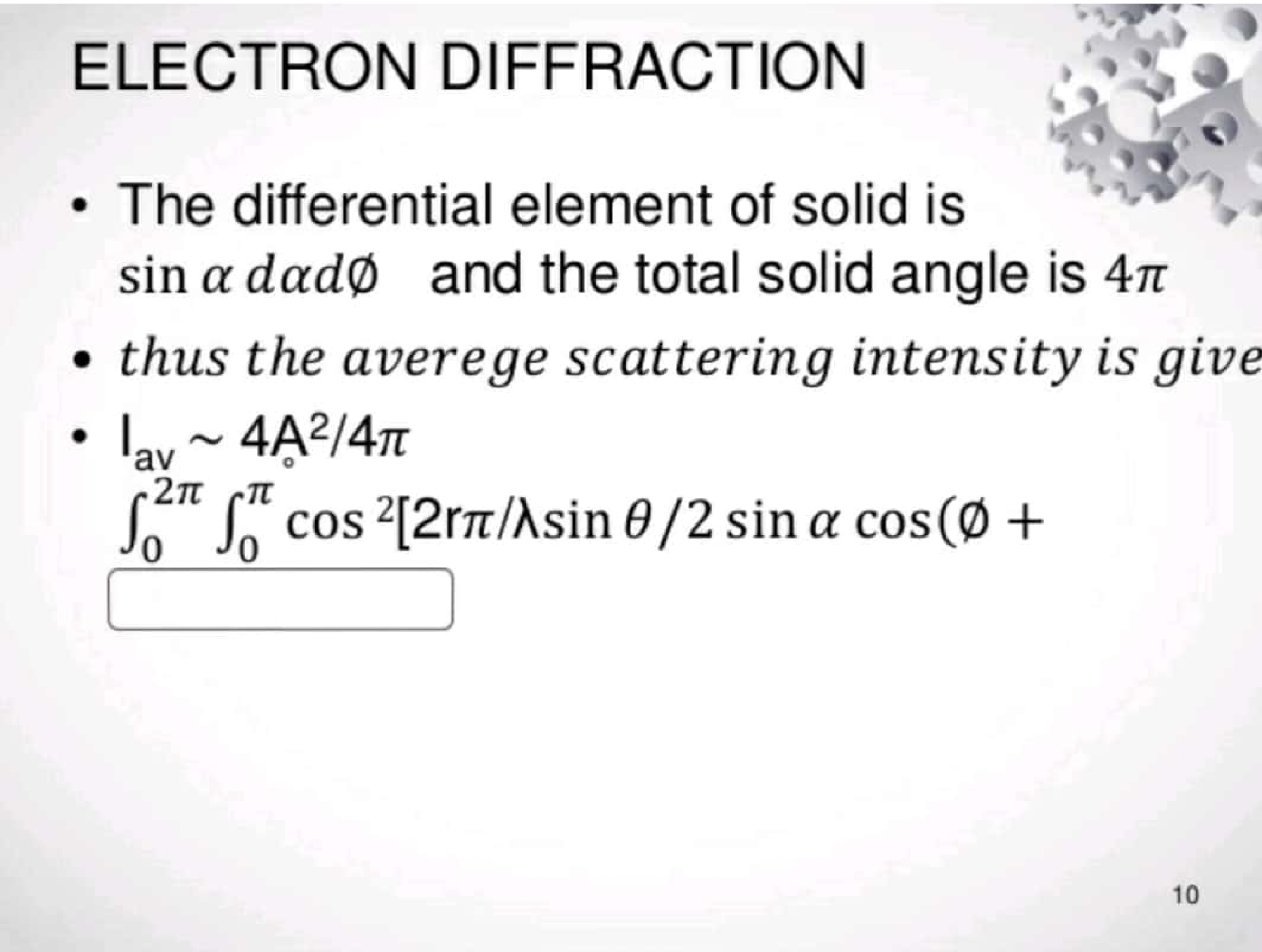
ELECTRON DIFFRACTION

- PM is perpendicular to AY and PN is perpendicular to the diffracted beam.
- δ=AN-AM
- δ=AP$\cos(\theta + \emptyset - 90)$ - AP$\cos(90 - \emptyset)$
- $\therefore \quad AP = r \sin \alpha$
- $\delta = r \sin \alpha \cos(\theta + \emptyset - 90) - r\sin \alpha \cos(90 - \emptyset)$
- $\delta = r \sin \alpha \, [\cos(\theta + \emptyset - 90) - \cos(90 - \emptyset)]$
- $\delta = r \sin \alpha [\cos -\{90 - (\theta + \emptyset)\} - \cos(90 - \emptyset)]$
- Formula $[\quad \cos -\theta = \cos \theta \,]$
- $\delta = r \sin \alpha \, [\cos(90 - \theta + \emptyset) - \cos(90 - \emptyset)]$
- Formula $[\cos(90 - \theta) = \sin \theta \;]$
- $\delta = r \sin \alpha \, [\sin(\theta + \emptyset) - \sin \emptyset)]$
- $\sin C - \sin D = 2[\cos \frac{C+D}{2} \times \sin \frac{(C-D)}{2}]$
- $\delta = r \sin \alpha \, . \, 2[\cos \frac{\theta+\emptyset+\emptyset}{} \times \sin \frac{(\theta+\emptyset-\emptyset)}{}]$



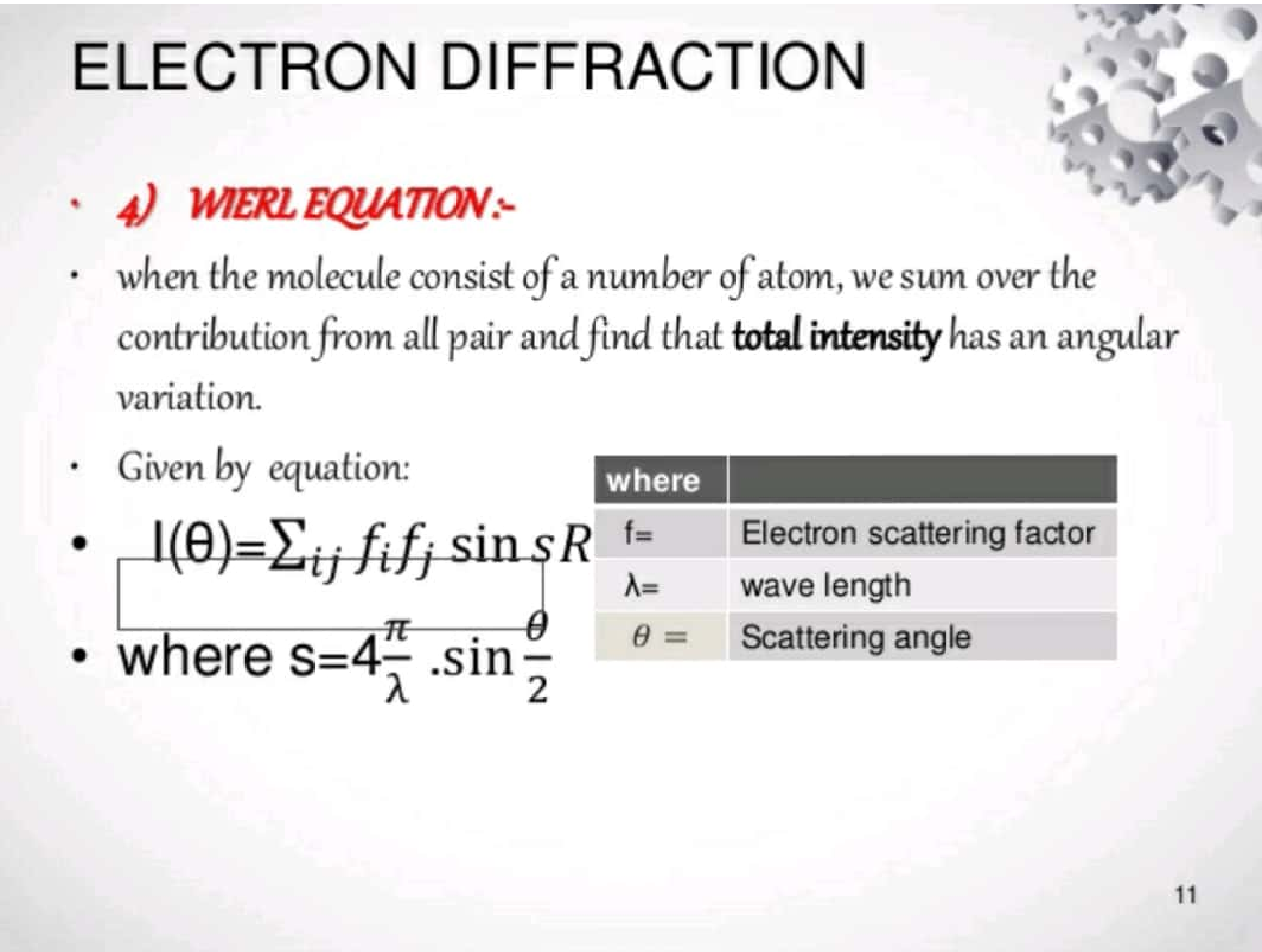
ELECTRON DIFFRACTION

- The difference in phase between to scattered wave is $(2\pi/\lambda)\delta$.
- Assuming the atoms A & B identical the resultant amplitude at P is
- $A=\underset{\circ}{A}+\underset{\circ}{A}e^{2\pi i\delta/\lambda}$
- $A=\underset{\circ}{A}(1+e^{2\pi i\delta/\lambda})$
- where $\underset{\circ}{A}$=atoms form factor for electron scattering(depands on the nuclear charge of the atom.)
- The intensity of radiation is proportional to square of the amplitude .
- $I=A^2$
- $I=A.\bar{A}$
- $\boxed{I=\underset{\circ}{A}(1+e^{2\pi i\delta/\lambda})} . \underset{\circ}{A}(1+e^{-2\pi i\delta/\lambda})$
- $I=\underset{\circ}{A}^2(1+e^{2\pi i\delta/\lambda}) .(1+e^{-2\pi i\delta/\lambda})$
- Formula $(1+e^{\theta})(1+e^{-i\theta}) = 2(1+\cos\theta)$



ELECTRON DIFFRACTION

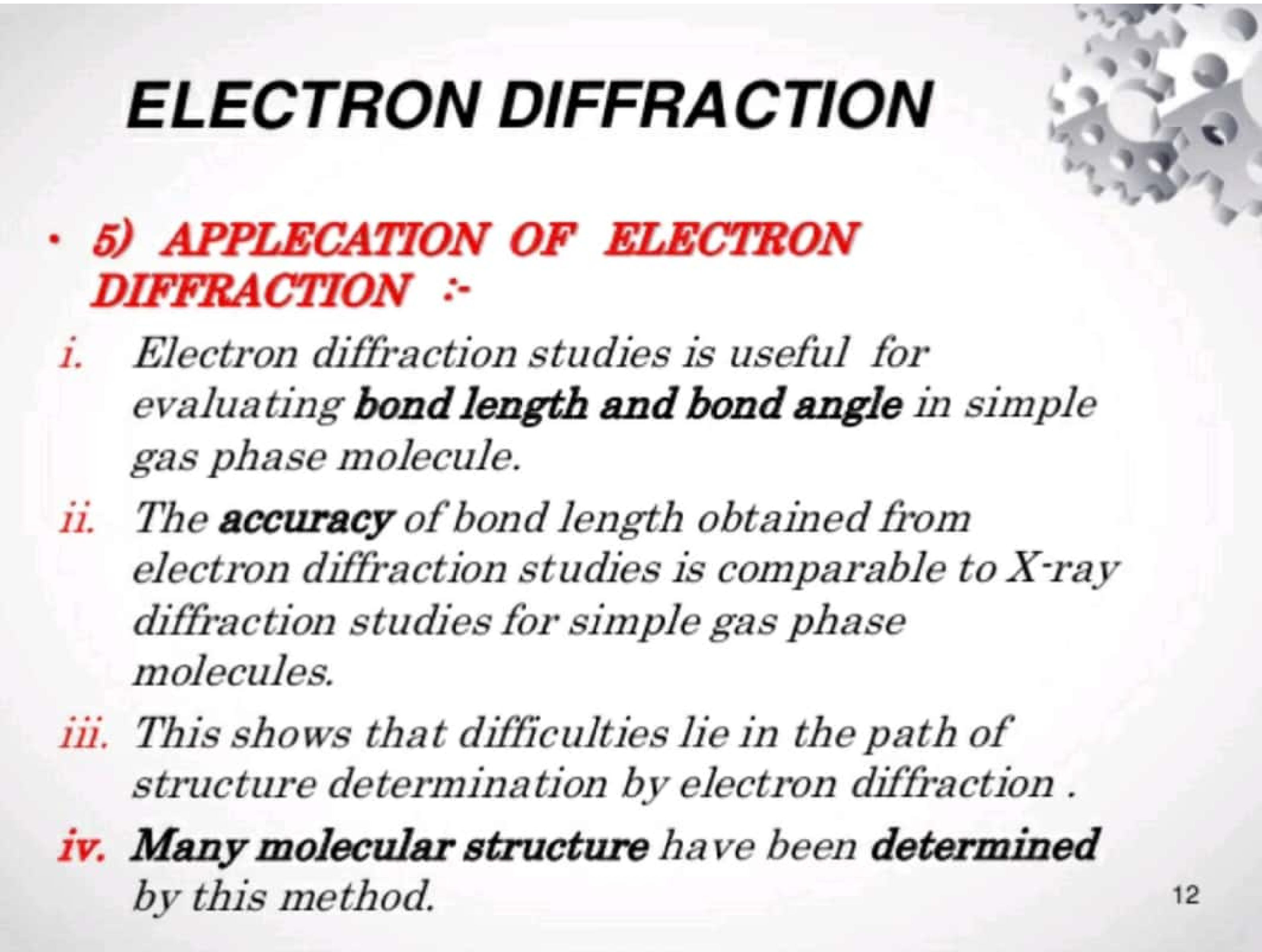
- The differential element of solid is $\sin\alpha \, d\alpha d\emptyset$ and the total solid angle is 4π
- *thus the averege scattering intensity is give*
- $I_{av} \sim 4\underset{\circ}{A}^2/4\pi \int_0^{2\pi}\int_0^{\pi} \cos^2[2r\pi/\lambda \sin\theta/2 \sin\alpha\cos(\emptyset +$



ELECTRON DIFFRACTION

- **4) WIERL EQUATION :-**
- when the molecule consist of a number of atom, we sum over the contribution from all pair and find that **total intensity** has an angular variation.
- Given by equation:
- $I(\theta)=\sum_{ij} f_i f_j \sin sR$
- where $s=4\frac{\pi}{\lambda}\ .\sin\frac{\theta}{2}$

where	
f=	Electron scattering factor
λ=	wave length
$\theta =$	Scattering angle



ELECTRON DIFFRACTION

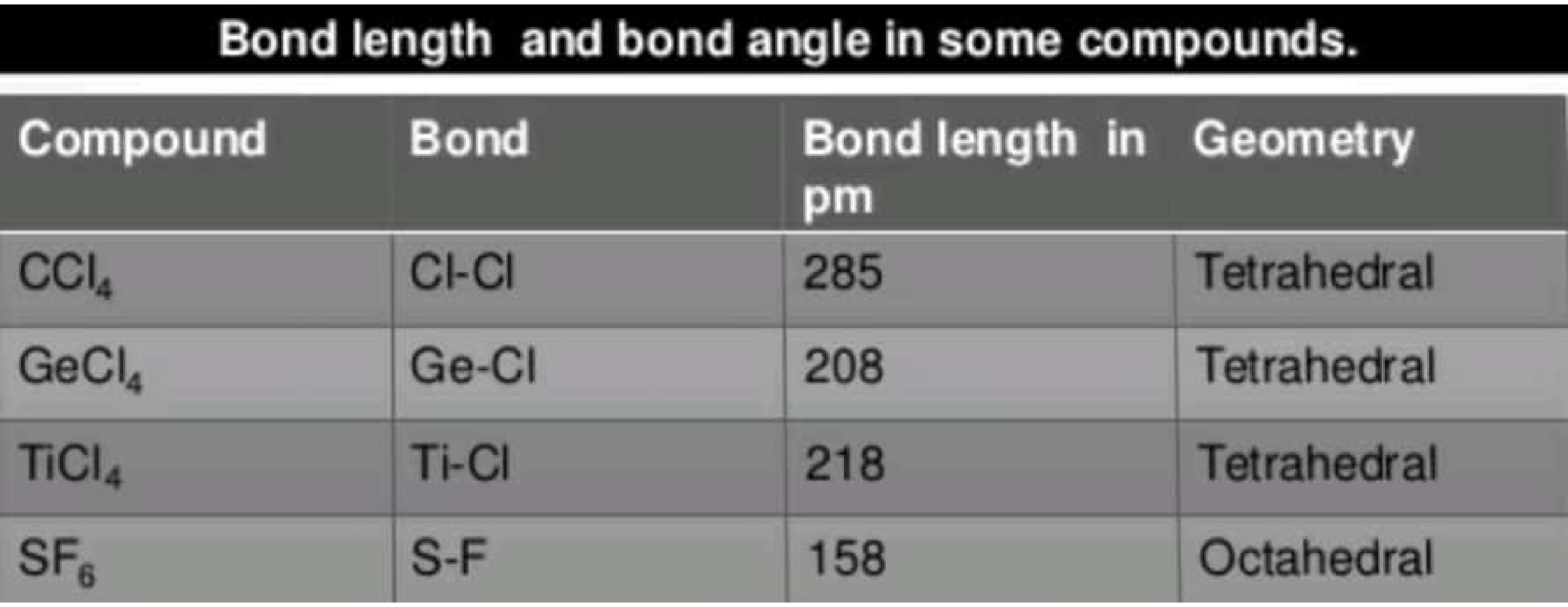
- ***5) APPLECATION OF ELECTRON DIFFRACTION :-***

i. *Electron diffraction studies is useful for evaluating* ***bond length and bond angle*** *in simple gas phase molecule.*

ii. *The* ***accuracy*** *of bond length obtained from electron diffraction studies is comparable to X-ray diffraction studies for simple gas phase molecules.*

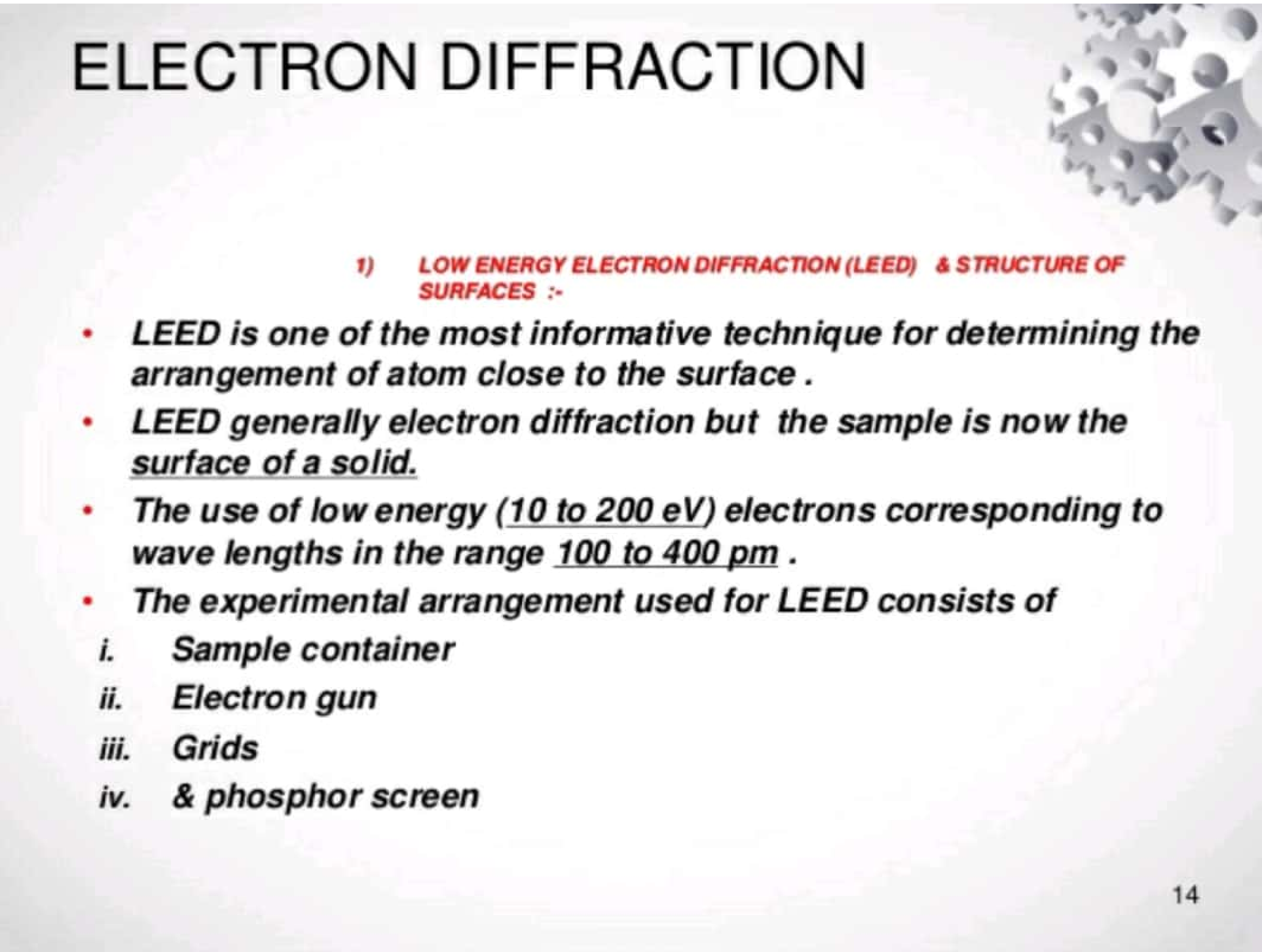
iii. *This shows that difficulties lie in the path of structure determination by electron diffraction .*

iv. ***Many molecular structure*** *have been* ***determined*** *by this method.*



Bond length and bond angle in some compounds.

Compound	Bond	Bond length in pm	Geometry
CCl_4	Cl-Cl	285	Tetrahedral
$GeCl_4$	Ge-Cl	208	Tetrahedral
$TiCl_4$	Ti-Cl	218	Tetrahedral
SF_6	S-F	158	Octahedral

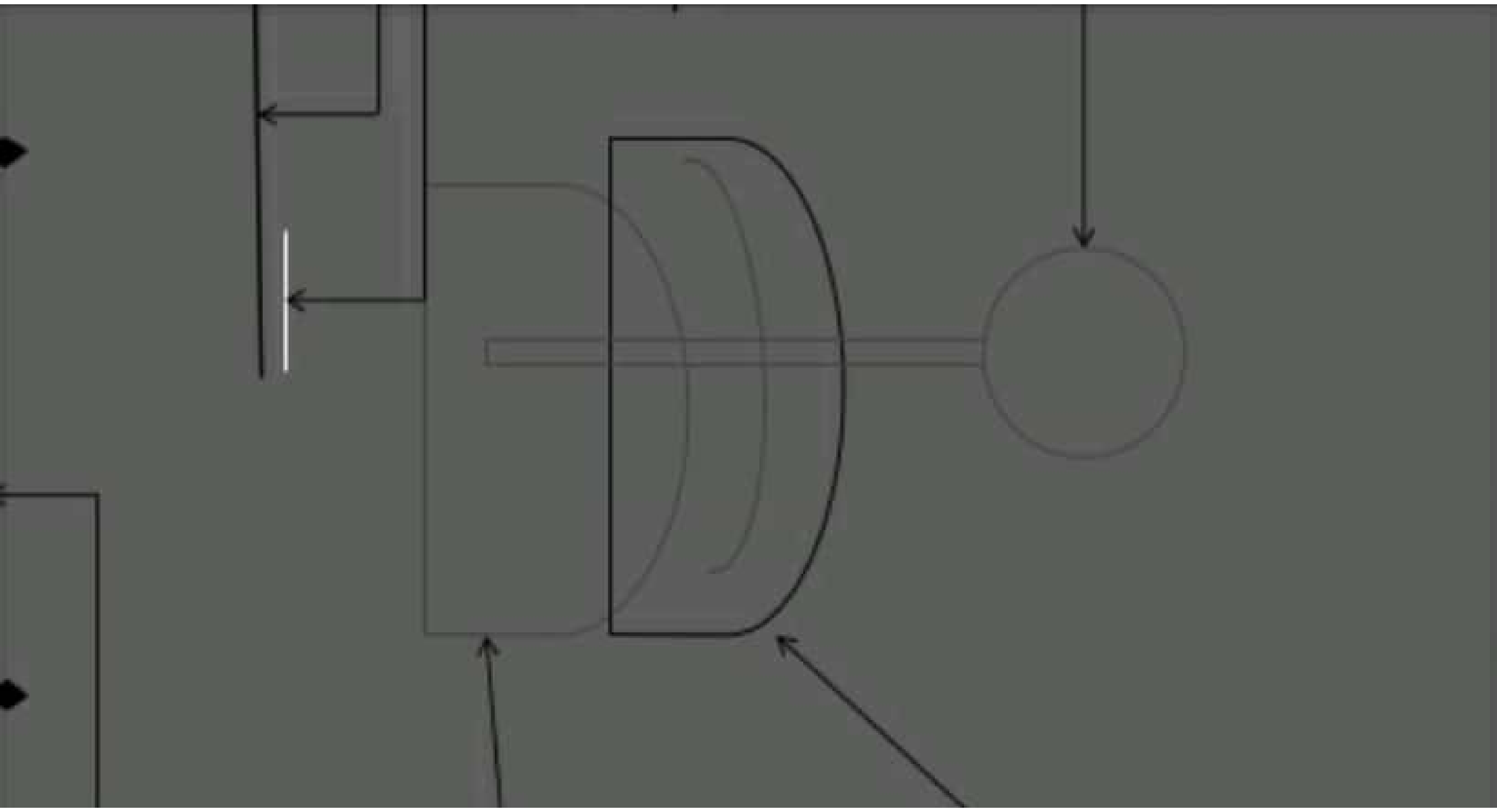


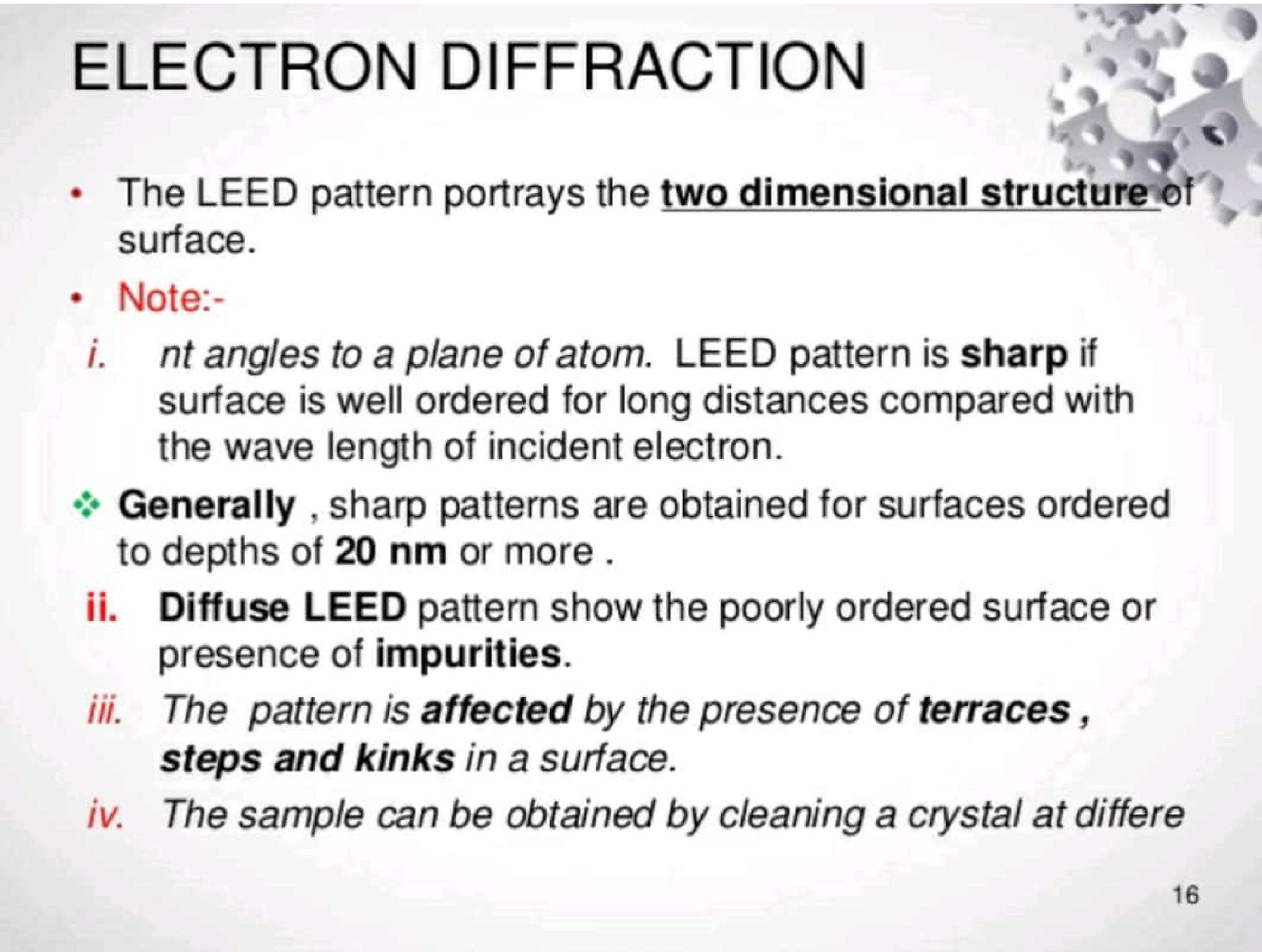
ELECTRON DIFFRACTION

1) LOW ENERGY ELECTRON DIFFRACTION (LEED) & STRUCTURE OF SURFACES :-

- ***LEED is one of the most informative technique for determining the arrangement of atom close to the surface .***
- ***LEED generally electron diffraction but the sample is now the surface of a solid.***
- ***The use of low energy (10 to 200 eV) electrons corresponding to wave lengths in the range 100 to 400 pm .***
- ***The experimental arrangement used for LEED consists of***

  i. ***Sample container***
  ii. ***Electron gun***
  iii. ***Grids***
  iv. ***& phosphor screen***





ELECTRON DIFFRACTION

- The LEED pattern portrays the **two dimensional structure** of surface.
- Note:-

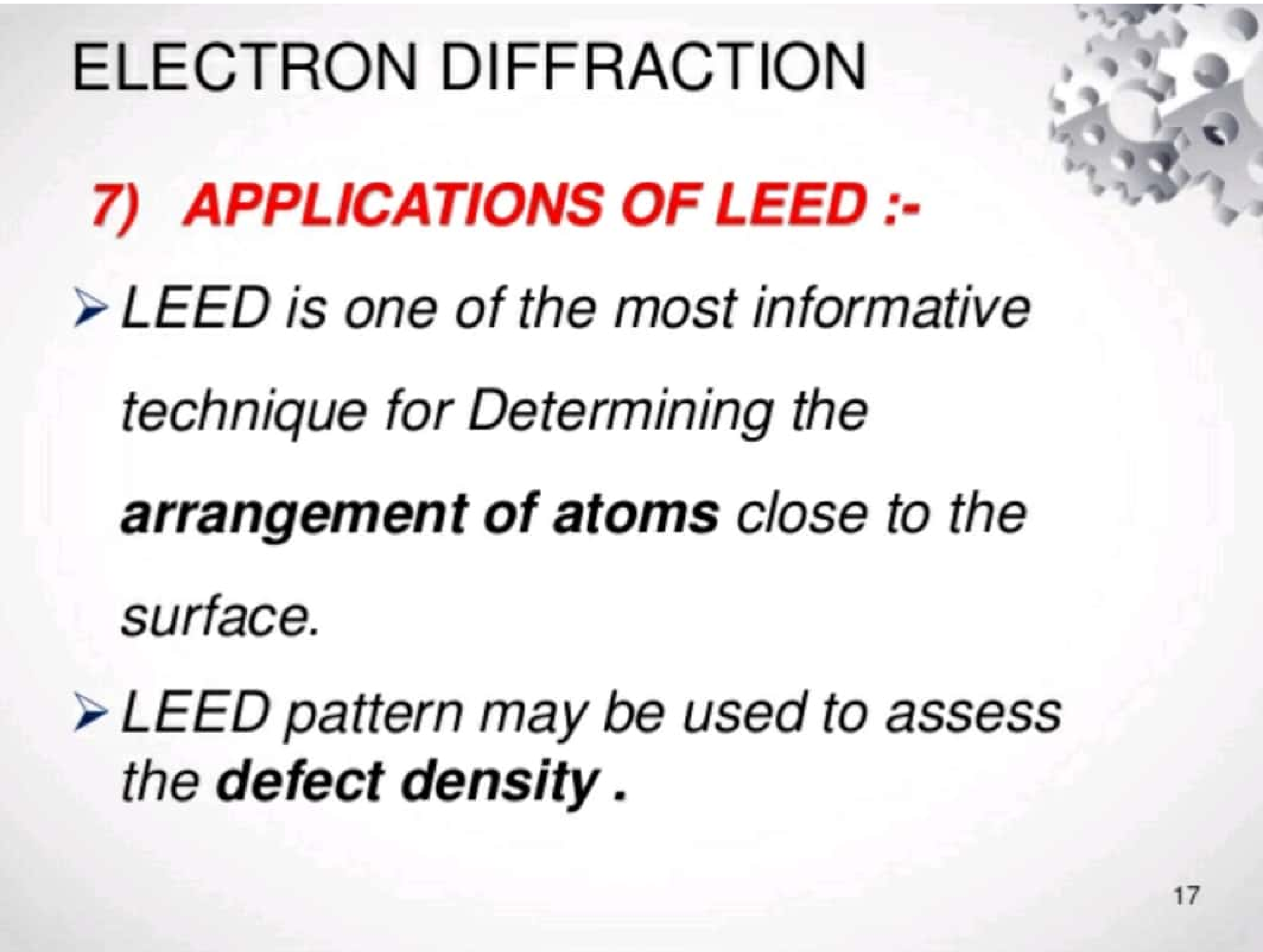
i. *nt angles to a plane of atom.* LEED pattern is **sharp** if surface is well ordered for long distances compared with the wave length of incident electron.

- **Generally** , sharp patterns are obtained for surfaces ordered to depths of **20 nm** or more .

ii. **Diffuse LEED** pattern show the poorly ordered surface or presence of **impurities**.

iii. *The pattern is **affected** by the presence of **terraces , steps and kinks** in a surface.*

iv. *The sample can be obtained by cleaning a crystal at differe*



ELECTRON DIFFRACTION

7) APPLICATIONS OF LEED :-

- *LEED is one of the most informative technique for Determining the* ***arrangement of atoms*** *close to the surface.*
- *LEED pattern may be used to assess the* ***defect density .***