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Mathematical Analysis of X-Ray Scattering Phenomenon in the Epoch of New Generation based Sources of Light

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Abstract:- This paper investigates the performance of x-ray scattering of new generation light sources and examines mathematically the phenomenon of scattering techniques. This research article demonstrates little interpreter kind of examples exemplifying the functioning of X-ray scattering. There exists versatile stages of edification and it is substantial that, an elementary authoritative classical modeling of elastic related scattering of an electromagnetic wave by a negatively charged electron is reasonably seems to be more precise. X-ray scattering proficiencies are basically belongs to a fellowship of non-devastating holomorphic techniques, which disclose the entropy about the various physical related properties of materials in particular. Mathematical analysis also has been incorporated in this paper so that one can analyze the patterns of x-ray scattering. Comparison has been done on wide-angle x-ray diffraction and small angle x-ray diffraction techniques which is the key element of this paper.

Keywords: Elastic scattering, classical modeling, new generation light sources and performance.

1. Introduction

It is well known fact that, there exists many diffraction methods basically employed in order to analyze the structural finding of particle size estimations [1-4]. In this paper, some of the x-ray scattering methods are being analyzed in the introduction section. From X-ray diffraction methods one can acquire data pertaining to phase quantization, phase identification, crystalline structure variations related to lattice parametric quantity, lattice deformation and periodicity assessments. In Fig 1, it is clearly shown the formation of X-ray scattering while, fig 2 depicts the method of occurrence of inelastic scattering.

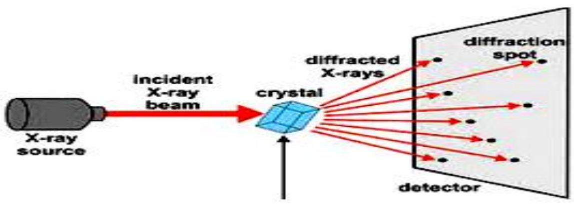

Fig. 1: X-ray diffraction Technique

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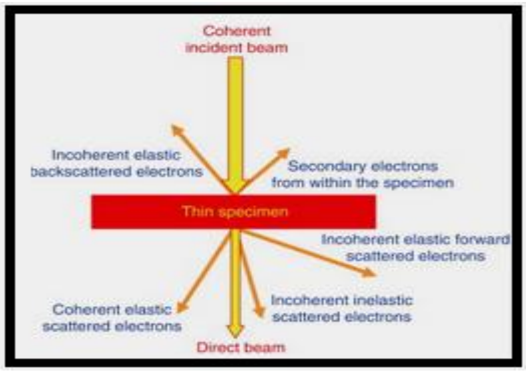

Fig. 2: Inelastic Scattering

In elastic scattering, the scattering angle is calculated with the help of Random number and further the elastic mean free path could be computed. Elastic scattering happens whenever there is no expiration of energy of incidental electron. The elastically scattered electron can alter the orientation but does not alter the value of wavelength (λ). Elastic scattering is used to analyze the crystalline structure whereas the inelastic scattering basically occurs when there exists an interaction which in turn causes loss of energy of electron. They have more wavelengths. The fig 3 represents the phenomenon of electron based scattering technique. In electron scattering analysis, an approximation of de-Broglie wavelength is considered. Bragg's law is called forth.

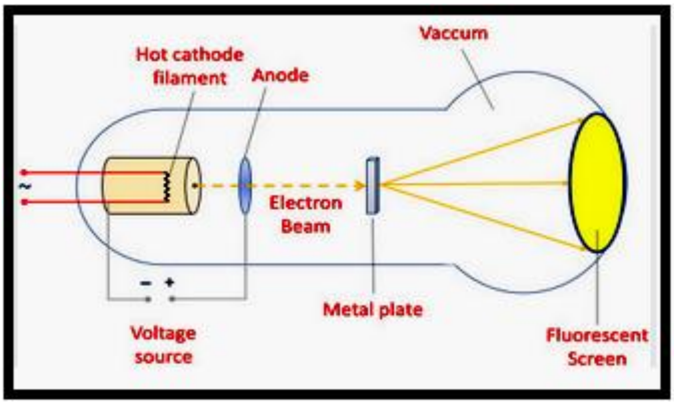

Fig. 3: Electron Scattering Technique

There exists another method namely neutron diffraction which is one kind of elastic scattering techniques, where the neutrons have the same amount of energy as that of electrons. Neutron scattering is employed to find the atomic structure of material. Fig 4, clearly depicts the method of Neutron scattering method.

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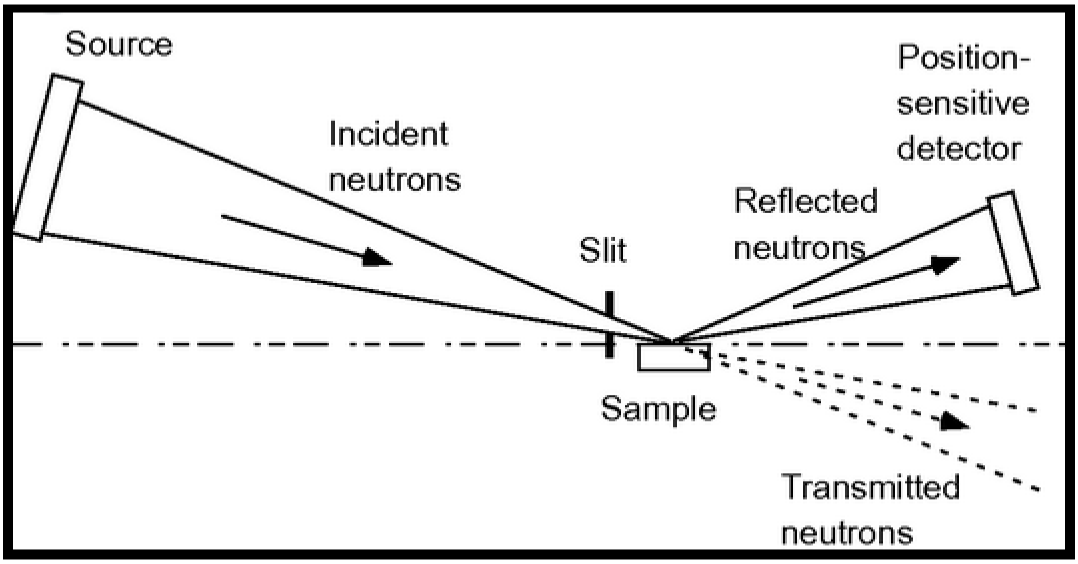

Fig. 4: Neutron Scattering Technique

Single crystal X-ray diffraction is the probably the oldest methods of crystallography. Fig 5 shows the pattern pertaining to single crystal diffraction.

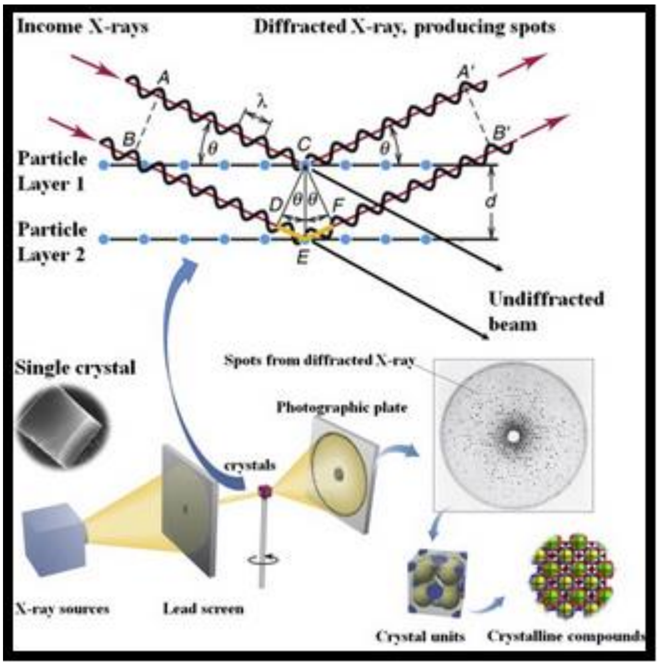

Fig. 5: Single crystal diffraction

Powder diffraction method is also one of the methods employed to analyze the x-ray diffractions.

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Powder diffractometer is used to study the structural delineation of materials.

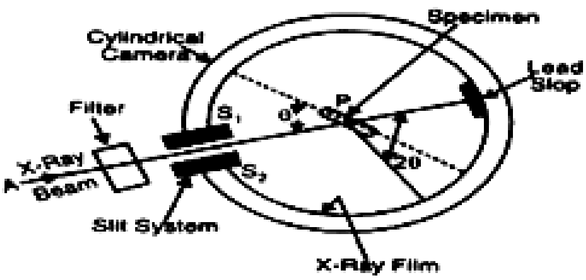

Fig. 6: Powder diffraction

Small Angle X-ray Scattering (SAXS) is also one of the analytical methods which basically provide the access to selective information approximately about the structure of different materials in nano-scale basis.

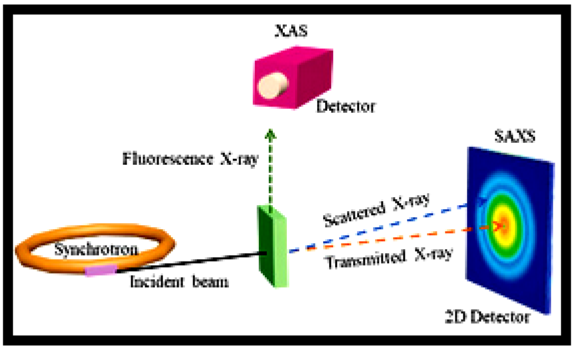

Fig.7 SAXS diffraction method

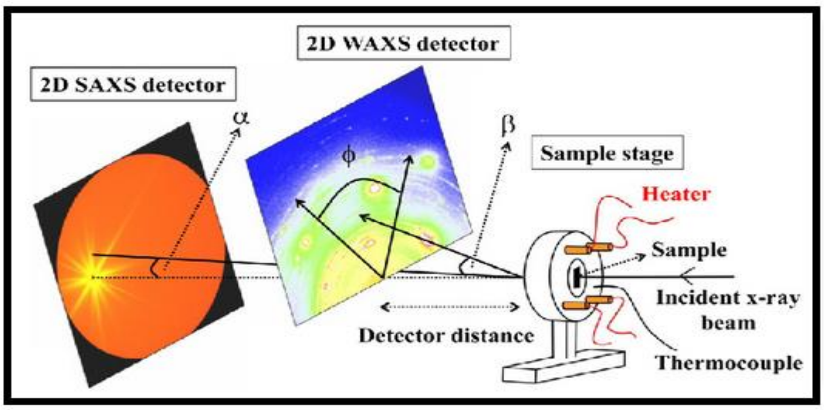

Fig.8 WAXS diffraction method

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There is another method called Wide area X-ray diffraction method which is used to determine the degree of crystalline structure. Fig 8 shows the method of WAXS.

2. MATHEMATICAL ILLUSTRATION OF X-RAY SCATTERING

The x-ray diffraction technique basically uses the Bragg's relation in order to analyze the patterns of x-ray beams.

Bragg's relation is given by, $n\lambda = 2d\sin\theta$

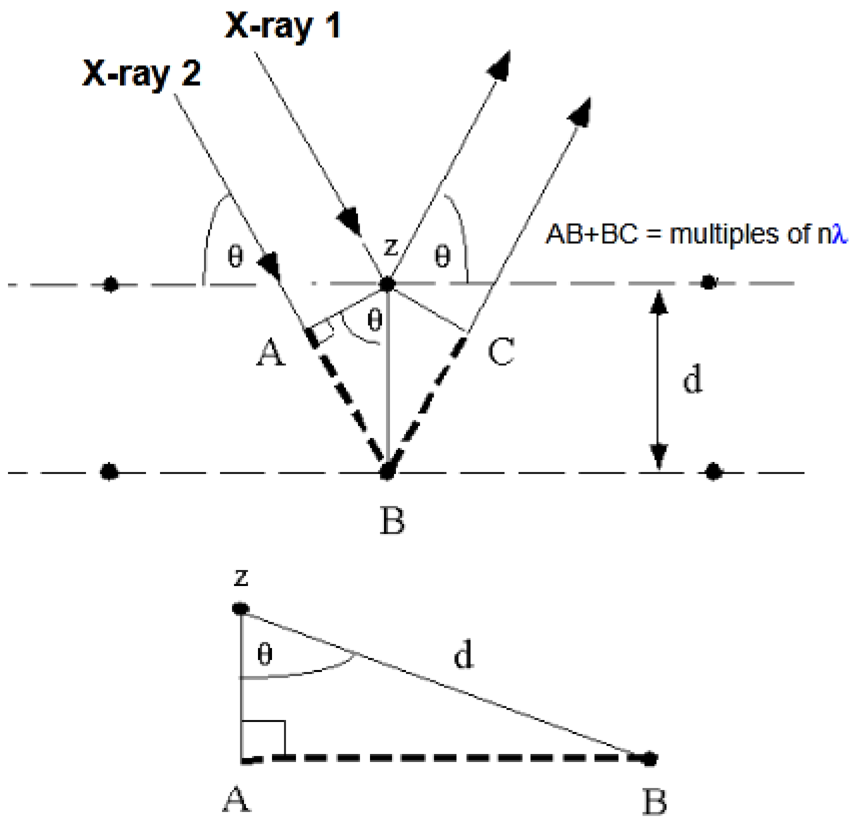

Fig.9 Bragg's relation illustration

Fig 9, demonstrates how Bragg's equation is derived and obtained.

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$$n\lambda = AB + BC$$
$$AB = BC$$
$$n\lambda = 2AB$$
$$\sin\theta = \frac{AB}{d}$$
$$AB = d\sin\theta$$
$$n\lambda = 2d\sin\theta$$

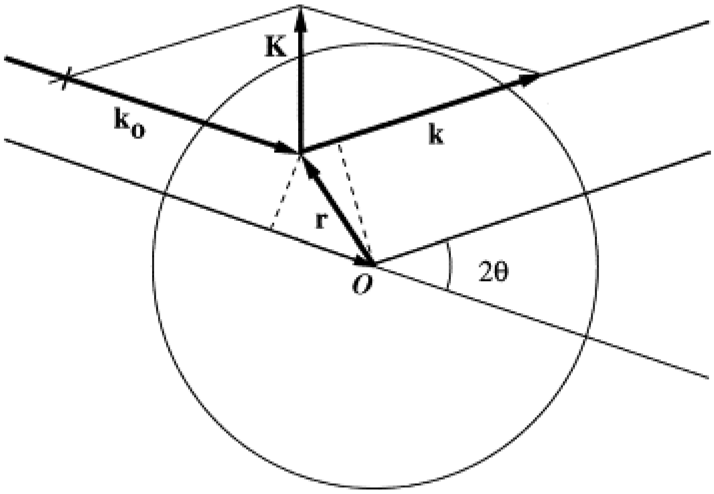

Fig.10 X-ray scattering cross section analysis

The scattering cross-section is represented by relation

$$\frac{d\sigma}{d\Omega} = d^2 K_p$$

Where K_p = polarization factor, Ω = solid angle.

The refractive index is calculated by using the formula given below:

$$r = 1 - n\left(\frac{\lambda^2}{2\pi}\right) df$$

Where r= refractive index, n=number of electrons per volume,

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The distribution factor of scattering can be computed by the relation given below:

$$f(K)=\int 4\pi r^2 \rho(r)\sin\left(\frac{Kr}{K}\right)dr$$

By using above normalization relation, one can calculate the scattering angle and distribution factor of scattering respectively.

The size of particles could be determined by:

$$D=\frac{K\lambda}{B\cos\theta}$$

Where D =size of the particle, B= width in radians, K = constant, θ=diffraction angle

Momentum transfer (S) can also be found by the relation depicted below:

$$S=\frac{4\pi\sin\theta}{\lambda}$$

X-ray diffraction patterns for amorphous materials and crystalline materials are depicted below:

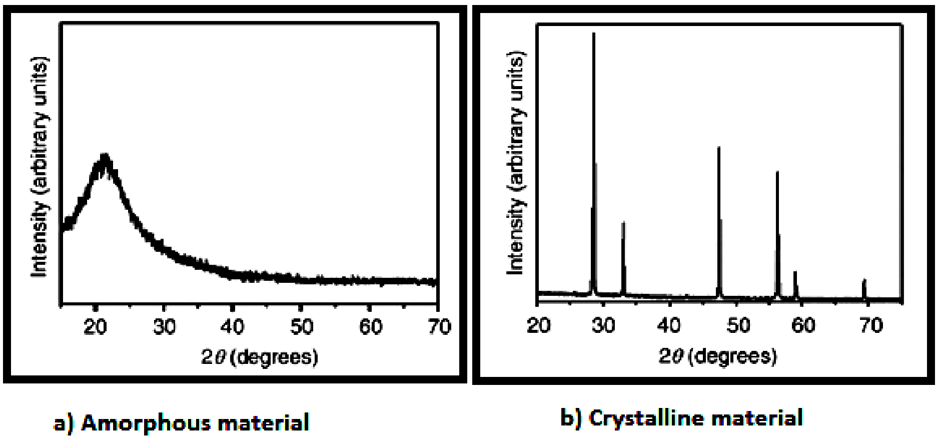

Fig.11 X-ray patterns for different materials

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3. Conclusion

In this paper, the point of focus is the mathematical treatment of x-ray diffraction method. Various methods have been analyzed to explain about the x-ray scattering techniques. Mathematical analysis also have been represented to analyze and find various parameters like refractive index, polarization factor, momentum transfer, size of the particle and distribution factor shall be calculated by the relations provided in this paper. One can easily analyze the Bragg's relation and its association with x-ray scattering phenomenon. The x-ray diffraction patterns are also represented in this paper respectively.

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