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Characterization of Nanomaterials by X-ray Diffraction Technique

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Abstract:

Nanomaterials are novel materials and plays an important role in various technology including solar cell, sensors, targeted drug delivery, miniaturized electronic components, high-efficiency catalysts, water purification membranes, and stronger, lightweight construction materials etc. X-ray diffraction method is a powerful tool to determine the crystal structure, lattice parameter, stresses, and crystallite size of the nanoparticles. We explored the Scherrer equation to analyze the size of nanoparticle and obtained various other parameters associated with size of nanoparticle. Moreover, we also explored the Williamson-Hall (W-H) Method to analyze the strain in lattice along size of nanoparticle.

Keywords: Nanoparticle, XRD, Scherrer equation, Williamson-Hall Method

1. Introduction

Nanomaterials, due to their unique properties, have demonstrated their potential to transform numerous fields of science, industry, and technology. Materials with a size of at least one dimension in the range of 1–100 nm are called nanomaterials. A key characteristic of nanomaterials is that their high surface-to-volume ratio leads to a significant increase in reactivity at the molecular level, resulting in electronic, optical, and chemical properties that differ from those of their bulk counterparts [1]. Due to these characteristics, they are being used in many types of technologies including solar cell, sensors, targeted drug delivery, miniaturized electronic components, high-efficiency catalysts, water purification membranes, and stronger, lightweight construction materials etc. Thus, Accurate and thorough characterization techniques are essential for fully grasping and leveraging the potential of nanomaterials. Nanomaterial characterization techniques involve examining and measuring the structural, chemical, physical, and optical properties of nanoscale materials. Here we will discuss different methods for the characterization of nanomaterials.

2. Development of Nanotechnology

1.The key processes employed in nanotechnology include the assembly, separation, and manipulation of materials at the scale of individual molecules or atoms.
2. Richard Feynman introduced the concept of nanotechnology in 1959.
3. Researcher Norio Taniguchi first used the term "nanotechnology" in a 1974 study. He explained in detail the fabrication of things and characteristics with nanometer-scale dimensions utilizing synthesis technologies.

3.Characterization of Nanomaterials

3.1 Dynamic Light Scattering (DLS)

The DLS method have been utilized for particle size determination of materials including solid particles, polymers, emulsions, and others. DLS measurement is based on the Brownian motion of particles which is the fundamental principle of the method.

The principle is that when particles continuously collide with solvent molecules, a certain amount of energy is transferred to the particles during these collisions, causing the particles to move. Therefore, based on the speed of the particles, diameter of the particle can be calculated by equation

$$D = \frac{K_B T}{6\pi\eta R_H} \quad \text{…….(1)}$$

where D is Translational diffusion coefficient [m^2 /s] "speed of the particles,"
kB = Boltzmann constant [m^2 kg/Ks^2],
T = Temperature [K],
η = Viscosity [Pa s],
R_H = Hydrodynamic radius [m].

3.2 X-ray-diffraction techniques

3.2.1 Scherrer equation

X-ray diffraction (XRD) is one of the most powerful techniques used for the characterization of nanomaterials. Numerus information about the materials is provided by XRD pattern. The information obtained from XRD patterns are crystalline structure, nature of the phase, lattice parameters and crystalline grain size. The peaks and related intensity visualized in diffraction pattern is compared with reference patterns namely JCPDS standard data to identify the materials. Thus, XRD pattern is a fingerprint of the materials.
The Scherrer equation is used to determine the mean crystalline size (t) of the particles from the XRD line broadening [

$$t = \frac{k\lambda}{\beta_c Cos\theta} \quad \text{…….. (2)}$$

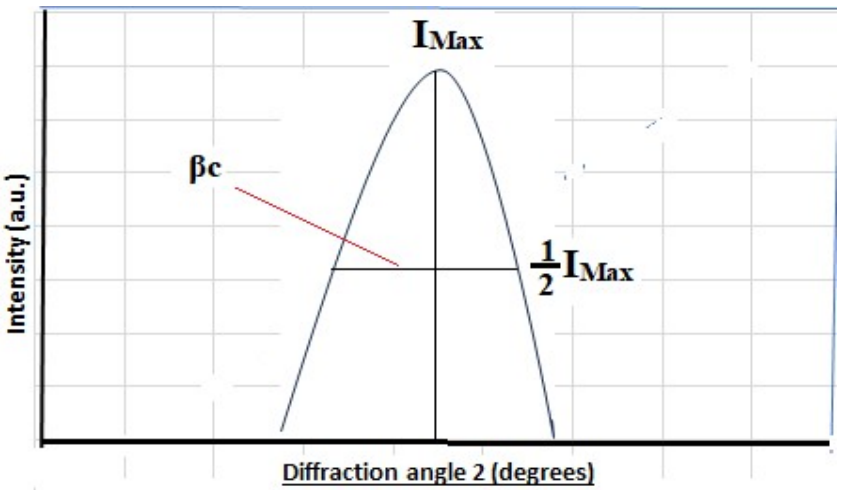

Figure 1: A typical XRD peak broadening of a nanomaterial: estimation of β_c

Where k = Scherrer constant, the shape of the crystalline domains can affect the Scherrer constant k, which is commonly believed to be 0.91.
λ = Wavelength of the X-ray source (Cu Kα = 0.1541 nm), The constant X-ray wavelength (λ) varies according on the type of X-rays used.
A constant crystallographic domain size should be obtained by analysing each peak independently.

β_c = Full width at half the maximum of the diffraction peak (FWHM) in radians of the X-ray diffraction peak, θ = Bragg (diffraction) angle. It is important to note that, in the Scherrer equation, the diffraction angle is taken in radians instead of degrees for the calculation. From equation (2) it is clear that β and L are mutually reciprocal. Figure 1 depicts greater the broadening smaller the crystallite size and vice-versa.
Besides, mean crystalline size (t) is very useful parameter which help to calculate the dislocation density by using the equation

$$\delta = \frac{1}{t^2} \quad \text{……..} \quad (3)$$

It is reported that the lattice defect increased as particle size decreased.
The number of unit cells is known as the volume of the nanoparticle. Therefore, by using the particle size obtained from Scherrer equation the volume of nanoparticles can be calculated as [4]

$$V = \left({}^{4}/_{3}\right)\pi\left({}^{t}/_{2}\right)^{3} \quad \text{……..} \quad (4)$$

For hexagonal particle the volume of the unit cell (v) is estimated by relation-

$$v = 3a^2c/2 \quad \text{……..} \quad (5)$$

Thus obtained the value of $a^2c = 2v/3$ is used to determine the number of unit cells present in a particle, using the following expression as [4]

$$n = 1.621\ (D^3/a^2c) \quad \text{……..} \quad (6)$$

where a and c are the lattice constants of hexagonal structure of nanoparticle.

In a molecule bond length is also an important parameter which also provide the information regarding crystal structure. The parameter indicates the bond strength and the bond dissociation energy. The analysis of bond length in a molecule can be calculated by the following equation [5]

$$L = \sqrt{\left(\frac{a^2}{3} + \left(\frac{1}{2} - u\right)^2\right) C^2} \quad \text{……..} \quad (7)$$

where u is a parameter of crystal has a hexagonal structure, and obtained by the relation

$$u = a^2/3c^2 + 0.25 \quad \text{……..} \quad (8)$$

3.2.1 Williamson-Hall (W-H) Method

As we saw the peak broadening is a main cause which is indication of smaller size of particle that can be seen in the Bragg's law as shown in figure 2 (a). In such a condition size of particle can be calculated by Scherrer equation. Besides, strain in the particle also affect the peak broadening.

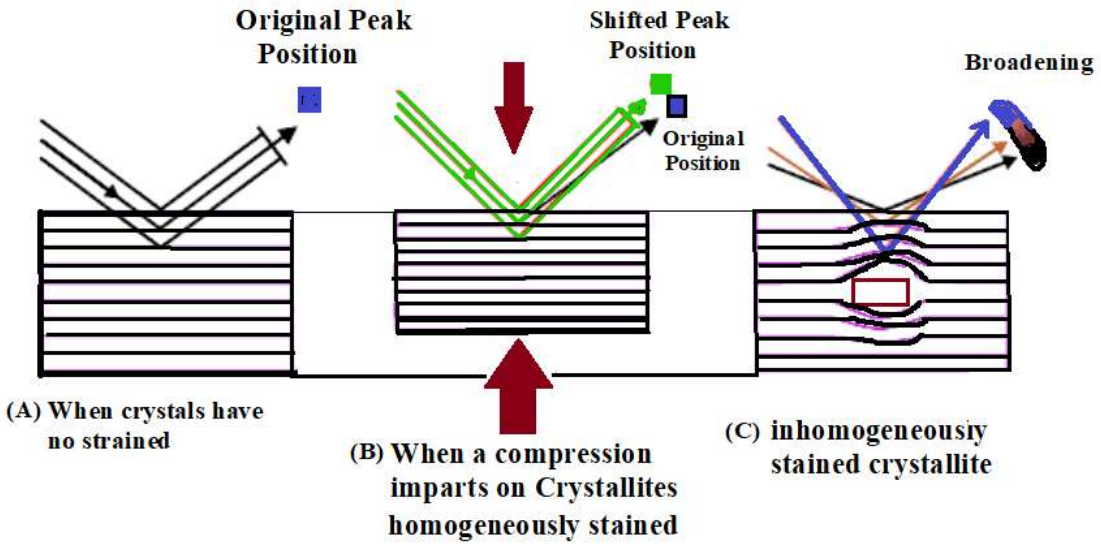

Figure 2: Peak broadening due to homogeneous and inhomogeneous strained

Strain on crystallite changes the d spacings by two ways-
(1) d spacings goes smaller due to a compressive stress, while
(2) it goes larger due to tensile stress,
Thus, it can be said that two components are primarily responsible for diffraction peak broadening: crystallite size and lattice strain. Using the Scherrer formula, the effect of crystal size on XRD peak broadening can be explained, but this formula does not account for the microstructure of the lattice.
The microstructural parameters can be evaluated by several ways including Williamson-Hall method, Warren-Averbach, Balzar and Enzo analysis, Halder-Wagner, size-strain plot, etc. In 1953, G.K. Williamson and W.H. Hall reported the model for crystal size and the associated intrinsic strain in the sample [6]. The proposed model is based on broadening, caused by both size broadening, βsize, and strain broadening, βstrain. Thus, βsize and βstrain broadening add-up which provides the total broadening of corresponding peaks.

$$\beta_{total} = \beta_{size} + \beta_{strain} \quad \text{.....(8)}$$

It is noted that βsize depends on 1/cosθ and βstrain on tan θ.

The values for β_{size} and β_{strain} can be written by the equations

$$\beta_{size} = \frac{k\lambda}{DCos\theta} \quad \text{.....(8)}$$

$$\beta_{strain} = 4\varepsilon tan\theta \quad \text{.....(9)}$$

Hence $$\beta_{total} = \frac{k\lambda}{DCos\theta} + 4\varepsilon tan\theta \quad \text{.....(10)}$$

Now multiplying Cosθ both side then equation (10) becomes

$$\beta_{total}\, Cos\theta = \frac{k\lambda}{D} + 4\varepsilon\, Sin\theta \quad \text{.....(11)}$$

Now by using XRD data profile taking the values of β_{total} Cosθ on y-axis and values of 4Sinθ on x-axis and plot a graph on excel sheet provides the information about crystallite size and lattice strain. A straight-line is fitted on the graph data, for the said materials with R^2 value nearly equal 1. When this equation is compared with the standard equation of a linear straight-line y = mx + c, the intrinsic strain is derived from the slope and the crystal size from the intercept.

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