

## Chapter 25

# Optical X-Ray Diffraction Data Analysis Using the Williamson-Hall Plot Method in Estimation of Lattice Strain-Stress

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### ABSTRACT

*Lattice stress and strain was analysed with estimated crystalline size of the synthesised ZnFe<sub>2</sub>O<sub>4</sub> nanoparticles from x-ray diffraction data using Williamson-Hall (W-H) method. This very peculiar method was used to analyse the other physical parameters such as strain, stress, and energy density. Values calculated from the W-H method include uniform deformation model, uniform deformation stress model, and uniform deformation energy density model. These are very useful methods to label each data point on the Williamson-Hall plot according to the index of its reflection. Particularly, the root mean square value of strain was calculated from the interplanar distance using these three models. The three models have given different strain values by reason of the anisotropic nature of the nanoparticles. The average grain size of ZnFe<sub>2</sub>O<sub>4</sub> nanoparticles estimated from FESEM image, Scherrer's formula, and W-H analysis is relatively correlated.*

### INTRODUCTION

Spinel oxide type AB<sub>2</sub>O<sub>4</sub>, where A and B represent two different ionic comparable cations, are a class of chemically and thermally stable materials that are suitable for a wide-ranging application such as the catalyst and magnetic materials. In the spinel structure, oxygen ions form a cubic closed structure, and

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cations A and B occupy two different crystallographic sites: tetrahedral and octahedral sites (Ashtaputre et al., 2005; Gupta, 1990; Harbour & Hair, 1979; Mitra, Chatterjee, & Maiti, 1998). In the distribution of cations, A and B, these two sites are influenced by the combination and nature of the two cations and are strongly dependent on the preparation and processing conditions. Spin cation distribution has been given a lot of attention because it allows an understanding of the correlations between the structure and properties such as color, diffusivity, magnetic behavior, and optical properties, which are heavily based on better occupation with these two metal sites (Hotchandani & Kamat, 1992). In the class of nanomaterials, zinc ferrite nanocrystalline spinel ( $\text{ZnFe}_2\text{O}_4$ ) is known as Zinc iron brown, commonly used as a catalyst, color filter for automotive lamps, and a pigment layer on luminescent materials due to their optical properties, thermal, chemical, peculiar stability, and photochemistry (Cullity & Stock, 2001; Ramakanth, 2007; Suryanarayana, 2004; Ungár, 2007). In recent years, much work has been done on the preparation of nanoscale  $\text{ZnFe}_2\text{O}_4$  for optical properties. A variety of methods, such as combustion (Warren & Averbach, 1950), Pechini method (Suryanarayana & Norton, 1998), sol-gel (Wasa, Kitabatake, & Adachi, 2004), and micro-emulsion (Zhang, Zhang, Xu, & Ji, 2006) have been successfully performed for the preparation of  $\text{ZnFe}_2\text{O}_4$  nanoparticles.

XRD diffraction peak broadening of the nanoparticle is an important parameter to estimate the three main patterns, such as crystalline size, stress, and strain (Qin & Szpunar, 2005). Crystallization of the perfect powder crystals should extend in all directions with infinity lattice points. But according to the crystallography defined that no crystals can be perfect because of their finite size. This deviation of the flawless nanocrystals can be detected from the line broadening of the individual x-ray diffraction peaks. The two main properties extracted from peak width analysis are (a) crystallite size and (b) lattice strain. Crystallite size is a measure of the size of a coherently diffracting domain. The crystallite size of the particles is not generally the same as the particle size due to the presence of polycrystalline aggregates (Ramakanth, 2007). The lattice strain is the measurement of the dispersion of the lattice constants arising from the deformation of the crystal, that is, the displacement of the lattice, and this is the main source of the other strain, such as the three junctions of the grain boundaries, assembling liabilities, coherency stresses. X-ray line broadening is used to examine the distribution, lattice displacements, reducing crystal sizes, and mixed composites, in addition to mechanical milling powders, induces greater strain (Suryanarayana & Norton, 1998). As already stated, X-ray diffraction grading analysis is a simple tool for estimating the size of the crystal and mainly the lattice strain, as well as the characteristics of the crystal. The values of the crystallite size and lattice strain obtained by using a pseudo-Voigt function, Rietveld purification, and Warren-Averbach analysis from the X-ray diffraction data (Warren & Averbach, 1952). Scherrer first introduced the idea that a crystallite size also examined that a single crystal comprised several grains or particles. Grain had a crystal within themselves, and the size of the crystalline particles differed from that of the grain. Lattice strain can be affected by the displacement of lattice location and point defects due to crystal defect (Dorf, 2003). Two types of lattice strains in the crystals (i.e., uniform and nonuniform strains) that cause the amplitude of the peak to be found in the same crystal lattice (Gul, Maqsood, Naeem, & Ashiq, 2010). Some methods to find deformation of the sized materials have represented by Scherrer (Salavati-Niasari, Davar, & Emadi, 2010), Williamson-Hall (W-H) (Bersuker, 1997), strain–size plot (SSP), and Warren-Averbach methods (Maurizio et al., 2010). The Scherrer and W-H methods set the Full-width Half Maximum (FWHM) values and integrated integral line broadening peaks, these are indicating from the Fourier coefficient profile in the Warren-Averbach method (Mimani, 2001). But in the Warren-Averbach method is mathematically complex (Irfan, Racik K, & Anand, 2018). Among these, the Williamson-Hall (W-H) analysis is a simplified, integrated Full-width

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