Supplementary File 1

1. Crystal Phase Analysis

These equations (Eq. S1 to Eq. S6) are used to measure various crystallographic parameters of the synthesized ZnO-NPs.

Unit cell parameter, $$\left(\frac{1}{d_{hkl}}\right)^2 = \frac{4}{3}\left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2} \quad (1)$$

Microstrain, $\varepsilon = \beta / 4 \tan\theta$ (2)

Dislocation density, $$\delta = \frac{1}{(D_c)^2} \quad (3)$$

Unit Cell volume, $$V = \frac{\sqrt{3}}{2} a^2 c \quad (4)$$

Specific surface area, $$s = \frac{6}{\rho \times D_c} \quad (5)$$

Preference growth, $$PG = \frac{RI_{sample} - RI_{standard}}{RI_{standard}} \quad (6)$$

Within the above equations, the variables h, k, and l correspond to the Miller indices of the crystal plane, while a and c represent the lattice parameters. The full width at half maximum (FWHM), crystallite size, peak height, shape factor, diffraction angle and density is denoted by β (in radians), D_c, H_{hkl}, k (0.9), θ (in degree) and ρ, respectively.

Supplementary File 2

2. Crystal size estimation using different XRD models.

2.1. Williamson–Hall Model

2.1.1 Uniform deformation model (UDM)

The UDM of the W-H approach is implemented when the stress arises from isotropic crystal deformation, resulting in the strain being consistently distributed across all crystallographic lattices. The equation representing the strain within a crystal is given in Eq. S7, and upon rearrangement with the Scherrer equation (Eq. 3), it yields the expression shown in Eq. S8.

$$\beta_{strain} = 4.\varepsilon.\tan(\theta) \quad (7)$$

$$\cos(\theta)\, \beta_{total} = (K\lambda)/D + 4.\varepsilon.\sin(\theta) \quad (8)$$

Within this expression, ε refers to strain, and the other parameters remain the same as previously denoted. The crystallite size can be determined from the intercept of the line by plotting 4sin(θ) on the X-axis and cos(θ)βtotal on the Y-axis, while the strain can be obtained from the slope by comparing Eq. 8 with the straight-line equation, y = mx + c and the obtained data were depicted in Fig. S1.

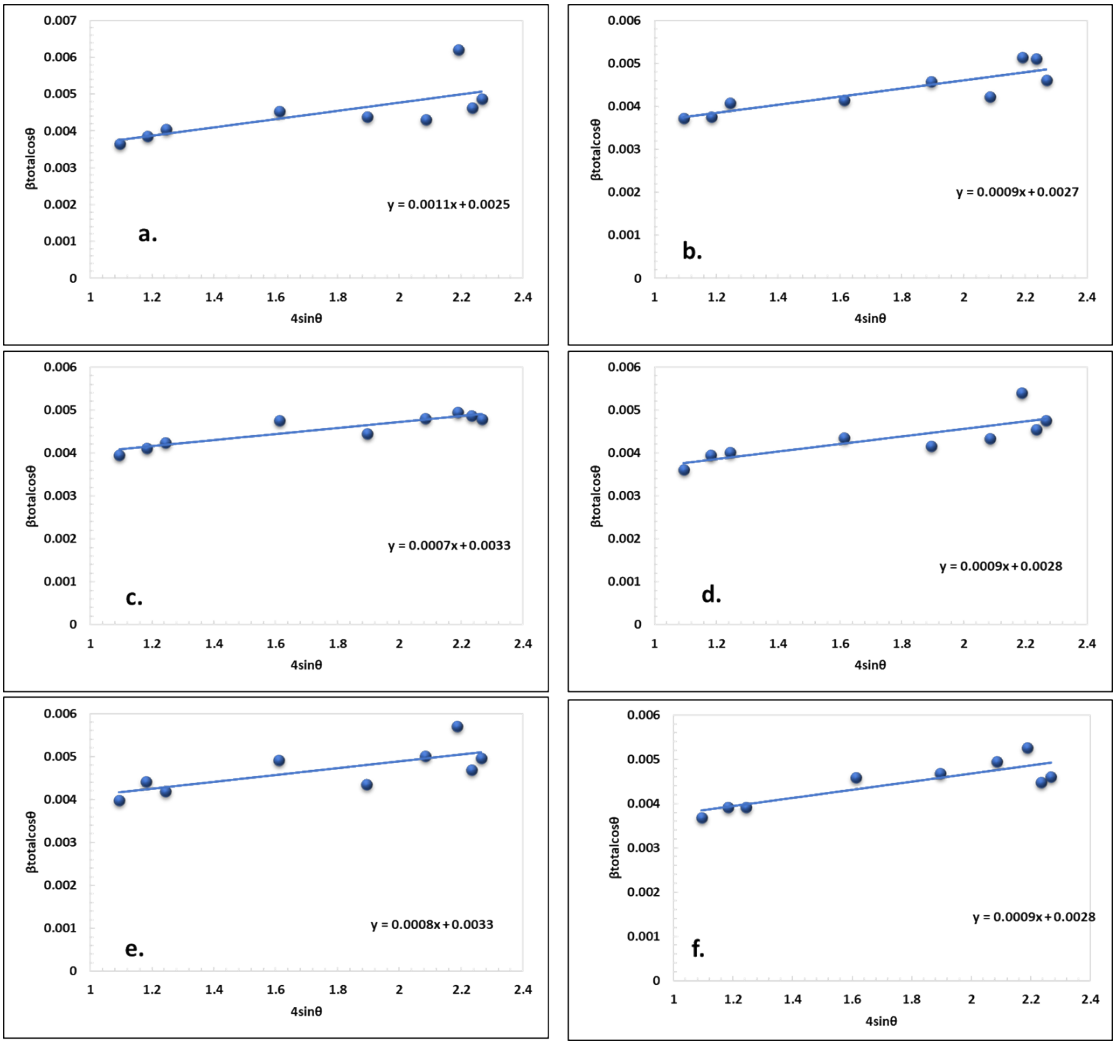

Fig. S1. Uniform deformation model for a. PZO b. AgZO c. CuZO d. CoZO e. FeZO and f. CaZO

2.1.2. Uniform stress deformation model (USDM)

The UDM makes the assumption that the crystal is the same in all directions because real crystals are not isotropic. In order to address this, the Uniform Stress Deformation Model (USDM) is created by updating the model to incorporate strain variations. The USDM approach posits that stress-induced deformation is equally distributed throughout the lattice in all

directions within the crystallites. Hooke's Law describes a direct relationship between strain (ε) and stress (σ), as shown in Eq. S9.

$$\sigma = Y_{hkl}.\ \varepsilon \tag{9}$$

Eq. S10, a revised form of Eq. S8, is obtained by incorporating the strain term into the equation.

$$cos(\theta)\ \beta_{total} = \frac{K\lambda}{D} + \frac{4.\sigma.sin(\theta)}{Y_{hkl}} \tag{10}$$

A comparison of Eq. 3 (Fig. S2) with the straight-line equation, y = mx + c, yields the stress from the slope, while the crystallite size can be found from the intercept of the line by plotting $\frac{4.sin(\theta)}{Y_{hkl}}$ on the X-axis and $cos(\theta)\ \beta_{total}$ on the Y-axis.

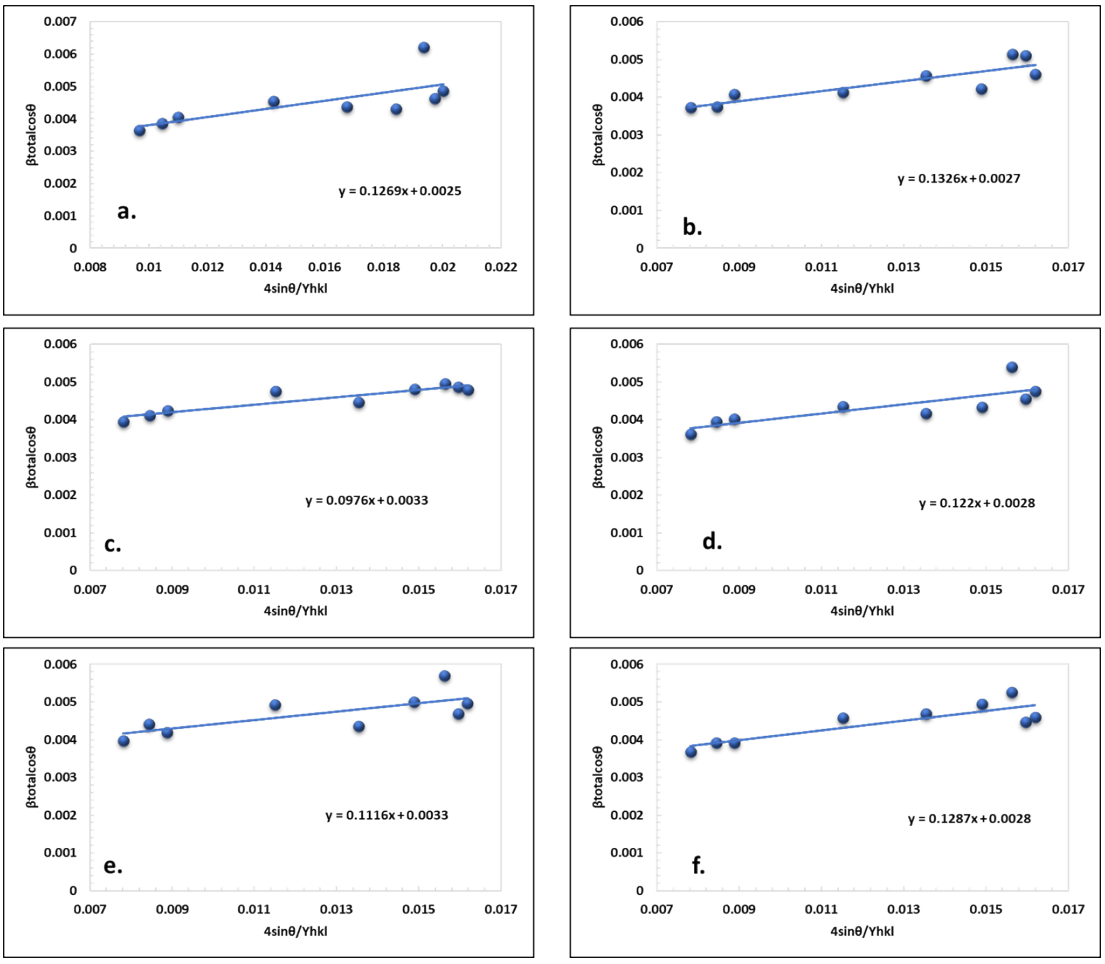

Fig. S2. Uniform stress deformation model for a. PZO b. AgZO c. CuZO d. CoZO e. FeZO and f. CaZO

2.1.3 Uniform deformation energy density model (UDEDM)

UDM and USDM are the methods based on the uniform strain and uniform strain, respectively. UDEDM is a method for studying stress and strain distribution, assuming evenly spread deformation energy to predict material behavior under stress [1]. Hooke's Law associated with energy density is presented as Eq. S11.

$$\mu = \varepsilon^2 \frac{Y_{hkl}}{2} \tag{11}$$

By rearranging Eq. S8 and plotting the value of strain (ε) in the equation, another equation, Eq. S12, is formed that includes the energy density term.

$$cos(\theta)\beta_{total} = \frac{K\lambda}{D} + 4.sin(\theta)\frac{\sqrt{2\mu}}{\sqrt{Y_{hkl}}} \tag{12}$$

By using the line's intercept ($\frac{K\lambda}{D}$) and slope ($\sqrt{2\mu}$), where $\frac{4.sin(\theta)}{\sqrt{Y_{hkl}}}$ plotted on the X-axis and $cos(\theta)\beta_{total}$ plotted on the Y-axis, the crystallite size and energy density can be found by comparing Eq. 12 with the straight-line equation, y = mx + c, portrayed in Fig. S3.

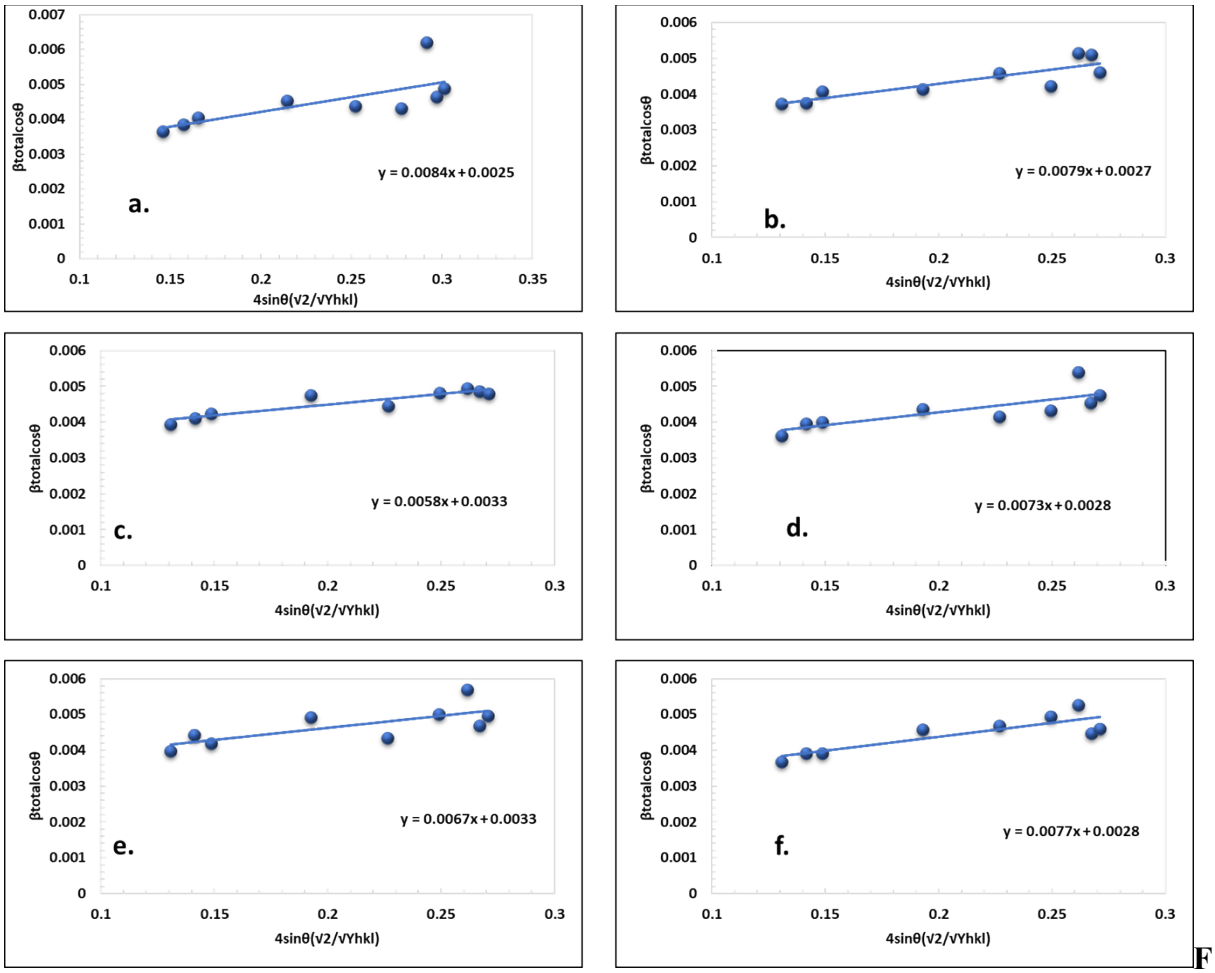

Fig. S3. Uniform deformation energy density model for a. PZO b. AgZO c. CuZO d. CoZO e. FeZO and f. CaZO

2.2. Scherrer's Model with a linear straight-line method.

The linear straight-line method of Scherrer's equation (LSLMSE) improves the usual way of determining crystallite size by using numerous diffraction peaks to increase accuracy instead of only one, as in the standard Scherrer equation [2]. In the LSLMSE method, the broadening of diffraction peaks is linearly related to factors such as the Bragg angle and wavelength. By plotting the full width at half maximum (FWHM) against a function of the Bragg angle, the slope of the resulting line can be used to determine the average crystallite size.

$$cos\theta = \frac{K\lambda}{D_L \beta} \tag{13}$$

The crystal size, denoted by D_L in this formula, is computed using the linear equation that comes from the Scherrer model. With the X-axis representing 1/β in radians and the Y-axis indicating cos(θ) in degrees, the values were produced using Eq. S13 (Fig. S4). The crystal sizes displayed

in Table 2 were determined using the slope, which is defined as m = Kλ/(DL), and this equation, which represents the linear form of a straight line (y = mx + c).

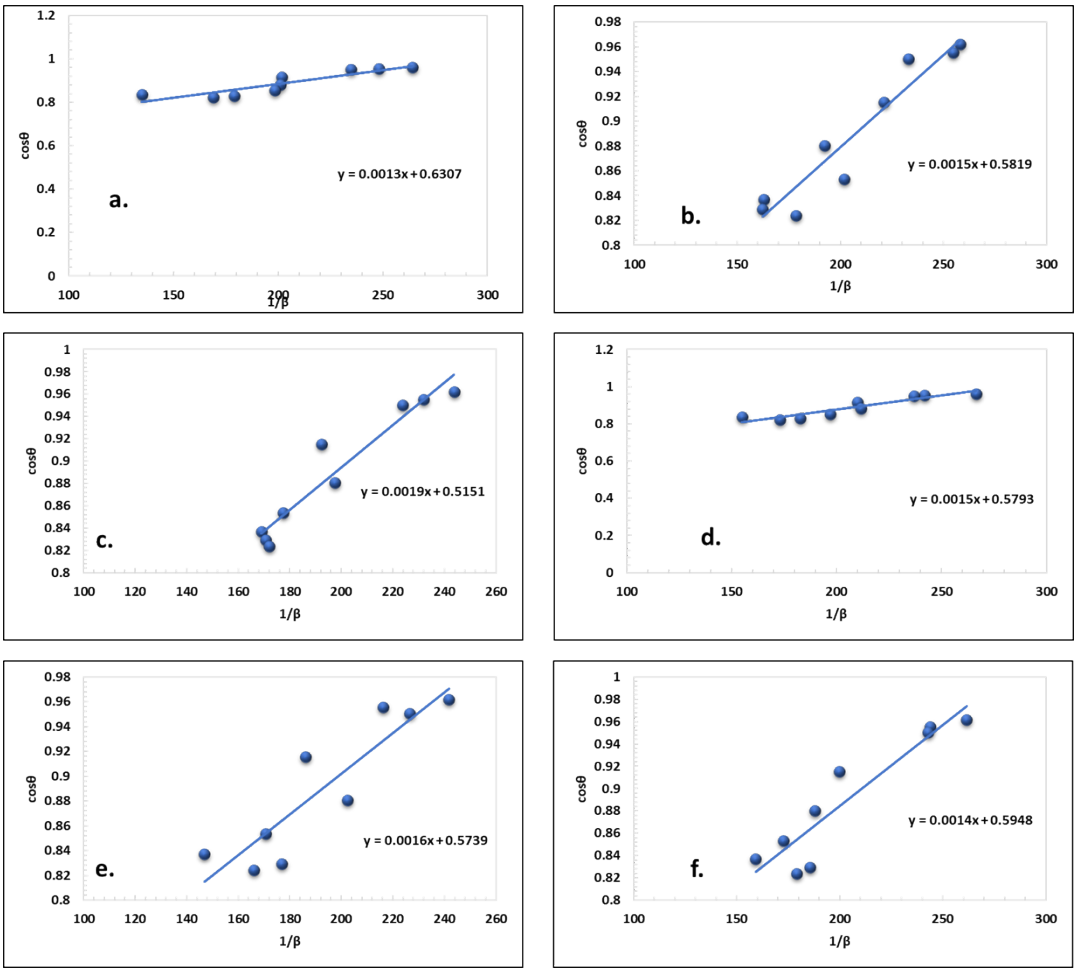

Fig. S4. Scherrer's Model with a linear straight-line method for a. PZO b. AgZO c. CuZO d. CoZO e. FeZO and f. CaZO

2.3. Monshi–Scherrer method

The Monshi-Scherrer model is particularly effective for assessing the crystallite sizes of nanoparticles because it emphasizes reducing errors and incorporates all diffraction peaks in the calculation which uses logarithmic values shown in Eq. S14 [3].

$$ln\beta = ln\frac{1}{Cos\theta} + ln\frac{K\lambda}{D_M} \tag{14}$$

In this context, D_M refers to the crystallite sizes determined using this particular method, with the associated parameters remaining consistent with those outlined previously. A graph was constructed (Fig. S5), from which the values were derived, plotting the natural logarithm of β on the X-axis and the natural logarithm of 1/Cosθ on the Y-axis, with measurements in radians and degrees, respectively.

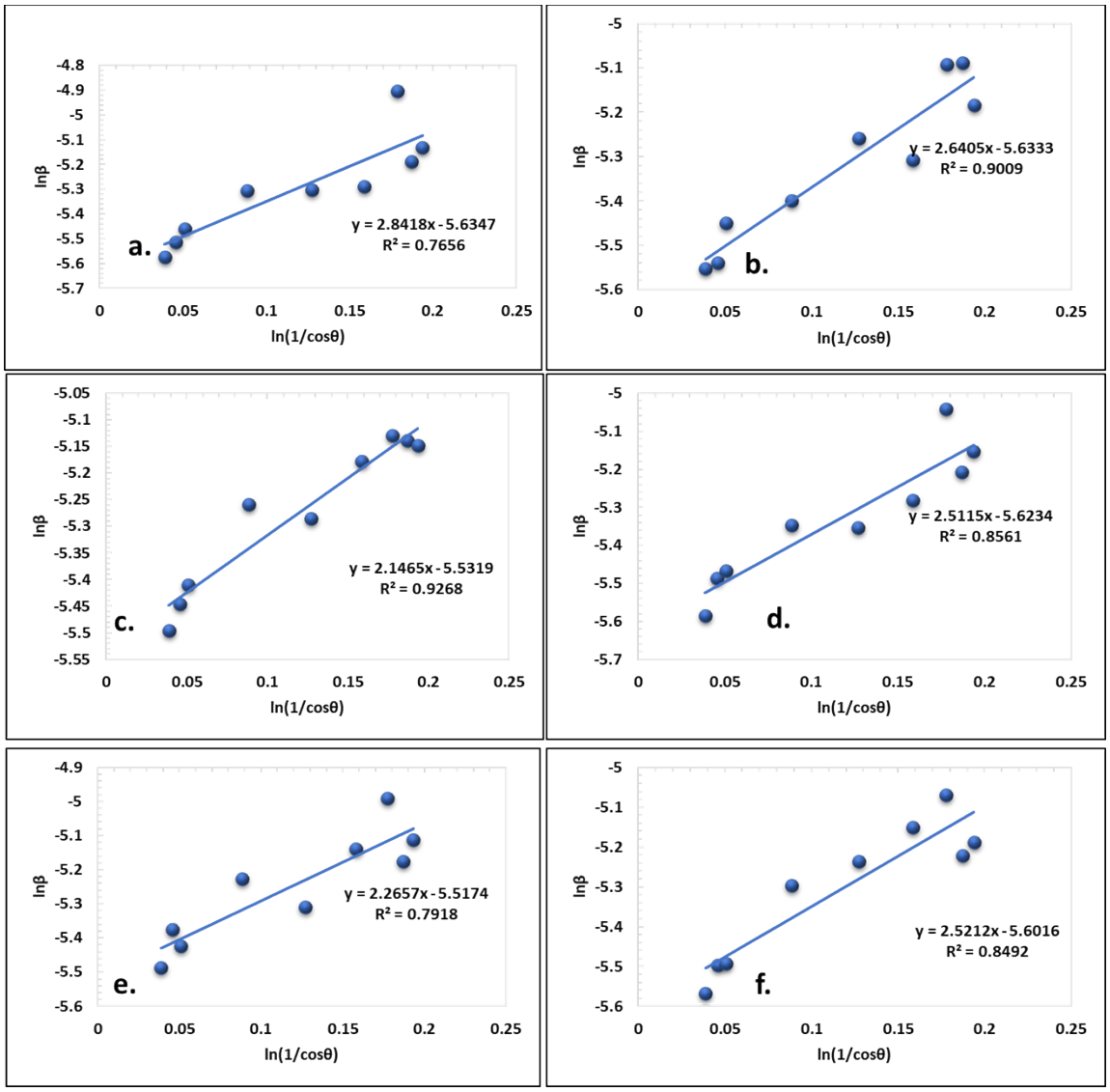

Fig. S5. Monshi–Scherrer method for a. PZO b. AgZO c. CuZO d. CoZO e. FeZO and f. CaZO

2.4. Shahadat-Scherrer Model

In the SSM technique, peak broadening as a consequence of instrumental effects and strain is deemed insignificant. Peak widening related to the crystal size is used to calculate the crystallite size using the Eq. S15 that passes through the coordinate origin [4].

$$cos\ \theta = \frac{K\lambda}{D_{s-s}} \times \frac{1}{FWHM} \tag{15}$$

A straight line can be obtained by plotting $\frac{1}{FWHM}$ on the X-axis and $cos\ \theta$ on the Y-axis and a graph was projected in Fig. S6. Another straight line is drawn by selecting a point at the origin, which is used to determine the crystallite size summarized in **Table 2.**

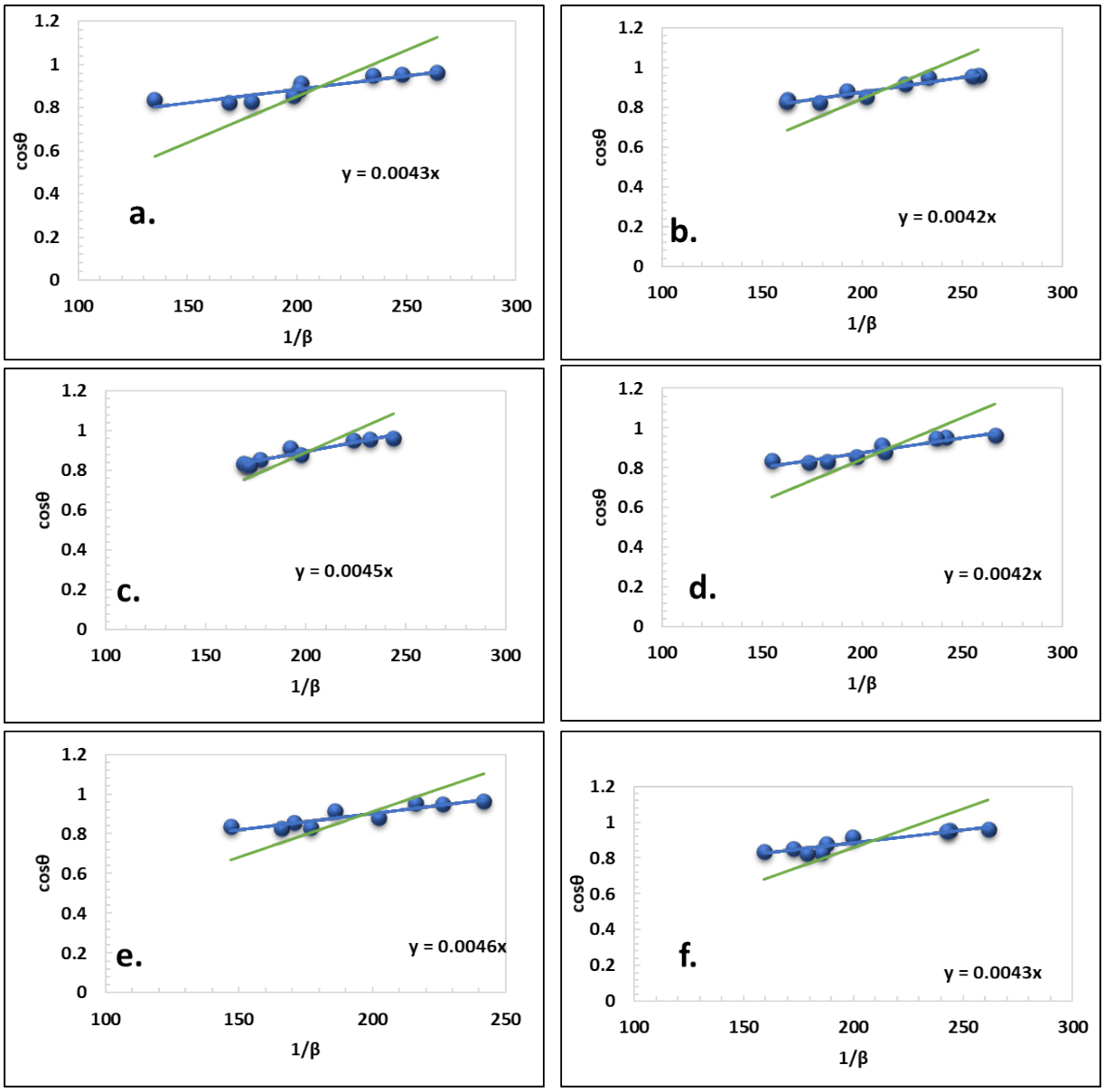

Fig. S6. Shahadat-Scherrer Model for a. PZO b. AgZO c. CuZO d. CoZO e. FeZO and f. CaZO

2.5. Size-Strain plot method

From the previous analysis, it is clear that peak broadening is linked to size and strain components, which are represented by the Lorentzian (β_L) and Gaussian (β_G) functions, as described in the published article (Eq. 16) [5]. This approach is ideal for XRD analysis, where minimal peak overlap occurs at lower angles in the powder diffraction method, making the defined low-angle range sufficient for predicting crystallite size and strain.

$$\beta_{total} = \beta_L + \beta_G \tag{16}$$

According to Eq. (16), Eq. (17) illustrates the size-strain graph shown in Fig. S7 utilized for determining mean strain and crystallite size.

$$(d_{hkl}\beta_{hkl}\,cos\theta)^2 = \frac{K\lambda}{D}(d_{hkl}^2\,\beta_{hkl}\,cos\theta) + \frac{\varepsilon^2}{4} \quad (17)$$

Average strain and size can be determined from the intercept of the line by plotting $(d_{hkl}^2\,\beta_{hkl}\,cos\theta)$ on the X-axis and $(d_{hkl}\beta_{hkl}\,cos\theta)^2$ on the Y-axis, while the size can be obtained from the slope by comparing Eq. (17) with the straight-line equation, y = mx + c.

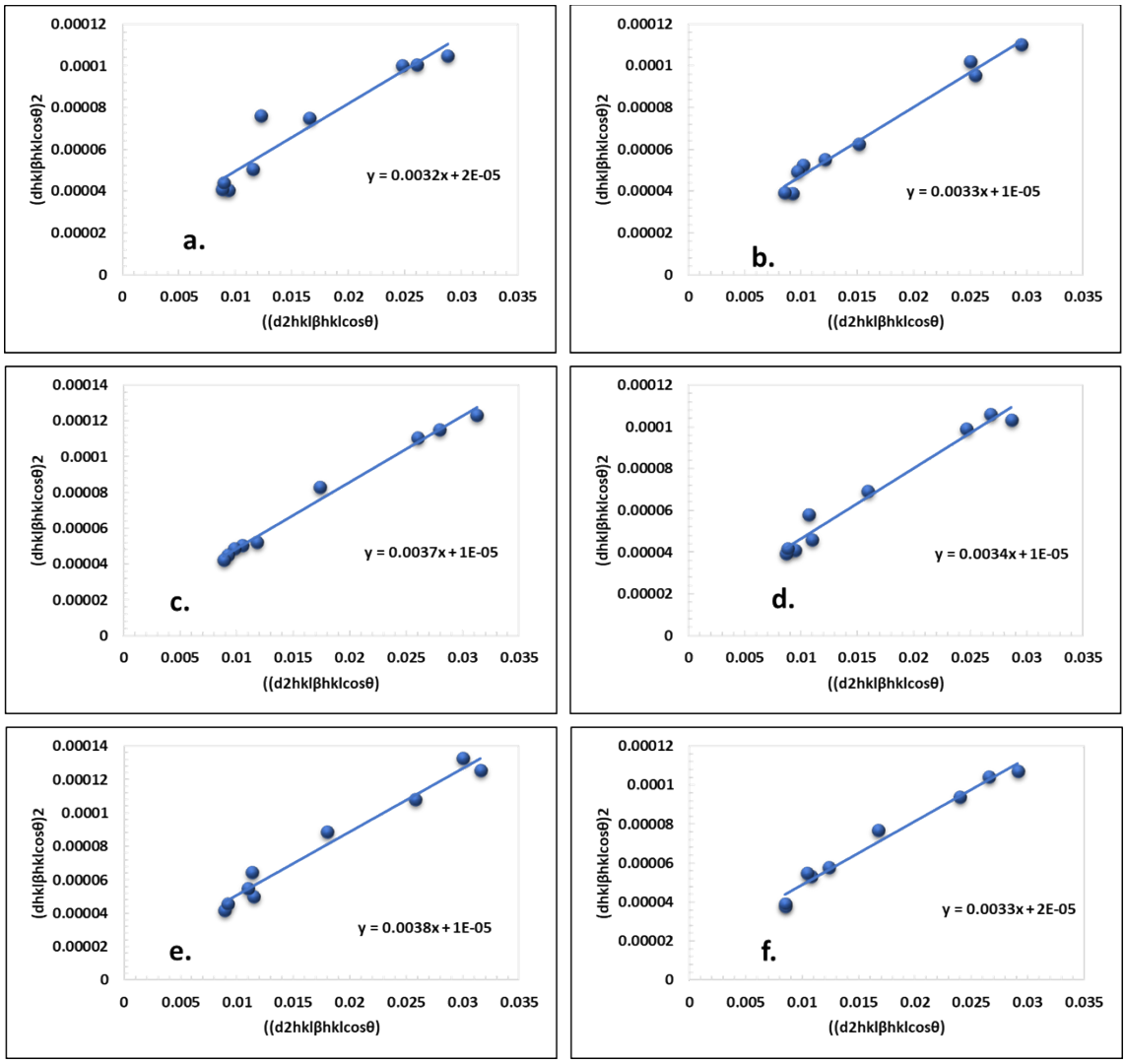

Fig. S7. Size-Strain plot method for a. PZO b. AgZO c. CuZO d. CoZO e. FeZO and f. CaZO

Supplementary File 3

3.1. EDAX analysis

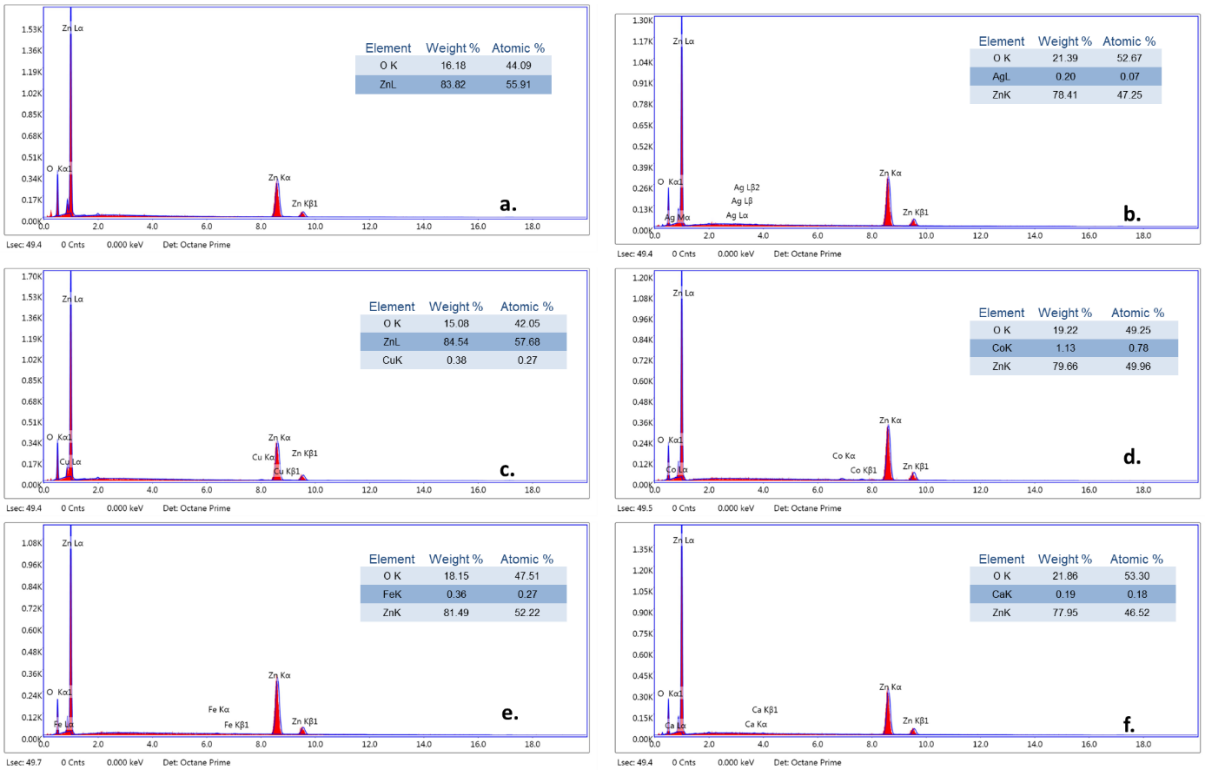

Fig. S8. EDAX analysis for a. PZO b. AgZO c. CuZO d. CoZO e. FeZO and f. CaZO

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