X-ray diffraction analysis by Williamson-Hall, Halder-Wagner and size-strain plot methods of CdSe nanoparticles- a comparative study

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HIGHLIGHTS
- Water soluble MPA capped CdSe nanocrystals have been chemically synthesized.
- XRD peak broadening analysis has been carried out by different models.
- Different models are modified W–H Plot, SSP method and H–W method.
- SSP and H–W method provide the best value for average size and intrinsic strain.
- These results match well with the morphological analysis from TEM, AFM and SEM.

GRAPHICAL ABSTRACT

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ABSTRACT

Cadmium selenide (CdSe) nanoparticles have been prepared by chemical method using sodium hydrogen selenide precursor and cadmium chloride. X-ray diffraction (XRD) study confirms the crystalline nature of the CdSe nanoparticles with Cubic Zinc-blende lattice structure, whereas transmission electron microscopy (TEM), scanning electron microscopy (SEM) and atomic force microscopy (AFM) analysis indicate the spherical morphology of the prepared nanoparticles, having an average size of approximately 36 nm. Here, Williamson-Hall (W–H), Size-Strain Plot (SSP), and Halder-Wagner Method (H–W) have been used to investigate the particle size and the intrinsic strain from the XRD peak broadening analysis. Further, in W–H method, different models have been considered for the determination of physical and microstructural parameters such as strain, stress, and energy density. The average particle size that has been determined from Williamson-Hall, Size-Strain, Halder-Wagner Methods are compared with HR-TEM, AFM, and SEM analysis.

1. Introduction

Semiconductor nanoparticles, in the dimension of 1–100 nm, possess unique size-dependent many physical properties, different from their bulk counterpart [1,2]. It is reported that elastic properties is one of the important physical properties, tuning of which, can modify many physical properties such as optical properties and surface properties and because of which, many semiconductor nanoparticles find enormous
application in different branches of science such as in the field of optoelectronics devices as light-emitting diodes [3], solar cells [4].

Cadmium selenide (CdSe) is one of the important group II-VI semiconductor nanoparticles having a direct band gap of 1.74 eV, with an exciton Bohr radius of 6 nm [5–7]. CdSe nanocrystals reported to exhibit cubic (zinc blende) and hexagonal (wurtzite) lattice structure [8], which can be prepared by many suitable synthesis methods [9–11]. In nanocrystals, there exists intrinsic strain because of size confinement and this important elastic property can be tuned by varying synthesis parameters, such as pH and concentration, which in turn affects the optical and other properties [12]. X-ray Diffraction (XRD) analysis of a nanocrystal can confirm the crystallinity of the sample, which shows different peaks, related to different reflection planes [13]. It is well known that because of size confinement in nanocrystals and presence of intrinsic strain, which originates due to size confinement, broaden the XRD peaks. Thus, a physical peak broadening primarily consists of two parts; size-dependent broadening and strain induced broadening [14]. The most common sources of the lattice strain are dislocation density, point defects, grain boundary junction, contact or sinter stress, and stacking faults [15–16]. So, from the XRD peak broadening analysis, the size of the nanocrystals as well as the value of the intrinsic strain, including other elastic properties such as stress, energy density, which are related to strain, can be determined indirectly. There are many methods for this, such as Williamson-Hall Method, Warren-Averbach Method and Balszar Method. Warren-Averbach and Balszar method consider Stokes fourier de-convolution method [27–31], whereas Williamson-Hall method uses the FWHM of the diffraction peak and hence, it is very easy and suitable one for determination of different elastic properties including strain, along with average size calculation.

Here, our interest lies in the determination of different elastic properties of the wet chemically synthesized CdSe nanocrystals, from their X-ray diffraction data, using Williamson-Hall (W-H) analysis, Size-Strain Plot (SSP) and Halder-Wagner (H-W) Method. Williamson-Hall analysis comprises of uniform deformation model (UDM), uniform stress deformation model (UDSM), and uniform deformation energy density model (UDEDM) to calculate the various elastic parameters such as strain, stress and energy density respectively. Again, size-strain plot considers the size broadened part as Lorentzian and the strain broadened part as Gaussian function of the XRD peak profile. The advantage of SSP model is that, it gives more importance to the low angle XRD reflection peak, where the accuracy and precision of the XRD data are high. Due to this, size estimation from the SSP model is more accurate than W-H method [23–25]. Halder-Wagner Method, on the other-hand, assumes the physical peak broadening as voigt function and considering that, average size and strain can be estimated from the XRD peak broadening [26].

In the present work, we have done a comparative study of various elastic parameters of chemically prepared CdSe nanocrystals based on the XRD peak broadening using different models of the W–H plot, along with SSP method and H–W method. Subsequently, their morphological analysis has been performed on high resolution Transmission electron microscopy (HR-TEM), atomic force microscopy (AFM) and field emission scanning electron microscopy (FE-SEM), where the average size obtained from these methods matches very well with the obtained results from XRD analysis.

2. Chemical synthesis

For the preparation of CdSe nanocrystals, selenium precursor has been prepared by dissolving 0.2 mmol of selenium powder and 0.5 mmol of sodium borohydride in 10 mL of distilled water, which is constantly stirred for 1 h at 600 rpm [27]. Under this vigorous reaction, selenium is reduced within a few minutes by forming a colorless sodium hydrogen selenide (NaHSe). Again, in another beaker, containing 30 mL of distilled water, 0.2 mmol of cadmium chloride and 1 mmol of 3-mercaptoproic acid (MPA) have been added and in that mixture, the selenium precursor solution as sodium hydrogen selenide (NaHSe) are mixed under stirring and heated approximately at 120 °C for 45 min. This rigorous reaction finally produces the CdSe nanoparticles, showing a reddish brown color and this prepared CdSe nanoparticles have been extracted from the mixture by filtering.

3. Results and discussion

3.1. X-ray diffraction analysis

The X-ray diffraction (XRD) profile of chemically prepared CdSe nanoparticles, in the range of 20° < 20 < 60° with a step size of 0.02° is shown in Fig. 1, which has been taken in Bruker D8 diffractometer, using CuKα1 radiation with the wavelength of 1.5406 Å, having the accelerating voltage of 40 kV. Diffraction pattern shows peaks at 25.41°, 30.11°, 42.44° and 50.18°, corresponding to the planes (111), (200), (220), and (311), which matches with the stick pattern of the Joint Committee on Powder Diffraction Standards (JCPDS), having the card no. 65–2891 of cubic CdSe nanocrystals [38]. From this diffraction data, both the particle size and the intrinsic strain have been calculated, which are discussed in the following section.

3.1.1. Scherrer method

X-ray diffraction peak gets broadens in the nanocrystals due to the crystalline size effect and intrinsic strain effect and this peak broadening normally consists of two parts physical broadening and instrumental broadening [29–32]. This instrumental broadening can be corrected using the following relation,

\[ p^2 = p_0^2 - \delta^2 \]  

Where \( p_0 \) is the measured broadening, \( p_1 \) is the instrumental broadening and \( \delta \) is the corrected broadening. Here, crystalline silicon has been used as a standard reference material for position calibration and instrumental broadening calculation. The instrumental broadening and physical broadening of the sample have been measured as full width at half maximum (FWHM). Using the corrected physical broadening, we can calculate the average particle size with the help of Scherrer equation [33–35].

\[ D = \frac{0.94 \lambda}{\beta I \cos \theta} \]

Fig. 1. XRD pattern of cubic CdSe nanoparticles with reference stick pattern of JCPDS card no. 65–2891.
Where \( \lambda \) is the incident radiation, \( D \) is the average particle size, which has been calculated as 41.95 nm. Rearranging the above equation, we can write,

\[
\cos \theta = \frac{0.941}{D} \beta_g
\]  
(3)

Now, plotting a graph of \( 1/\beta_g \) vs \( \cos \theta \) for CdSe nanoparticles, as shown in Fig. 2, known as the Scherrer plot, average particle size can be calculated from the slope of the graph, which is found as 41.12 nm.

3.1.2. Williamson-Hall analysis

Scherrer formula considers only the effect of crystallite size on the XRD peak broadening, but it doesn’t tell anything about the microstructures of the lattice i.e. about the intrinsic strain, which gets developed in the nanocrystals due to the point defect, grain boundary, triple junction and stacking faults [19,21]. There are many methods such as Williamson’s Hall method, Warren-Averbach method etc., which considers the effect of the strain induced XRD peak broadening and can be used for the calculation of the intrinsic strain along with the particle size. Among these methods, Williamson-Hall (W-H) method is a very easy and simplified one [20,24]. According to which, physical line broadening of X-ray diffraction peak occurs due to the size and microstrain of the nanocrystals and the total broadening can be written as,

\[
\beta_{\text{total}} = \beta_{\text{size}} + \beta_{\text{strain}}
\]  
(4)

In the present work, average particle size and microstrain have been calculated using modified W-H equation such as UDM, USDM and UDEDM, which are discussed in the following sections.

3.2. Uniform deformation model (UDM)

Uniform deformation model (UDM) considers uniform strain throughout the crystallographic direction, which gets introduced in the nanocrystals due to crystal imperfections. In other words, UDM considers strain, which is isotropic in nature [22]. This intrinsic strain actually affects the physical broadening of the XRD profile and this strain induced peak broadening can be expressed as,

\[
\beta_{\text{strain}} = 4 \varepsilon \tan \theta
\]  
(5)

So, the total broadening due to strain and size in a particular peak having the hkl value, can be expressed as,

\[
\beta_{\text{hkl}} = \beta_{\text{size}} + \beta_{\text{strain}}
\]  
(6)

Where, \( \beta_{\text{hkl}} \) is the full width at half of the maximum intensity for different diffraction planes.

This equation (6), on re-arranging we get,

\[
\beta_{\text{hkl}} \cos \theta = \frac{k \lambda}{D} + 4 \varepsilon \sin \theta
\]  
(7)

Equation (7) is an equation of a straight line and is known as the uniform deformation model (UDM) equation, which considers the isotropic nature of the crystals. Fig. 3 shows the plotting of this equation (7), with the term \((4 \sin \theta)\) along X-axis and \((\beta_{\text{hkl}}, \cos \theta)\) along Y-axis corresponding to each diffraction peak for CdSe nanoparticles. This plotted straight line is a good fitted line, corresponding to all the values, as the correlation coefficient value of \( R^2 \) is 0.8816. The slope of this straight line provides the value of the intrinsic strain, whereas the intercept gives the average particle size of the CdSe nanocrystals. The origin of the lattice strain is attributed mainly to the lattice expansion or lattice contraction in the nanocrystals due to size confinement, because the atomic arrangement gets slightly more rigid due to size confinement, compared to their bulk counterpart. On the other hand, many defects also get created at the lattice structure due to the size confinement and this in turn results in the lattice strain. The average particle size has been determined from the uniform deformation model approximately as 45 nm. Again, slope of the UDM plot has been found to be positive, which indicates the lattice expansion [14] and hence produce an intrinsic strain in the nanocrystals. From the slope, intrinsic strain has been calculated as \( 0.87 \times 10^{-3} \).

3.3. Uniform stress deformation model (USDM)

UDM model is based on the assumption that sample is homogeneous and isotropic in nature, which is not actually justified for a real crystal. Now, as a crystal is anisotropic, Williamson-Hall equation should be modified by an anisotropic term and here for this, an anisotropic strain has been considered. This modified model is the uniform stress deformation model (USDM), where lattice deformation stress has been considered uniform along all the lattice plane directions containing a small microstrain [13].

According to Hooke’s law, stress and strain have a linear relationship, where stress is expressed as \( \sigma = \varepsilon \times Y_{\text{hkl}} \), \( Y_{\text{hkl}} \) being the modulus of elasticity or Young’s modulus. So, strain can be expressed as

- Fig. 2. Scherrer plot for CdSe nanoparticles.
- Fig. 3. UDM plot for CdSe nanoparticles.
\[ e = \frac{\sigma}{Y_{bkl}} \]  

A small amount of internal stress arises with the intrinsic strain in the crystals due to size confinement. USDM considered stress induced broadening in the XRD peak and anisotropic nature of Young’s modulus [36]. Putting the value of \( e \) in equation (7) and on rearrangement, we get

\[ \beta_{bkl} \cos \theta = \frac{k_0}{D} + 4\pi \frac{\sin \theta}{Y_{bkl}} \]  

(9)

This is the modified W-H equation and is known as uniform stress deformation model, which considers the uniform stress in every crystallographic direction.

Here, Young’s modulus \( Y_{bkl} \) can be expressed for cubic crystal as [13],

\[ \frac{1}{Y_{bkl}} = S_{11} - 2 \left[ (S_{11} - S_{12}) - \frac{1}{2} S_{44} \right] \left[ \frac{\sqrt{h^2 + k^2 + l^2}}{(h^2 + k^2 + l^2)^{\frac{3}{2}}} \right] \]  

(10)

Where \( S_{11}, S_{12}, S_{44} \) are known as elastic compliances of cubic CdSe and can be computed from the elastic stiffness constant \( C_{11}, C_{12} \) and \( C_{44} \) [14], which are as follows

\[ S_{11} = \frac{C_{11} + C_{12}}{(C_{11} - C_{12})(C_{11} + 2C_{12})} \]  

(11)

\[ S_{12} = \frac{-C_{12}}{(C_{11} - C_{12})(C_{11} + 2C_{12})} \]  

(12)

\[ S_{44} = \frac{1}{C_{44}} \]  

(13)

The value of the stiffness constants \( C_{11}, C_{12}, C_{44} \) for cubic CdSe is \( 86.2 \times 10^{-10} \text{ N/m}^2, 30.3 \times 10^{-10} \text{ N/m}^2 \) and \( 36.8 \times 10^{-10} \text{ N/m}^2 \) respectively [37]. Using the stiffness constant values from equations (11)-(13), the elastic compliances values have been calculated as \( 0.014 \times 10^{-10}, -0.0036 \times 10^{-10} \) and \( 0.0271 \times 10^{-10} \) respectively. Using these compliances values, the Young’s modulus value have been calculated for \((111), (200), (220) \) and \((311) \) peak as \( 89.28, 71.42, 77.51 \) and \( 78.71 \text{ MPa} \) respectively and from these values, average Young’s modulus has further been calculated as \( -79.233 \text{ MPa} \).

Plot of equation (9), with the term \((4\pi \sin \theta / Y_{bkl})\) along X-axis and \((\beta_{bkl} \cos \theta)\) along Y-axis corresponding to each peak in the XRD pattern for CdSe nanoparticles, is shown in Fig. 4. The slope of this plotted straight line provides the value of stress, whereas the intercept gives the average particle size of the CdSe nanocrystals. The average particle size and stress have been determined from the uniform stress deformation model approximately as 41 nm and 73.8 MPa respectively.

3.4. Uniform deformation energy density model (UDEDM)

UDM model assumes the isotropic nature of the crystal, whereas the USDM model assumes a linear relationship between stress and strain, as per Hook’s law. But, in real crystals, isotropic nature and linear proportionality between stress and strain, cannot be considered, as because different defects, dislocations, and agglomerates create imperfections in almost all crystals. So, a different model is required, which should be used for the study of the different microstructures of crystals. Here, Uniform deformation energy density model (UDEDM) model is used for this purpose, which considers the uniform anisotropic lattice strain in all crystallographic direction and the cause of that uniform anisotropic lattice strain is the density of deformation energy [38].

According to Hook’s law energy density \( (u) \) is related to strain with the relation

\[ u = \frac{\varepsilon^2}{2} \frac{Y_{bkl}}{2} \]  

(14)

Again, we know stress and strain are related as \( \sigma = \varepsilon \sqrt{Y_{bkl}} \). So, the intrinsic strain can be written as a function of energy density,

\[ \varepsilon = \sqrt{\frac{2u}{Y_{bkl}}} \]  

(15)

Where \( Y_{bkl} \) is the anisotropic Young’s modulus.

Putting the value of \( e \) in equation (7) and on re-arrangement we get,
\[ \beta_{hkl, \text{cos} \theta} = \frac{k \lambda}{D} + 4 \sigma \sin \theta \sqrt{\frac{2}{Y_{hkl}}} \]  \hspace{1cm} (16)

Equation (16) is a straight line equation and is known as the uniform deformation energy density model (UDEDM) equation [31]. From this model, energy density value of the crystals can be calculated as per equation (16). Plot of this equation (16), with the term \((4 \sin \theta \sqrt{2 \mu / Y_{hkl}})\) along X-axis and \((\beta_{hkl, \text{cos} \theta})\) along Y-axis corresponding to each diffraction peak for CdSe nanoparticles, is shown in Fig. 5. The intercept of the plotted straight line provides the average size as 38.19 nm, whereas the slope gives the energy density value as 48.38 KJm\(^{-3}\).

3.4.1. Size-strain plot (SSP)

Williamson-Hall method actually considers the broadening of peaks as a function of diffraction angle (20), which is assumed to be combined effect of size induced broadening and strain induced broadening. But there are models, which deals with the peak profile analysis. Size-Strain plot (SSP) is one such method, which considers that XRD peak profile is a combination of Lorentzian function and Gaussian function, where size broadened XRD profile is labelled as a Lorentz function and strain broadened profile is labelled as Gaussian function [21]. So, the total broadening of SSP can be expressed as

\[ \beta_{hkl} = \beta_L + \beta_G \]

Where \(\beta_L\) and \(\beta_G\) are the peak broadening due to Lorentzian and Gaussian function respectively.

Further, SSP method always provides a better result for isotropic broadening, as it gives more importance to low angle reflections, where the accuracy and precision are more, than that in higher angles. This is because, at higher angles, XRD data are of lower quality and peaks are generally highly overlapped at higher diffracting angles.

So, the SSP calculation is performed using the equation [38], as follow

\[ (d_{hkl})^2 = \frac{k \lambda}{D} (d_{hkl})^2 + \frac{\varepsilon^2}{4} \]  \hspace{1cm} (17)

where \(d_{hkl}\) is the lattice distance between the (hkl) planes and for the cubic crystal,

\[ d_{hkl}^2 = \frac{a^2}{h^2 + k^2 + l^2} \]  \hspace{1cm} (18)

Now, using equation (17), a plot is drawn with \((d_{hkl}, \beta_{hkl, \text{cos} \theta})\) term along X-axis and \((\beta_{hkl}, \beta_{hkl, \text{cos} \theta})^2\) along Y-axis corresponding to each diffraction peak, which is shown in Fig. 6. The slope of the straight line provides the average size as 38.09 nm, whereas the intercept gives the intrinsic strain of the CdSe nanocrystals as \(1.78 \times 10^{-3}\).

3.4.2. Halder-Wagner Method

In the SSP method, the size broadening of the XRD peak profile has been assumed as a Lorentzian function, whereas strain broadening, as Gaussian function. But actually, XRD peak is neither Lorentzian function nor Gaussian function, as XRD peak region matches well with the Gaussian function, whereas its tail falls off too rapidly without matching and on the other hand, tails of the profile fits quite well with Lorentz function, but that fails to match the XRD peak region [39,40].

So, to overcome this difficulty, the Halder-Wagner method is used, which is based on the assumption that peak broadening is a symmetric Voigt function [40,41], as it is a convolution of Lorentzian function and Gaussian function [21]. So, for Voigt function, the full width at half maximum of the physical profile can be written as per Halder-Wagner Method as

\[ \beta_{hkl} = \beta_L + \beta_G \]  \hspace{1cm} (19)

Where, \(\beta_L\) and \(\beta_G\) are the full width at half maximum of the Lorentzian and Gaussian function. This method has the advantage that it gives more weight to the peaks at low and mid angle range, where the overlapping of the diffracting peaks is very less. Now, the relation between the crystallite size and lattice strain according to Halder-Wagner Method is given by,

\[ \left( \frac{\beta_{hkl}}{d_{hkl}} \right)^2 = \frac{1}{D} \beta_{hkl}^2 + \frac{\varepsilon^2}{4} \]  \hspace{1cm} (20)

Fig. 5. UDEDM plot for CdSe nanoparticles.
Where $\beta_{hkl} = \beta_{hkl} \cos \theta / \lambda$ and $d_{hkl} = 2d_{hkl} \sin \theta / \lambda$.

Plot of equation (20), with $(\beta_{hkl} / d_{hkl}^2)$ term along X-axis and $(\beta_{hkl} / d_{hkl}^2)^2$ along Y-axis for each peak of the XRD pattern, is shown in Fig. 7. The slope of the plotted straight line provides the average size, whereas the intercept gives the intrinsic strain of the CdSe nanocrystals. The average particle size has been calculated from the plot as 36.67 nm, which matches well with that obtained from SSP model, whereas calculated value of strain from Halder-Wagner plot is found out to be $5.61 \times 10^{-3}$, which is about 5 times more than the strain value obtained from other models as discussed above. This increase in estimated strain value is actually because of the contribution of low and mid angle XRD data. Further, calculated higher value of strain as obtained in Halder–Wagner method, may be attributed to the lattice dislocations [41], which play a significant role in broadening of the reflection peaks at lower angles.

**Table 1** provides all the calculated values of average size and the intrinsic strain, including other elastic parameter. It is clear from this table that average size calculated from UDED, SSP and H–W method are comparable.

### 3.5. Morphological study

#### 3.5.1. HR-TEM study

Morphology of CdSe nanoparticles has been studied by TEM (JEOL JEM-2100 model instrument) operating at 200 kV of accelerating voltage. Fig. 8(a) shows the HRTEM image of the prepared CdSe nanoparticles, along with the particle-size distribution graph as in Fig. 8(b). The average particle size has been obtained from the size distribution graph as 36.23 nm and that is in good agreement with average size obtained from UDED, SSP and H–W method with a variation less than 5%. Fig. 8(c) shows the HR-TEM image of a single CdSe nanoparticle and Fig. 8(d) gives the inter-planar spacing of 0.412 nm for (111) reflection plane showing edge dislocation of this plane.

#### 3.5.2. AFM analysis

Morphology and the surface texture analysis of chemically synthesized CdSe nanocrystals have been studied using the atomic force microscopy (AFM), which has been carried out by a Bruker AFM, Model: INOVA. For this, the sample has been prepared by spin coating deposition on a silicon wafer. For spin coating, water is taken as solvent and for evaporation to take place, the sample is kept at room temperature for almost 5 h. Fig. 9 shows the 3D AFM micrograph of the CdSe nanocrystals, which reveals the average particle size of the CdSe nanoparticles as 38.5 nm.

Additionally, it is also apparent from the 3D image that the surface is very dense and particles are dispersed uniformly, having an average roughness (Ra) of the surface as 3.6 nm. This average roughness is very useful for understanding the general variation in the height profile, which is actually the mean height as computed over the entire area. Surface texture of the sample is the irregularities in the surface, which mainly comprises of roughness, waviness and flaws. Fig. 10 shows the texture, waviness and average roughness analysis over the $6 \times 6 \mu m^2$ area...
Table 1
Geometrical parameters of chemically prepared CdSe nanoparticles using different Models.

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<tr>
<th>Scherrer Method</th>
<th>Williamson-Hall Method</th>
<th>Size-Strain Plot</th>
<th>Halder Wagner Method</th>
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<td></td>
<td>UDM</td>
<td>UDDM</td>
<td>UDEDHM</td>
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<td>Size D (nm)</td>
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<td>44.47</td>
<td>41.36</td>
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Fig. 8. (a) HR-TEM image of prepared CdSe nanoparticles. (b) Size distribution graph. (c) HRTEM image showing spherical morphology. (d) Interplanar spacing of CdSe nanoparticle of (111) plane showing edge dislocation of (111) plane.

area of the CdSe nanoparticles. The result of AFM study, regarding the average size is in per with the XRD result.

3.5.3. SEM study
Finally, the particle size, along with surface morphology of CdSe nanoparticles has been investigated by field emission scanning electron microscopy (FE-SEM), having Model no. - Sigma 300, Carl Zeiss. Fig. 11 shows the FE-SEM image, containing nanoparticles of uniform size distribution, with an average size of 36.2 nm. The particle size calculated from the FE-SEM image is in close agreement with TEM data and AFM data. All the calculated values of the average particle size as calculated from TEM, AFM and FE-SEM are given in Table 2.

Fig. 12 shows the distribution of the average particle size, as calculated from different models using the XRD peak broadening and from different morphological study. It has been observed that particle size estimated from the UDEDHM, SSP and H-W method, which are in the range of 36 nm–39 nm, shows a good resemblance with the average particle size calculated from the morphological study using HR-TEM, AFM and FE-SEM. So, it may be concluded that the average particle size of chemically synthesized CdSe nanoparticles lies in between 36 and 39 nm.

4. Conclusion

MPA capped CdSe nanoparticles have been prepared by chemical route, which is further studied through X-ray diffraction analysis for...
Fig. 9. AFM micrograph of chemically synthesized CdSe nanoparticles.

Fig. 10. Texture and roughness analysis of CdSe nanoparticles using AFM.

their crystallinity and structural properties. XRD peak broadening analysis has been performed to calculate the various elastic properties of the CdSe nanocrystals such as intrinsic strain, stress, energy density, using Scherrer plot, different models of Williamson-Hall plot, Size-Strain Plot and Halder-Wagner Method, along with the determination of the average particle size. The average particle size of CdSe nanoparticles from the TEM and SEM study has been found as 36.23 nm and 36.2 nm, whereas, that of the spin coated CdSe nanoparticles from AFM study, has been found as 38.5 nm. After comparing all these studies, it has been found that, the average size calculated from Size-Strain Plot and Halder-Wagner Method matches very well with the average size observed in HR-TEM, AFM and SEM studies. Different elastic properties have been

<table>
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<th>Table 2</th>
<th>Average particle size of CdSe nanoparticles from morphology study.</th>
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<tr>
<td>Morphology Study</td>
<td>Average Particle Size (nm)</td>
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<td>TEM</td>
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<tr>
<td>SEM</td>
<td>36.2</td>
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Fig. 11. FE-SEM image of CdSe nanoparticles.

Fig. 12. The distribution of the average particle size calculated from XRD and morphological study.
calculated with the different models of W–H method, such as UDM, USDM and UDEDM models. So far, strain calculation is concerned, SSP provides the best result, whereas W–H method gives a very high value of strain, as because, it considers the contribution of low and mid angle XRD data, along with the attribution from the lattice dislocations. Finally, the distribution of the average particle size, calculated from different models using the XRD peak broadening and the morphological study from HR-TEM, AFM and SEM, show that average size lies in the range 36–39 nm.

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