ABSTRACT

Computational program "Crystal-2" in Visual Basic 6.0 was designed and applied to identify the specification for three crystal structures includes the lattice parameters (a, b, c), the axial angles (α, β, γ), the Filling Factor(FF) foe CdS, the Average Grain Size (AGS) for CdS, and the Elastic Strain (ε) for CdS and CdTe.

This program will give us a complete description on crystal structure for three crystal structures material by inserting a data which include the values of Miller indices (hkl), the diffracted angle (2θ) from ASTM data for cadmium sulfide, beryllium and compare the calculated values with the values of ASTM data used material.

This program is includes many special calculations for a certain material such as cadmium sulfide that used to examine the cubic system and calculated lattice parameters were found to be a ≈ 5.82 Å, b ≈ 5.83 Å and c ≈ 5.81 Å and there is a drift error about $D \approx \mp 4.365314 \times 10^{-5}$ Å when is compared with the published values, and to examine orthorhombic system by using ASTM data for cadmium sulfide as example the calculated values were found to be a ≈4.169 Å, b ≈ 2.791 Å and c ≈ 5.413 Å, with a drift error about $D \approx \mp 8.28014 \times 10^{-4}$ Å, also the tetragonal system is also examined for beryllium and the calculated values were found to be a ≈ 1.36 Å, b ≈ 1.36 Å, and c ≈ 3.58 Å with a drift error $D \approx \mp 5.743535 \times 10^{-4}$ Å, and the average grain size is also calculated for CdS by using the Scherrer's formula ,the filling factor is determined for Cadmium Sulfide, and the elastic strain by using the Hall-Williamson method for CdS and CdTe.

Acknowledgments

Appendix -1-
A computational program to determine some of crystal structure specification.

Public TTH(100) As Single
Public H(100) As Single
Public K(100) As Single
Public L(100) As Single
Public TH(100) As Single
Public Alpha(100) As Single
Public Beta(100) As Single
Public Gamma(100) As Single
Public A1(100, 101) As Single
Public X(100) As Single
Public Delta(100) As Single
Public AL(100) As Single
Public BE(100) As Single
Public GA(100) As Single
Public DIS As Single
Public w, y, r As Single
Public a, b, c As Long

- Calculations of the lattice parameters (a, b, c):

Private Sub Command1_Click()
Text1.Text = 30
Text2.Text = 0.00001
Text3.Text = 1.7889
N = Val(Text1.Text)
d = Val(Text2.Text)
lemda = Val(Text3.Text)
PI = 4 * Atn(1)
M = 4
TTH(1) = 23.19: H(1) = 1: K(1) = 1: L(1) = 0
TTH(2) = 25.26: H(2) = 0: K(2) = 2: L(2) = 0
TTH(3) = 27.3: H(3) = 1: K(3) = 1: L(3) = 1
TTH(4) = 28.85: H(4) = 0: K(4) = 0: L(4) = 2
TTH(5) = 29.18: H(5) = 0: K(5) = 2: L(5) = 1
TTH(6) = 37.28: H(6) = 1: K(6) = 1: L(6) = 2
TTH(7) = 38.75: H(7) = 0: K(7) = 2: L(7) = 2
TTH(8) = 39.35: H(8) = 2: K(8) = 0: L(8) = 0
TTH(9) = 43.38: H(9) = 1: K(9) = 3: L(9) = 0
TTH(10) = 47.42: H(10) = 2: K(10) = 2: L(10) = 0
TTH(11) = 49.56: H(11) = 2: K(11) = 0: L(11) = 2
TTH(12) = 49.56: H(12) = 2: K(12) = 2: L(12) = 1
TTH(13) = 51.33: H(13) = 0: K(13) = 2: L(13) = 3
TTH(14) = 52.03: H(14) = 0: K(14) = 4: L(14) = 0

```
For I = 1 To N
TH(I) = TTH(I) / 2
Next I
For I = 1 To N
TH1 = TH(I) * PI / 180
ALpha(I) = (lemda * H(I)) ^ 2
Beta(I) = (lemda * K(I)) ^ 2
Gamma(I) = (lemda * L(I)) ^ 2
Delta(I) = (0.5 * Cos(TH1) ^ 2) * ((1 / Sin(TH1))) + 1 / TH1
Next I
S11 = 0: S12 = 0: S13 = 0: S14 = 0: S15 = 0
S21 = 0: S22 = 0: S23 = 0: S24 = 0: S25 = 0
S31 = 0: S32 = 0: S33 = 0: S34 = 0: S35 = 0
S41 = 0: S42 = 0: S43 = 0: S44 = 0: S45 = 0
For I = 1 To N
T = TH(I) * PI / 180
z = Sin(T) ^ 2
S11 = S11 + ALpha(I) ^ 2
S12 = S12 + ALpha(I) * Beta(I)
S13 = S13 + ALpha(I) * Gamma(I)
S14 = S14 + ALpha(I) * Delta(I)
S15 = S15 + ALpha(I) * z
S22 = S22 + Beta(I) ^ 2
S23 = S23 + Gamma(I) * Beta(I)
S24 = S24 + Delta(I) * Beta(I)
S25 = S25 + z * Beta(I)
S33 = S33 + Gamma(I) ^ 2
S34 = S34 + Gamma(I) * Delta(I)
S35 = S35 + Gamma(I) * z
S44 = S44 + Delta(I) ^ 2
S45 = S45 + z * Delta(I)
Next I
'-------------------------------------------------------------------------------
'Generate Matrix of size M AND M+1 COLUMNS
'-------------------------------------------------------------------------------
A1(1, 1) = S11: A1(1, 2) = S12: A1(1, 3) = S13: A1(1, 4) = S14: A1(1, 5) = S15
A1(2, 1) = S12: A1(2, 2) = S22: A1(2, 3) = S23: A1(2, 4) = S14: A1(2, 5) = S25
A1(3, 1) = S13: A1(3, 2) = S23: A1(3, 3) = S33: A1(3, 4) = S34: A1(3, 5) = S35
A1(4, 1) = S14: A1(4, 2) = S24: A1(4, 3) = S34: A1(4, 4) = S44: A1(4, 5) = S45
For K1 = 1 To M - 1
For I = K1 + 1 To M
A2 = A1(I, K1) / A1(K1, K1)
For j = 1 To M + 1
A1(I, j) = A1(I, j) - A2 * A1(K1, j)
Next j
Next I
```

```
Next K1
For I = 1 To M
For j = 1 To M + 1
If Abs(A1(I, j)) < d Then A1(I, j) = 0
Next j: Next I
X(M) = A1(M, M + 1) / A1(M, M)
For K1 = 2 To M
I = M + 1 - K1
s = 0
For j = I + 1 To M
s = s + A1(I, j) * X(j)
Next j
X(I) = (A1(I, M + 1) - s) / A1(I, I)
Next K1
A0 = X(1)
B0 = X(2)
C0 = X(3)
d0 = X(4)
AP = 1 / (2 * A0 ^ 0.5)
BP = 1 / (2 * B0 ^ 0.5)
cp = 1 / (2 * C0 ^ 0.5)
Text7.Text = Round(AP, 2)
Text8.Text = Round(BP, 2)
Text9.Text = Round(cp, 2)
 Text4.Text = AP
 Text5.Text = BP
 Text6.Text = cp
 a = Int(AP)
 b = Int(BP)
 c = Int(cp)
 'Text7.Text = a
 'Text8.Text = b
 'Text9.Text = c
 Text10.Text = d0


'*************************************************************************
************

End Sub

Private Sub Command2_Click()
Form3.Show
End Sub
```

```
Private Sub Command3_Click()
End
End Sub

Private Sub Command4_Click()
Form1.Show
End Sub

Private Sub Text1_Click()
Dim H1 As Integer
Text1.Text = H1
End Sub




Private Sub Text2_Click()
Dim d As Integer
Text2.Text = d


End Sub

Private Sub Text3_Click()
Dim w1 As Integer
Text3.Text = w1

End Sub
```

- Calculations of the axial angles (α, β, γ):

```
Private Sub Command1_Click()
PI = 4 * Atn(1)
M = 4
N = Val(Form2.Text1.Text)
a = Val(Form2.Text7.Text)
b = Val(Form2.Text8.Text)
c = Val(Form2.Text9.Text)
For I = 1 To N
TH1 = TH(I) * (PI / 180)
H1 = 1: K1 = 3: L1 = 3
HA = H1 / a: KB = K1 / b: LC = L1 / c
HKL = (HA ^ 2 + KB ^ 2 + LC ^ 2) ^ (0.5)
DIS = 1 / HKL
E1 = DIS * (HA)
E2 = (1 - E1 ^ 2) ^ 0.5
E3 = E2 / E1
```

```
AL(I) = Atn(E3)
H1 = 1: K1 = 3: L1 = 3
HA = H1 / a: KB = K1 / b: LC = L1 / c
HKL = (HA ^ 2 + KB ^ 2 + LC ^ 2) ^ (0.5)
DIS = 1 / (HKL)
F1 = DIS * (KB)
F2 = (1 - F1 ^ 2) ^ 0.5
F3 = F2 / F1
BE(I) = Atn(F3)
H1 = 1: K1 = 3: L1 = 3
HA = H1 / a: KB = K1 / b: LC = L1 / c
HKL = (HA ^ 2 + KB ^ 2 + LC ^ 2) ^ (0.5)
DIS = 1 / (HKL)
V1 = DIS * LC
V2 = (1 - V1 ^ 2) ^ (0.5)
V3 = V2 / V1
GA(I) = Atn(V3)

RD = 180 / PI
w = (AL(I) * 2) * RD
y = (BE(I) * 2) * RD
r = (GA(I) * 2) * RD

Form3.Text1.Text = (w)
 Form3.Text2.Text = (y)
Form3.Text3.Text = (r)

Next I
If (a <> b) And (b <> c) And (w <> y) And (w <> r) And (y <> r) Then reply =
MsgBox("     Triclinic system  ", vbOKCancel, "result")
If reply = vbOK Then Form8.Show
If (a <> b) And (a <> c) And (b <> c) And (w = 90) And (w = y) And (r <> 90) Then
MsgBox (" Monoclinic system   "), , "result"
If (a <> b) And (a <> c) And (b <> c) And (w = y) And (w = r) Then MsgBox ("
orthorhombic system        "), , "result"
If (a = b) And (a <> c) And (w = y) And (w = r) Then MsgBox ("    Tetragonal system
"), , "result"
If (a = b) And (a = c) And (w = y) And (w = r) Then reply = MsgBox("     cubic system
", vbOKCancel, "   Result   ")
If reply = vbOK Then Form7.Show
If (a = b) And (a <> c) And (w = y) And (w = 90) And (r = 120) Then MsgBox
("Hexagonal system"), , "result"
If (a = b) And (a = c) And (w <> 90) And (y <> 90) And (r <> 90) And (w = r = y <> 90)
Then reply = MsgBox("    rhombohedral system      ", vbOKCancel, "  Result  ")
'MsgBox ("ggggggggggg"), , "result"
```

```
End Sub

Private Sub Command2_Click()
Form4.Show
End Sub

Private Sub Command3_Click()
End
End Sub

Private Sub Command1_Click()
```
- Calculations of the average grain size (AGS):
```
lmda = Val(Text13.Text)
Q = Val(Text14.Text)
band = Val(Text15.Text)
AGS = (0.9 * lmda / (band * Cos(Q)))
Text1.Text = AGS
'MsgBox (AGS), , "The Av. grain size ="
End Sub

Private Sub Command2_Click()
Form5.Show
End Sub

Private Sub Command3_Click()
End
End Sub

Private Sub Command4_Click()
Form3.Show
End Sub

Private Sub Text13_Click()

Text13.Text = H2

End Sub

Private Sub Text14_Click()
Text14.Text = n3
End Sub

Private Sub Text15_Click()
Text15.Text = n4
End Sub
```

```
Private Sub Command1_Click()
    • Calculations of the filling factor (FF) and the elastic strain (ε):
PI = 4 * Atn(1)
R1 = Val(Text16.Text)
R2 = Val(Text17.Text)
n1 = Val(Text18.Text)
n2 = Val(Text19.Text)
TV = a * b * c
vo1 = (4 / 3) * PI * ((R1) ^ 3) * n1
vo2 = (4 / 3) * PI * ((R2) ^ 3) * n2
FF = ((vo1 + vo2) / TV) * 100
'MsgBox (FF), , "The filling factor ="
Text1.Text = FF

End Sub

Private Sub Command2_Click()
Form6.Show
End Sub

Private Sub Command3_Click()
End
End Sub

Private Sub Command4_Click()
Form4.Show
End Sub

Private Sub Text16_Click()
Text16.Text = N5
End Sub

Private Sub Text17_Click()
Text17.Text = n6
End Sub

Private Sub Text18_Click()
Text18.Text = n7
End Sub

Private Sub Text19_Click()
Text19.Text = n8
End SubPrivate Sub Command1_Click()
Form9.Show
End Sub
```

```
Private Sub Command2_Click()
End
End Sub

Private Sub Command3_Click()
Form5.Show
End Sub
Private Sub Command1_Click()
Form3.Show
End Sub
Private Sub Command1_Click()
End
End Sub
```

4.1 Conclusion:

This chapter is demonstrating the main conclusions obtained from the results which can be extracted from designing a computer program that determine the crystal structure. We improved this program from its original formula and we conclude the following statements:

1. The accurate determination of the lattice parameters (a, b, c) by using the least square method and fitting the values by the fitting least squares method, and the calculation of the axial angles (α, β, γ) by using equation 2.8 axial angles and by demanding the (hkl) for a certain plane.

2. The average grain size (AGS) by demanding the bandwidth and the diffracted angle (θ) for the CdS X-ray chart by using Scherrer's formula as in equation 2.25.

3. The filling factor (FF) by taking into account the number of atoms per unit cell and the radius atom those consist the material for CdS using equation 2.26 which is in the BCC.

4. The elastic strain (ε) from Hall-Williamson method AS IN EQUATION 2.29 by plot a graph between $(\dfrac{\beta_{1/2}\cos\theta}{\lambda})$ and $(\dfrac{2\sin\theta}{\lambda})$ for the most intense peak for CdS X-ray diffraction chart the peak are (100) and (002) and for CdTe X-ray diffraction chart the peaks are (111) and (220).

4.2 Future work:

1. Determine the lattice types for other crystal systems.
2. Determine the structure factor.

1.1 Introduction:

A crystal is a solid materials which composed of certain atoms those are arranged in an ordering repetitive array and posses a short and along range order the general features of solid materials classified into amorphous and crystalline the last one is divided into polycrystalline and single crystal [1].

1. Amorphous: are solid materials which have irregular arrangement of atoms over relatively large atomic distance, and amorphous (meaning literally without form). Therefore amorphous materials are characterized by atomic or molecular structure that are relativity complex and become ordered only with some difficulty. The producing of amorphous is very simple through different technique such as different deposition technique especially on the substance has amorphously state. The ordering in amorphous solids is limited to a few molecular distances represented by short range order.

2. Crystalline

   A: Single crystal: in which the arrangement of atoms are perfectly repeated or extend throughout the entirely of specimen without interruption, in other words, it posses along range order and all unit cells interlock in the same way and have the same orientation, a photograph of several single crystal is shown in figure 1.1.[1]

Fig.1.1 Explain a photograph of several single crystal of fluorite CaF_2 [1].

B: Polycrystallines: which are composed of a collection of many different crystalline on it cell. Various stages in the solidification of a polycrystalline are represented in figure 1.2 [1].

Initially, small crystals form at various positions these have random crystallographic orientations so it contains a short and long range order in both crystalline and amorphous solids forms depends on the ease with which a random atomic structure can transform to an ordered state during solidification. The above crystalline types are distinguished by the size of ordered regions with the materials.

In polycrystalline, the solid is made-up of grains which are highly ordered crystalline regions of irregular size orientation. Single crystal has long-range order, in which the special atomic arrangement extends throughout the entire material. Many important properties of materials are found to depend on the structure of crystals [1]. The producing of polycrystalline phase is simpler than the single crystal and it can be noticed in the powder technology and thin films and such alloys, whereas its properties is better than the amorphous state but is not efficient with respect to single crystal, that is return to the grains and grain boundaries
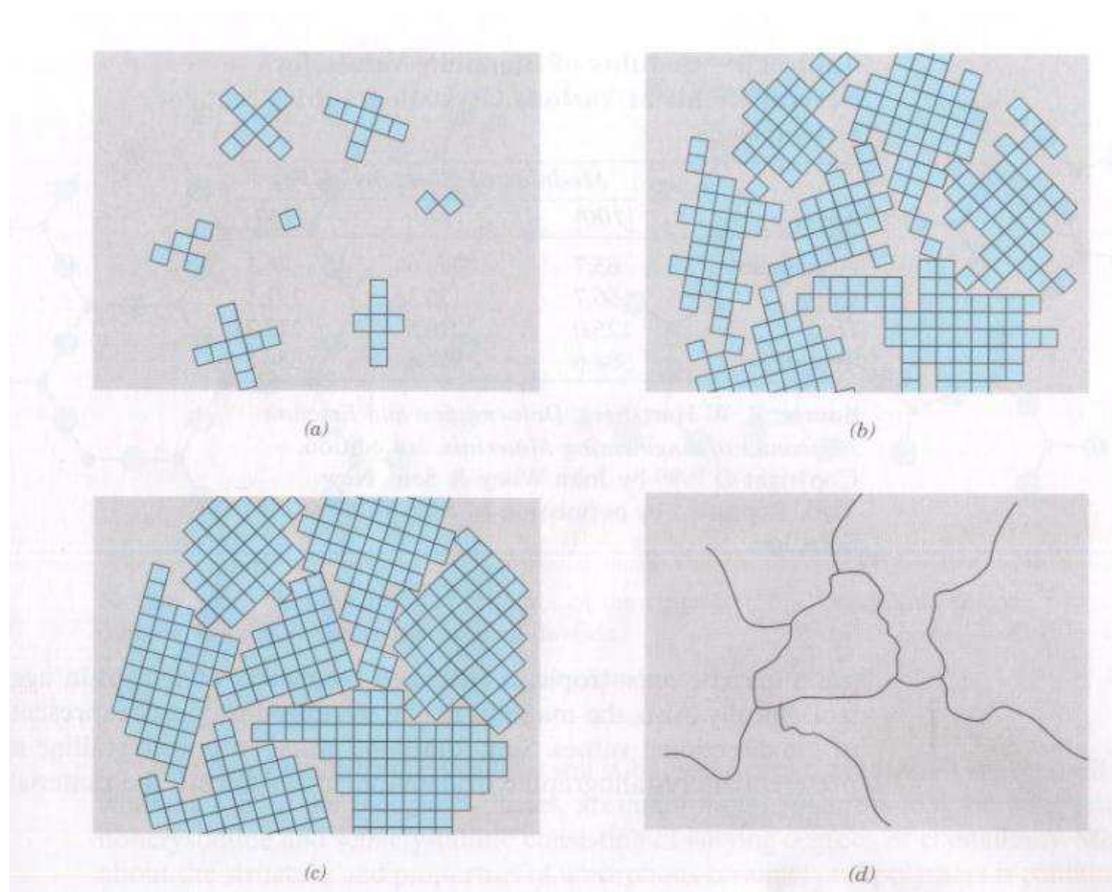
Fig. 1.2 shows a schematic diagram of the stages in the solidification of a polycrystalline materials.(a) small crystallite nucleai.(b) growth of the crystallites. (c) Up on completion of solidification, grains having irregular shapes have formed, (d) the grain structure as it would appear under the microscopic as dark lines [1].

1.2 Crystal structure of cadmium sulfide:

Cadmium sulfide (CdS) is an important II-VI compound semiconductor with an energy band gap of 2.42 eV, and can be used for fabrication of optoelectronic devices such as large area solar cells, laser diodes, and optical switches, Group V–VI compounds have widely been studied because of their excellent properties like photoconductivity, photosensitivity and thermoelectric power.

The absorption coefficient of the order of 104 to 105 cm−1 the low intensity and broad diffraction peak shows that the as-deposited thin films are either nanocrystalline and/or amorphous in nature. The diamond structure may be viewed as two fcc structures displaced from each other by one-quarter of a body diamond. The cubic cadmium sulfide structure result when Cd atoms are placed on one fcc lattice and S atoms on the other fcc lattice, as in figure 1.3 the coordinates of Cd atoms are $000; 0\frac{1}{2}\frac{1}{2}; \frac{1}{2}0\frac{1}{2}; \frac{1}{2}\frac{1}{2}0;$ the coordinates of the S atoms are $\frac{1}{4}\frac{1}{4}\frac{1}{4}; \frac{1}{4}\frac{3}{4}\frac{3}{4}; \frac{3}{4}\frac{1}{4}\frac{3}{4}; \frac{3}{4}\frac{3}{4}\frac{1}{4}$ [2].

o Cd

•   S

Fig.1.3 Crystal structure of cubic Cadmium Sulfide [2].

1.3 Crystal structure of cadmium telluride:

Polycrystalline thin-film CdTe has applications due to its near-optimum band gap, high absorption coefficient, and relative ease of film formation. CdTe deposited by a variety of techniques over a wide range of deposition temperatures, bonding in the II–VI and III–V compound semiconductors such as CdTe, there is no clear evidence for the valence electron distribution in the valence electrons in CdTe represents the localized nature of the valence electron.

Experimental observations for the localized valence electrons in CdTe is not easy because of the difficulties in growing high quality single phase single crystals because of its large X-ray absorption effects and large numbers of core electrons relative to only a few valence electrons. CdTe single crystal growth has mostly been focused on the preparation of bulk crystals of appreciable size and on epitaxial fields. However control of the electrical properties of this material has not yet been achieved as in figure 1.4 [3].

- Te
o Cd

Fig.1.4 crystal structure of cadmium telluride CdTe [3].

1.4 Crystal structure of beryllium:

Beryllium is a unique metal with unusual properties of technological and scientific importance. Its physical properties are useful to the nuclear power industry (as a neutron multiplier), beryllium exhibits an unusually high Debye temperature that leads to a large specific conductance and has thus been identified as a "hyperconductor" with favorable properties for efficient transmission of electrical power. This combination of unique properties and unusual behavior contribute to the characterization of beryllium as an "anomalous" metal. Scientifically beryllium has been the subject of a great deal of interest because of its simple atomic configuration and anomalous behavior, beryllium have hcp, bcc, and liquid phase as in figure 1.5 [4].
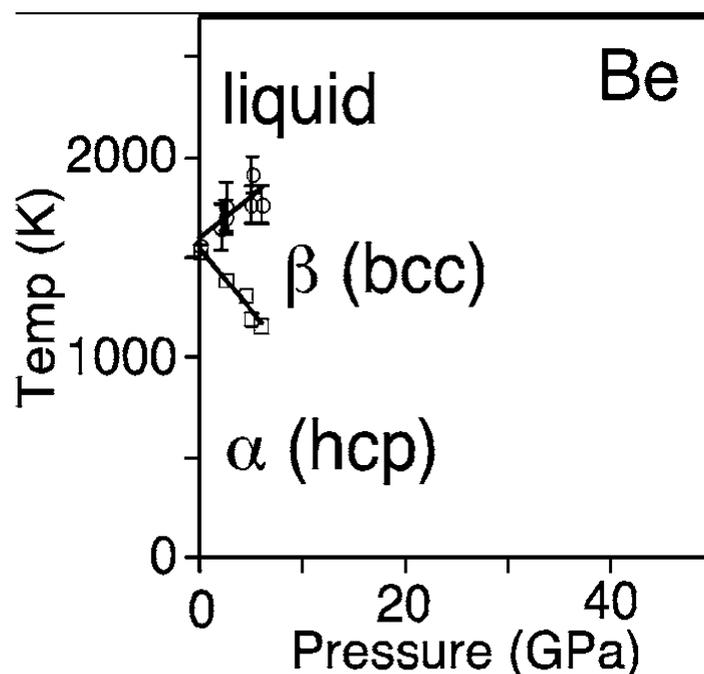

Fig.1.5 Phase diagram of beryllium the hcp, bcc, and liquid phase lines [4].

Fig.1.6 Phase diagram of beryllium the a) hcp, b) bcc [4].

1.5 Laue's Diffraction Law:

Laue's equations for diffraction are deal with the diffraction between atoms, and it is equivalent to Bragg's law for diffraction. There are three Von Laue equations for a crystal with cell parameters (a, b, c),

$$a(\cos\alpha - \cos\alpha_\circ) = h\lambda$$
$$b(\cos\beta - \cos\beta_\circ) = k\lambda \qquad\qquad (1.1)$$
$$c(\cos\gamma - \cos\gamma_\circ) = l\lambda$$

Where $\alpha_\circ$, $\beta_\circ$, and $\gamma_\circ$ are the angles of the incident ray, and α, β, and γ are the angles of the reflected ray. $\cos\alpha_\circ$, $\cos\beta_\circ$, $\cos\gamma_\circ$ are the direction cosines or orthogonal of the incident ray and $\cos\alpha$, $\cos\beta$, $\cos\gamma$ are the direction cosines or orthogonal of the reflected ray in the crystal axis So, we must also satisfy

$$\cos^2\alpha_\circ + \cos^2\beta_\circ + \cos^2\gamma_\circ = 1$$
$$\qquad\qquad (1.2)$$
$$\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1$$

Using that the angle between the incident and reflected ray is (2θ)

$$2\cos 2\theta = \cos\alpha\cos\alpha_\circ + \cos\beta\cos\beta_\circ + \cos\gamma\cos\gamma_\circ \qquad\qquad (1.3)$$

By squaring equation (1.3) we get

$$\frac{h^2\lambda^2}{a^2} = \cos^2\alpha - 2\cos\alpha\cos\alpha_\circ + \cos^2\alpha_\circ$$

$$\frac{k^2\lambda^2}{b^2} = \cos^2\beta - 2\cos\beta\cos\beta_\circ + \cos^2\beta_\circ \qquad (1.4)$$

$$\frac{l^2\lambda^2}{c^2} = \cos\gamma - 2\cos\gamma\cos\gamma_\circ + \cos^2\gamma_\circ$$

So that

$$\left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right]\lambda^2 = 1 - 2(\cos\alpha\cos\alpha_\circ + \cos\beta\cos\beta_\circ + \cos\gamma\cos\gamma_\circ) + 1 \qquad (1.5)$$

$$\left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right]\lambda^2 = 2(1 - \cos 2\theta) \qquad (1.6)$$

$$\left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right]\lambda^2 = 4\sin^2\theta \qquad (1.7)$$

Taking into account the square root of the equation (1.7) one can conclude the following equation

$$\lambda\left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right]^{\frac{1}{2}} = 2\sin\theta \qquad (1.8)$$

Which is the same as Bragg equation mentioned for it's order of diffraction by considering that for tetragonal and orthorhombic structure

$$d_{hkl} = \frac{1}{\sqrt{\dfrac{h^2}{a^2} + \dfrac{k^2}{b^2} + \dfrac{l^2}{c^2}}} \qquad (1.9)$$

So, only at a certain location will be constructive interference – get a set of bright spots in the diffraction pattern and, with lots of patience and effort, can use them to deduce the crystal lattice structure [5].

3.1 Introduction:

In this chapter the efficiency of this program was examined by the application for many materials data and discuses the results conclude in comparable with the standard values investigated in previous references. For some materials the most important role contains the successful of the main program construction represented by the calculation of the lattice parameters (a, b, c), and the axial angles between them (α, β, γ), those parameters give more details about the identification of the crystal system. In order to develop this program from the last program applied in previous references [6]. The values of filling factor, the average grain size and the elastic strain from a certain input data concluded from X-ray chart applied by diffractometer apparatus were calculated for certain materials.

3.2 The Identification of crystal structure:

When the beam of X-ray with wavelength (λ) incident on a surface of a certain material whether if it is thin film or bulk materials, there are many diffracted angles (2θ), applied as a function of different scattering intensity which represent the planes contains in the crystal structure defined by Miller indices. Through the intensity the diffraction angles (2θ) and the dependent Miller indices the lattice parameters of the crystal structure can be calculated based physically on the concept of Bragg's law. The data applied for (CdS) thin film as shown in table 3.1 [24]. The program produce the following data (a, b, c) and (α, β, γ) and defining the type of crystal structure in comparable with the data obtained from the ASTM data sheet labeled by the card number 10-0454 [24].

The proof of the successful our program represented by the following points:

1) The coincidence of the calculated values (a,b,c) with theoretical values.

2) The minimization of the drift error (D) that emplized the accuracy of calculated lattice constant with the theoretical values.

3) The investigation of angles between axis (α, β, γ), those emplized the type crystal structure mentioned above.

Table 3.1 Indicates the ASTM data of CdS represented by card number 10-0454 [24].

λ =1.5418 Å					
a=b=c = 5.82 Å					
$\alpha = \beta = \gamma$ =90°					
$2\theta°$	intensity	hkl	$2\theta°$	intensity	hkl
26.506	100	111	81.004	30	422
30.807	40	200	86.905	30	511
43.960	80	220	97.060	5	440
52.132	60	311	102.89	20	531
54.581	10	222	113.99	5	620
64.029	20	400	120.54	5	533
70.357	30	331	141.86	10	711
72.802	10	420			

The calculated values of CdS are a=5.82 Å, b = 5.83 Å, c = 5.81 Å, and a drift error D= 4.365314 $\times 10^{-5}$, and the calculated angles are ($\alpha = \beta = \gamma = 90°$), for a cubic system.

The expert on another type of Bravais lattice such as orthorhombic system was applied through the data that listed in table 3.2 for cadmium sulfide (CdS) those were mentioned in the ASTM-card number 40-1049 [25]. The operating of the program exhibited the calculated lattice parameters as follow: a=4.169 Å, b=2.791 Å, c=5.413 Å, with a drift error about D=$\pm 8.28014 \times 10^{-4}$ Å, and the angles between axis (α, β, γ), are defined as $\alpha = \beta = \gamma = 90°$, for orthorhombic system.

Table 3.2 includes the ASTM data of CdS represented by card number 40-1049 [25].

λ =1.54056 Å a = 3.711 Ǻ b =2.201 Ǻ c = 6.719 Ǻ					
2θ°	intensity	hkl	2θ°	intensity	hkl
24.807	62	100	77.855	2	204
26.507	91	002	80.237	9	300
28.182	100	101	83.252	14	213
36.620	29	102	86.308	7	302
43.681	48	110	91.495	8	205
47.839	50	103	96.162	3	220
50.882	8	200	102.26	5	222
51.824	31	112	102.87	6	116
52.796	15	201	104.52	2	304
54.584	5	004	107.64	9	215
58.278	3	202	112.33	4	107
60.839	3	104	115.85	7	313
66.772	15	203	118.45	3	400
69.264	5	210	120.16	2	401
70.862	8	211	126.28	2	216
72.382	4	114	135.48	4	403
75.478	9	105	141.21	4	321

The Tetragonal phase of Beryllium (Be) also used in such a way to prove the successful of our program through the dependent of ASTM-Card number 01-1291[49], for Beryllium (Be) listed in table 3.3 [26]. It was clear that the obtained results were a=1.36 Ǻ, b=1.36 Ǻ, and c= 3.58 Ǻ, with a drift error D= $\pm 5.743535 \times 10^{-4}$ Ǻ.

Table 3.3 include the ASTM data 0f Beryllium (Be) represented by card number 01-1291 [26].

$(\lambda)=1.54056$ Ǻ a=b=2.285 Ǻ, c=3.584 Ǻ		
2θ°	intensity	hkl
46.034	20	100
50.976	14	002
52.879	100	101
70.783	12	102
85.015	12	110
98.082	12	103
103.62	2	200
106.71	8	112

The presence of difference between the calculated values and the ASTM values and that because the Be is hexagonal phase and also the

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calculated values of the angles (α, β, γ) are not equaling 90° because the equation that we used to calculated the axial angles can only be used for the cubic, tetragonal and the orthorhombic system and for that we have a large value of the drift error in the calculated values. Table 3.4 includes a comparison between the crystal-2 calculated values of certain material with their ASTM data values such as $(Ba_{0.4}Sr_{0.2}Ca_{0.4})TiO_3$ [27], Ag_8Se_6 [28] and $(Ce_3Zn_{22})100U$ [29].

Table 3.4 includes the crystal-2 and the ASTM values.

sample	Crystal-2	ASTM data
$(Ba_{0.4}Sr_{0.2}Ca_{0.4})TiO_3$	a = 3.90 Å b = 3.93 Å c = 3.93 Å D = $\pm 4.901616 \times 10^{-5}$ Å $\alpha = \beta = \gamma = 90°$ Cubic system.	a = 3.910 Å b = 3.910 Å c = 3.910 Å $\alpha = \beta = \gamma = 90°$ Cubic system.
Ag_8Se_6	a = 10.438 Å b = 12.989 Å c = 6.083 Å D = $\pm 1.402066 \times 10^{-3}$ Å $\alpha = \beta = \gamma = 90°$ Orthorhombic system.	a = 10.388 Å b = 12.981 Å c = 6.0499 Å $\alpha = \beta = \gamma = 90°$ Orthorhombic system.
$(Ce_3Zn_{22})100U$	a = 8.924 Å b = 8.920 Å c = 21.377 Å D = $\pm 4.846672 \times 10^{-7}$ Å $\alpha = \beta = \gamma = 90°$ Tetragonal system.	a = 8.930 Å b = 8.930 Å c = 21.36 Å $\alpha = \beta = \gamma = 90°$ Tetragonal system.

3.3 Filling factor (FF):

The investigation of the above formula depends to insert the number of atoms per unit cell, the lattice parameters (a, b, c) and the ionic radius for the used sample such as cadmium sulfide (CdS) the calculated value of the filling factor of (CdS) is about 60.22% that means the CdS is BCC where the value of the filling factor about 68% that means we have error about 7.78 % between the calculated value and the theoretical value.

3.4 Average grain size (AGS):

It was clear from chapter one, that the polycrystalline samples, such as thin film or powder, specified by a different shapes of grain size distributed randomly in the formation of the sample under study. It is necessary to calculate the average value of grain size based on Scherrer's formula represented by equation 2.25, Cadmium Sulfide (CdS) is used to calculate the average grain size by take in to account the most probable intensity of a certain peak mentioned by the angle of diffraction (2θ), and the calculated value of AGS for the CdS is about AGS= 178.24 Ǻ, at diffraction angle θ =13.2°, and the band width was about $\beta_{1/2}$ = 0.0087 rad., with λ = 1.5405 Ǻ. by compared the calculated value of the AGS for CdS with the theoretical value which in range (85 – 205 Ǻ) [30].

3.5 Elastic Strain:

There are many physical parameters used to study the mechanical properties of solid materials, one of these parameters defined by elastic strain (ε). The theoretical formula that was dependent in our research

called Hall-Williamson method are used as mentioned in equation 2.29 was used to determine elastic strain for CdS and CdTe, for CdS, the most intense reflections were (002) and (100) and for CdTe the most intense reflections were (111) and (220) so by plot a graph between, $(\dfrac{\beta_{1/2}\cos\theta}{\lambda})$ and $(\dfrac{2\sin\theta}{\lambda})$ define the slope which is equal to (ε), for CdS the value of the elastic strain is equal to $\varepsilon = 1.0621$ as shown in figure 3.1 , and for CdTe the elastic strain is $\varepsilon = 1.6277$.

Table 3.4 includes the information of the (CdS) X-ray diffraction chart [22].

$(\dfrac{\beta_{1/2}\cos\theta}{\lambda})$	$(\dfrac{2\sin\theta}{\lambda})$	(hkl)
0.0044	0.278	111
0.0054	0.296	002

Table 3.5 includes the information of the (CdTe) X-ray diffraction chart [22].

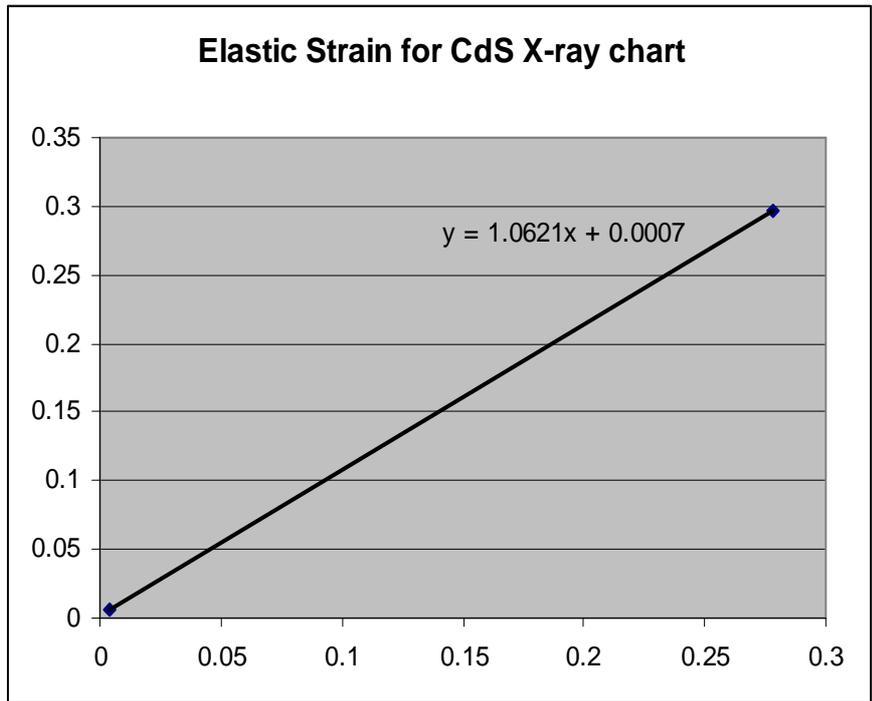| $(\dfrac{\beta_{1/2}\cos\theta}{\lambda})$	$(\dfrac{2\sin\theta}{\lambda})$	(hkl)
0.0033	0.266	111
0.0064	0.434	220

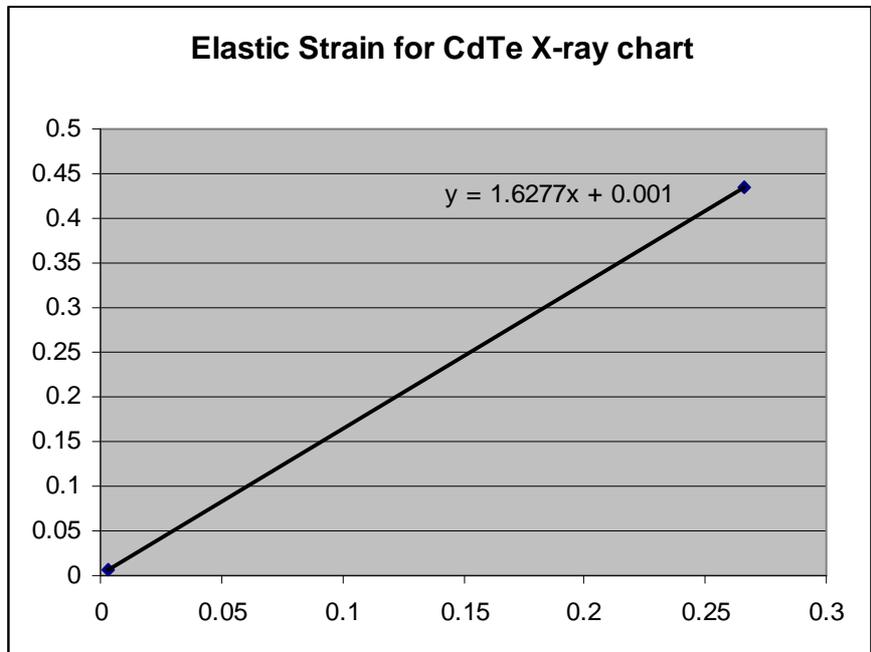Fig. 3.1 Elastic Strain for CdS X-ray chart.

Fig.3.2 Elastic Strain for CdTe X-ray chart.

2.1 Introduction:

The program investigated through our research project that is dealing with the complete definition of crystal structure which named by crystal-2. The process of calculations observed that the angles of Bragg reflections determined by X-ray powder diffraction using various types of analysis. These reflections have been assigned by Miller indices in terms of a particular crystal system, the program crystal-2 evaluates the dimensions of the corresponding crystallographic unit cell, the angles (α, β, γ), the average grain size, the filling factor and the elastic strain.

2.2 The main construction of crystal-2:

To calculate the lattice parameters (a, b, c) we used Cohen's Least Squares method which is a mathematical method that is dependent in the main construction of the program, for the determination of crystal lattice parameters from a set of measured angles of diffraction and corresponding Miller indices [6]. The considerance of calculated position, ($\theta_{calc.}$) with the practical angle of diffraction for a certain Miller indices (hkl) when X-ray beam with a wavelength (λ) irradiates a material is given by:

$$\sin^2 \theta_{calc.} = \left[\frac{\lambda^2}{4a^2} h^2 + \frac{\lambda^2}{4b^2} k^2 + \frac{\lambda^2}{4c^2} l^2 \right] \qquad (2.1)$$

Then the difference between the observed and calculated can be written, when more than one X-ray wavelength is considered, as the angle of diffractions can be represented by the following equation:

$$\sin^2 \theta_{obs.-calc.} = \sin^2 \theta_{obs.} - (Ah^2\lambda_n^2 + Bk^2\lambda_n^2 + Cl^2\lambda_n^2) \qquad (2.2)$$

Where (A,B,C) represent ($\frac{1}{4a^2}$, $\frac{1}{4b^2}$, $\frac{1}{4c^2}$). Whereas (λ_n) refers to an experimentally wavelength. The processing of equation (2.2) showed the presences of two parameters represented by a "drift error" (D), and the extrapolation function (δ) as appeared in equation (2.3)

$$\sin^2 \theta_{obs.-calc.} = \sin^2 \theta_{obs.} - (Ah^2\lambda_n^2 + Bk^2\lambda_n^2 + Cl^2\lambda_n^2 + D\delta) \qquad (2.3)$$

The calculated value of (D) has been normally a very small value may be positive or negative sing.

The method of Least Squares method produced a best values of A, B, and C that satisfy equation (2.3). The rearrangement of equation (2.3) tends to the following equation, by considering that this equation is applied under the minimum condition value of summation

$\sum [\sin^2 \theta_{obs.} - (A\alpha + B\beta + C\gamma + D\delta)]^2$ Where $\alpha = h^2\lambda_n^2$, $\beta = k^2\lambda_n^2$ and $\gamma = l^2\lambda_n^2$. If consider that there is a set of equal values to the summation denotes by (E) then, the partial differentiation of equation can be represented by equation (2.4)

$$\frac{\partial E}{\partial A} = -2\sum \alpha(\sin^2\theta_{obs.} - A\alpha - B\beta - C\gamma - D\delta)$$

$$\frac{\partial E}{\partial B} = -2\sum \beta(\sin^2\theta_{obs.} - A\alpha - B\beta - C\gamma - D\delta)$$

(2.4)

$$\frac{\partial E}{\partial C} = -2\sum \gamma(\sin^2\theta_{obs.} - A\alpha - B\beta - C\gamma - D\delta)$$

$$\frac{\partial E}{\partial D} = -2\sum \delta(\sin^2\theta_{obs.} - A\alpha - B\beta - C\gamma - D\delta)$$

By considering the equation (2.4) has a minimum value as we applied then

$$\frac{\partial E}{\partial A} = 0 \quad : \quad \frac{\partial E}{\partial B} = 0 \quad : \quad \frac{\partial E}{\partial C} = 0 \quad : \quad \frac{\partial E}{\partial D} = 0$$

Hence

$$-2\sum \alpha(\sin^2\theta_{obs.} - A\alpha - B\beta - C\gamma - D\delta) = 0$$

$$-2\sum \beta(\sin^2\theta_{obs.} - A\alpha - B\beta - C\gamma - D\delta) = 0$$

(2.5)

$$-2\sum \gamma(\sin^2\theta_{obs.} - A\alpha - B\beta - C\gamma - D\delta) = 0$$

$$-2\sum \delta(\sin^2\theta_{obs.} - A\alpha - B\beta - C\gamma - D\delta) = 0$$

$$D = \left[(0.5 \times \cos^2 \theta) \times \frac{1}{\sin \theta} + \frac{1}{\theta} \right] \qquad (2.6)$$

Where (D) is the drift error in the calculations of the lattice parameters [19].

The rearrangement of last equations producing equations (2.7) which are:

$$\sum A\alpha^2 + \sum B\alpha\beta + \sum C\gamma\alpha + \sum D\alpha\delta = \sum \alpha \sin^2 \theta_{obs.}$$

$$\sum A\alpha\beta + \sum B\beta^2 + \sum C\beta\gamma + \sum D\beta\delta = \sum \beta \sin^2 \theta_{obs.}$$

$$(2.7)$$

$$\sum A\alpha\gamma + \sum B\beta\delta + \sum C\gamma^2 + \sum D\gamma\delta = \sum \gamma \sin^2 \theta_{obs.}$$

$$\sum A\alpha\delta + \sum B\beta\delta + \sum C\gamma\delta + \sum D\delta^2 = \sum \delta \sin^2 \theta_{obs.}$$

The mathematical solution of equation (2.7) given us the accurate of calculated values of A, B and C and reduced parameters represented by a, b and c which is called the lattice parameters, as well as D the drift error. These equations can be solved by the method mentioned by a previous reference [44]. The calculated values of axial angles (α, β, γ) in the unit cell is also obtained by the following equations; then the determination of lattice constants and the angles (α, β, γ) play an important role in the specification the type of crystal structure belong to Bravais lattice

$$\alpha = \cos^{-1}(\frac{dh}{a})$$

$$\beta = \cos^{-1}(\frac{dk}{b}) \qquad (2.8)$$

$$\gamma = \cos^{-1}(\frac{dl}{c})$$

To fitting the values we get by using the Least-Square Curve- Fitting by assuming that we will be given a table of (n + 1) points which will be fitted with a curve, having an equation of the form

$$P_m(x) = a_m x^m + a_{m-1} x^{m-1} + \ldots\ldots\ldots + a_2 x^2 + a_1 x + a_0 \qquad (2.9)$$

Let us relax the requirements on $P_m(x)$ somewhat by permitting forms other than just polynomials. In general, let us permit the fitted curve to have form

$$P_m(x) = a_m g_m(x) + a_{m-1} g_{m-1}(x) + \ldots\ldots\ldots + a_1 g_1 + a_0 g_0 \qquad (2.10)$$

Where the functions $g_m(x)$ and $g_0(x)$ are assumed to be some known functions of (x).

We can easily return to an mth-degree polynomial as a special case by merely letting

$$g_m(x) = x^m$$

$$g_{m-1}(x) = x^{m-1}$$

$$g_1(x) = x^1$$

$$g_0(x) = 1$$

The functions $g_i(x)$ must all be linearly independent. To prove this statement, suppose that it were not true and that some $g_i(x)$ could be written as a linear combination of some $g_j(x)$ and $g_k(x)$ like this:

$$g_i(x) = b_j g_j(x) + b_k g_k(x) \qquad (2.11)$$

For some constants b_j and b_k. Then we could simply eliminate the $g_i(x)$ term from equation (2.10) altogether, and substitute the right-hand-side of equation (2.11) instead. This is equivalent to adding b_j and b_k to the existing coefficients a_j and a_k. We could eliminate any part of $g_i(x)$ from the expression for $P_m(x)$, equation (2.10) by adjusting a_j and a_k to compensate.

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We can now see that the functions

$$g_m(x) = x^m$$

$$g_{m-1}(x) = x^{m-1}$$

$$g_1(x) = x^1$$

$$g_0(x) = 1$$

are linearly independent, since they can not be obtained from each other by linear combinations.

Let us return to the basic problem, we have a table of (n+1) points, and seek equation (2.10) to match the (n+1) given points in such a way that, if we formed a set of deviations. One for each tabulated x_i ,

$$s_0 = p_m(x_0) - f(x_0)$$
$$s_1 = p_m(x_1) - f(x_1)$$
$$s_2 = p_m(x_2) - f(x_2)$$
$$s_n = p_m(x_n) - f(x_n)$$

Or, in general terms, the set of deviations

$$s_i = p_m(x_i) - f(x_i) \qquad \text{For i} = 0, 1, 2, \ldots\ldots, \text{n} \qquad (2.12)$$

The sum of the squares of these (n+1) deviations should be a minimum:

$$\sum_{i=0}^{n} (s_i)^2 = \text{a minimum} \qquad (2.13)$$

The summation in equation (2.5) can also be written as

$$\sum_{i=0}^{n} (s_i)^2 = \sum_{i=0}^{n} [p_m(x_i) - f(x_i)]^2 \qquad (2.14)$$

$$\sum_{i=0}^{n} (s_i)^2 = \sum_{i=0}^{n} [a_m g_m(x_i) + \ldots\ldots\ldots + a_0 g_0(x_i) - f(x_i)]^2 \qquad (2.15)$$

Let us find the partial derivative of the summation with respect to each of (m+1) variables a_i, and set each of these derivatives equal to zero:

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$$\frac{\partial}{\partial a_0} \sum_{i=0}^{n} (\delta_i)^2 = 0$$

$$\frac{\partial}{\partial a_1} \sum_{i=0}^{n} (\delta_i)^2 = 0$$

$$\frac{\partial}{\partial a_m} \sum_{i=0}^{n} (\delta_i)^2 = 0$$

Or in general terms, we can write

$$\frac{\partial}{\partial a_j} \sum_{i=0}^{n} (\delta_i)^2 = 0 \qquad \text{for } j = 0, 1, 2,\ldots,m \qquad (2.16)$$

The series has a finite number of terms, and so the derivative of a sum is equal to the sum of the derivatives of the terms. Thus we can write equation (2.8) as

$$\frac{\partial}{\partial a_j} \sum_{i=0}^{n} (\delta_i)^2 = \sum_{i=0}^{n} \frac{\partial}{\partial a_j} (\delta_i)^2 = \sum_{i=0}^{n} 2\delta_i \frac{\partial \delta_i}{\partial a^j} = 0$$

Or,

$$\sum_{i=0}^{n} \delta_i \frac{\partial \delta_i}{\partial a_j} = 0 \qquad \text{for } j = 0, 1, 2,\ldots,m \qquad (2.17)$$

The differentiation of any δ_i with respect to a_j is easy when we note that

$$\delta_i = p_m(x_i) - f(x_i)$$
$$= a_m g_m(x_i) + a_{m-1} g_{m-1}(x_i) + \ldots\ldots + a_j g_j(x_i) + \ldots\ldots + a_1 g_1(x_i) + a_0 g_0(x_i) - f(x_i) \quad (2.18)$$

When we differentiate with respect to a_j, we assume that every other term in equation(2.10) is constant except the term containing a_j, so that all other terms drop out upon differentiating, and

$$\frac{\partial \delta_i}{\partial a_j} = 0 + 0 + \ldots + \frac{\partial}{\partial a_j} a_j g_j(x_i) + 0 + \ldots + 0 + \frac{\partial \delta_i}{\partial a_j} = g_j(x_i) \qquad (2.19)$$

Now we substitute equation (2.19) into equation (2.17), and obtain the (m+1) equations

$$\sum_{i=0}^{n} \delta_i g_j(x_i) = 0 \qquad \text{for j = 0, 1, 2,……,m} \qquad (2.20)$$

Substituting equation (2.12) into (2.20), we have

$$\sum_{i=0}^{n} [p_m(x_i) - f(x_i)] \, g_j(x_i) = 0 \qquad \text{for j=0, 1, 2,…….,m} \qquad (2.21)$$

And then substituting equation (2.10) into (2.21) we have

$$\sum_{i=0}^{n} [a_m g_m(x_i) + ... + a_1 g_1(x_i) + a_0 g_0(x_i) - f(x_i)] \, g_j(x_i) = 0$$

$$\text{for j=0,1,…,m} \qquad (2.22)$$

Multiplying through on the left-hand side

$$\sum_{i=0}^{n} [a_m g_m(x_i) g_j(x_i) + ... + a_1 g_1(x_i) g_j(x_i) + a_0 g_0(x_i) g_j(x_i) - f(x_i) g_j(x_i)] = 0$$

$$\text{for j = 0, 1, 2,……, m}$$

We now break up the left-hand side into separate sums:

$$\sum_{i=0}^{n} a_m g_m(x_i) g_j(x_i) + ... + \sum_{i=0}^{n} a_1 g_1(x_i) g_j(x_i)$$

$$+ a_0 \sum_{i=0}^{n} g_0(x_i) g_j(x_i) = \sum_{i=0}^{n} f(x_i) g_j(x_i)$$

$$\text{for j = 0, 1, 2,…., m} \qquad (2.23)$$

equation (2.23) finally provides a useful result. To simplify the process a bit and make it more suitable for computer solution, we note that the coefficient of a_k in the jth equation is

$$\alpha_{kj} = \sum_{i=0}^{n} g_k(x_i) g_j(x_i) \qquad \text{for k = 0, 1, 2, …., m}$$

$$\text{j = 0, 1, 2,…..., m} \qquad (2.24)$$

since j and k in equation (2.24) can be interchanged, we have also the result that $\alpha_{kj} = \alpha_{jk}$ which reduces the work required to compute these coefficients by about half.

We now have a workable scheme for finding the least-squares fit. Using equation(2.23) we solve for the (m+1) unknown a's, which exist and are unique if we choose the g(x) functions properly, and then substitute the resulting values into equation (2.10) to give us the desired expression for $p_m(x)$. [20]

2.3Average Grain Size (AGS):

The average grain size can be obtained, depends on the mathematical formula applied in the program which is known as Scherrer's formula [21]. The x-ray chart of (CdS) as shown for example in figure 2.1 and X-ray chart of CdTe AS IN FIGURE 2.2[22] which exhibited a number of peaks, by evaluating the bandwidth of the most dense peak represented with a higher intensity of diffraction at a certain angle (2θ),

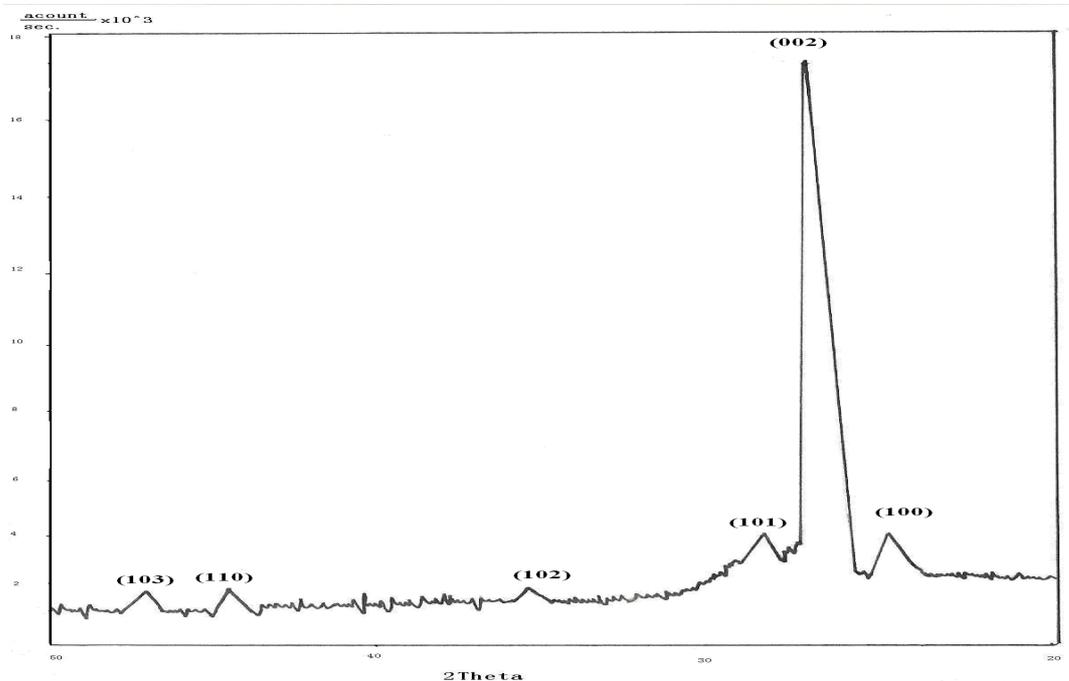$$AGS = \frac{0.9\lambda}{\beta_{1/2}\cos\theta} \tag{2.25}$$

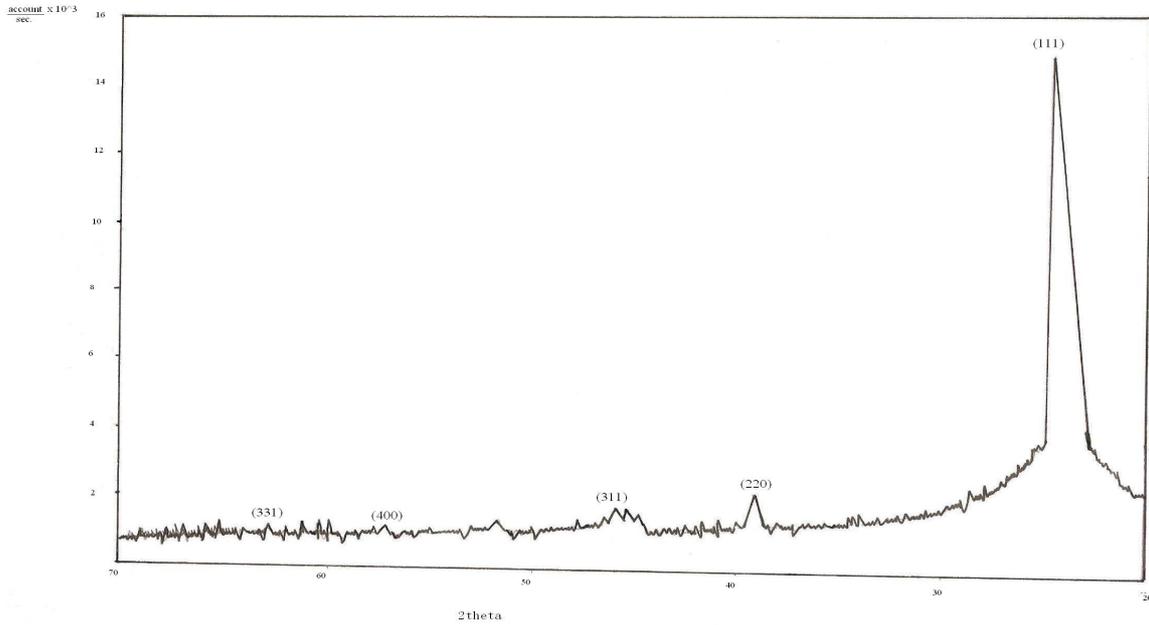Fig.2.1 Showed X-ray chart for CdS [22].

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Fig.2.2 Showed X-ray chart for CdTe [22].

2.4 Filling Factor (FF):

The applying of a simple relation that was studied previously in solid state physics which represented the packing ratio of the atoms or molecules with respect to the volume of the geometrical shape. It is necessary to apply the number of atoms or molecules per unit cell, the occupied volume by atoms or molecules, the total volume $[\vec{a} \cdot (\vec{b} \times \vec{c})]$ of the geometrical unit cell, then the filling factor can be obtained by the following equation [1]:

$$FF = \left[\frac{volume \; occupid \; by \; atoms}{total \; volume} \right] \times 100\% \qquad (2.26)$$

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$$FF = \left[\frac{(\frac{4}{3}r^3\pi) \times N}{total} \right] \times 100 \,\%.$$

(2.27)

Where (r) represents the radius of the atom, and (N) represents the number of atoms per unit cell.

2.5 The Elastic Strain (ε):

The elastic strain and the particle size can be obtained from the Hall-Williamson method [15].

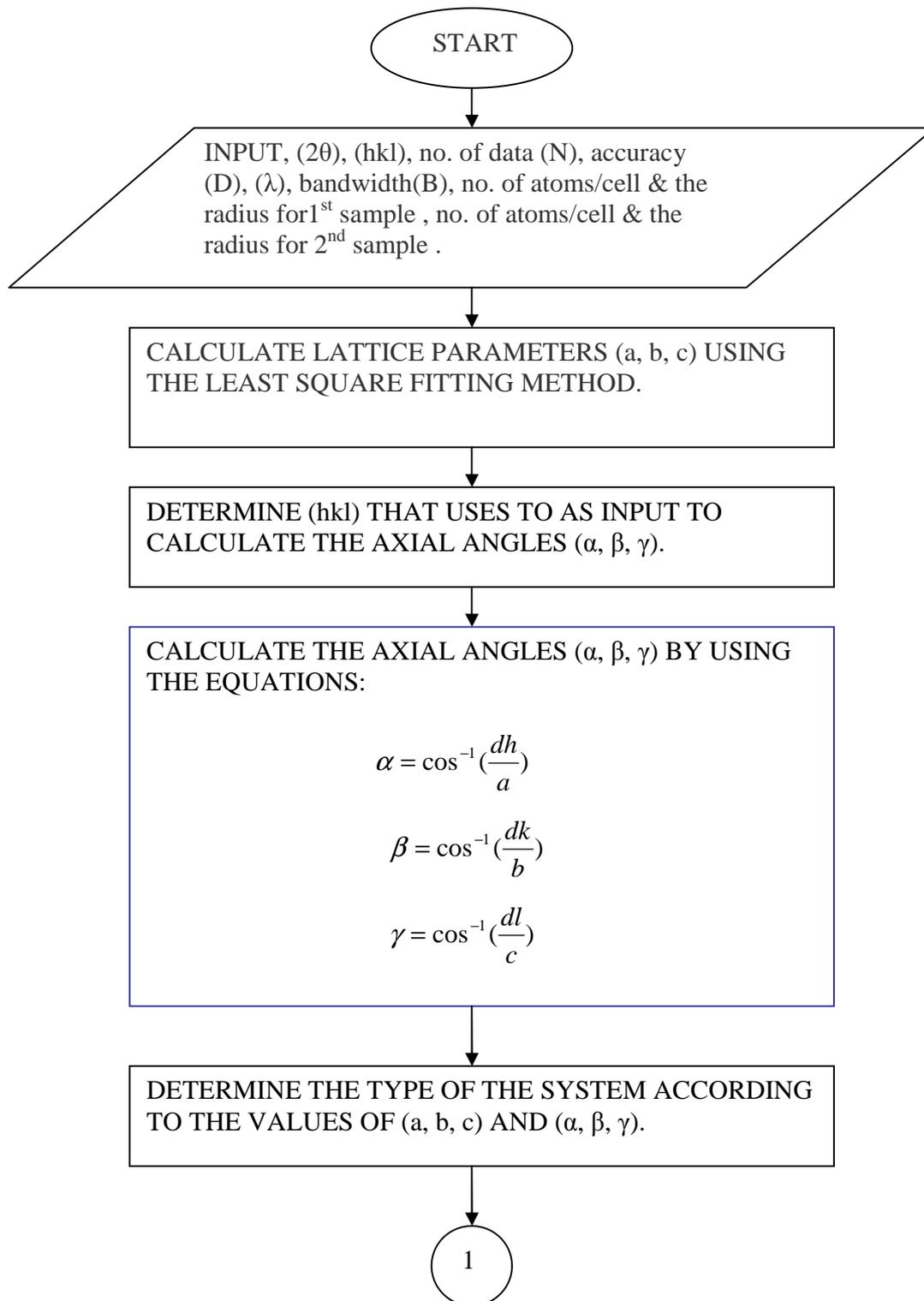$$(\frac{\beta_{1/2}\cos\theta}{\lambda})^2 = (\frac{0.89}{d})^2 + 16\varepsilon^2(\frac{\sin\theta}{\lambda})^2$$

(2.28)

Or,

$$\frac{\beta_{1/2}\cos\theta}{\lambda} = \frac{1}{D_V} + 2\varepsilon(\frac{2\sin\theta}{\lambda})$$

(2.29)

The elastic strain can be obtained by plot a graph between $(\frac{\beta_{1/2}\cos\theta}{\lambda})$ and $(\frac{2\sin\theta}{\lambda})$ and by equaling the slope with (ε), the value of the elastic strain can be obtained and from intercept the particle size can be obtained [23].

2.6 program design:

A computer program crystal-2, is in visual basic 6 is designed and applied to identify the information about crystal structure through the calculations of

1- The lattice parameter (a, b, c) using equation 2.7 by Evaluating the values of A, B, and C where (A, B, C) represents ($\frac{1}{4a^2}$, $\frac{1}{4b^2}$, $\frac{1}{4c^2}$).

2- The axial angles (α, β, γ) of unit cell by using equation 2.8.

3- The average grain size which can be evaluated from scherrer's formula as in equation 2.25.

4- The filling factor can be evaluated from equation 2.27, and the elastic strain which can be evaluated from the Hall-Williamson method as in equation 2.28. This program consists of many calculations as shown in figure 2.3.
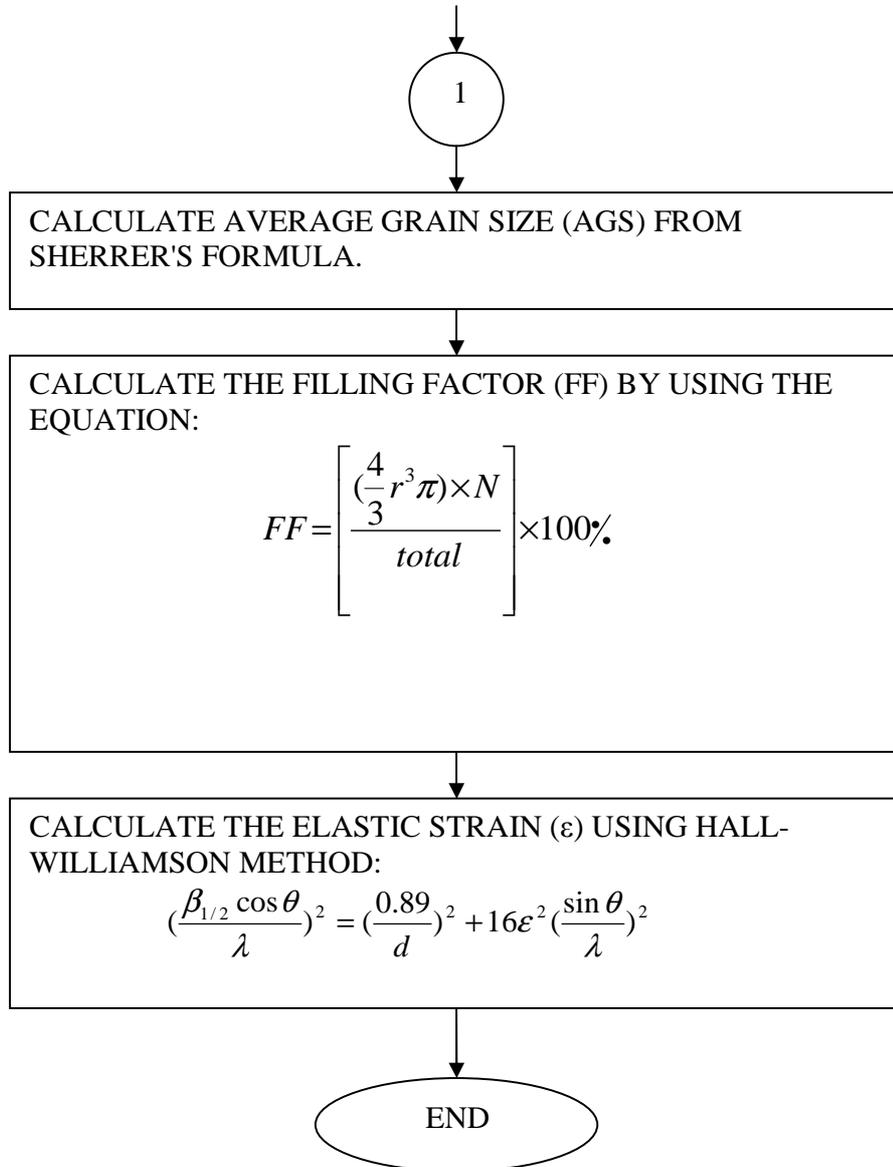
START

INPUT, (2θ), (hkl), no. of data (N), accuracy (D), (λ), bandwidth(B), no. of atoms/cell & the radius for1st sample , no. of atoms/cell & the radius for 2nd sample .

CALCULATE LATTICE PARAMETERS (a, b, c) USING THE LEAST SQUARE FITTING METHOD.

DETERMINE (hkl) THAT USES TO AS INPUT TO CALCULATE THE AXIAL ANGLES (α, β, γ).

CALCULATE THE AXIAL ANGLES (α, β, γ) BY USING THE EQUATIONS:

$$\alpha = \cos^{-1}(\frac{dh}{a})$$

$$\beta = \cos^{-1}(\frac{dk}{b})$$

$$\gamma = \cos^{-1}(\frac{dl}{c})$$

DETERMINE THE TYPE OF THE SYSTEM ACCORDING TO THE VALUES OF (a, b, c) AND (α, β, γ).

1

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                          ┌───┐
                          │ 1 │
                          └───┘
                            │
                            ▼
┌─────────────────────────────────────────────────────┐
│ CALCULATE AVERAGE GRAIN SIZE (AGS) FROM              │
│ SHERRER'S FORMULA.                                   │
└─────────────────────────────────────────────────────┘
                            │
                            ▼
┌─────────────────────────────────────────────────────┐
│ CALCULATE THE FILLING FACTOR (FF) BY USING THE       │
│ EQUATION:                                            │
│                                                      │
│                                                      │
└─────────────────────────────────────────────────────┘
```

CALCULATE THE FILLING FACTOR (FF) BY USING THE EQUATION:

$$FF = \left[\frac{(\frac{4}{3} r^3 \pi) \times N}{total} \right] \times 100\%.$$

CALCULATE THE ELASTIC STRAIN (ε) USING HALL-WILLIAMSON METHOD:

$$(\frac{\beta_{1/2} \cos\theta}{\lambda})^2 = (\frac{0.89}{d})^2 + 16\varepsilon^2 (\frac{\sin\theta}{\lambda})^2$$

END

Fig. 2.3 The flow diagram of crystal-2 program.

2.7 Input data:

1. to determine a, b, c and the axial angles (α, β, γ) we need to input:

for CdS the Bragg's angle, the miller indices, and the atomic displacement.

2. to determine the average grain size (AGS) we need to input

for CdS $\beta_{1/2}$=0.0087 rad., θ=13.2° and λ=1.5405Å.

3. to determine the filling factor (FF) we need to input

for CdS the number of atoms per unit cell for Cd and S are N_{cd}=4, N_s=4, a = b = c = 5.82 Å, for cubic structure and the ionic radius for Cd and S are r_{cd}=0.095 nm, r_s=0.184 nm.

4. to determine the elastic strain (ε) we need to input

For CdS $\beta_{1/2}$ at (100) = 0.00698 rad. And θ = 12.4° with λ=1.5405Å.

$\qquad$ $\beta_{1/2}$ at (002) = 0.0087 rad. And θ = 13.2° with λ=1.5405Å.

For CdTe $\beta_{1/2}$ at (111) = 0.00524 rad. And θ = 11.85° with λ=1.5405Å.

$\qquad$ $\beta_{1/2}$ at (220) = 0.01047 rad. And θ = 19.55° with λ=1.5405Å.

2.8 Output:

The important outputs parameter includes:

$\qquad$ a- The crystal structure:

$\qquad\qquad$ 1- The cell parameters (a, b, c).

$\qquad\qquad$ 2- The axial angles (α, β, γ).

$\qquad$ b- The average grain size (AGS).

$\qquad$ c- The filling factor (FF).

$\qquad$ d- The elastic strain (ε).

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A Computational Program to Determine Some of Crystal Structure Specifications

A Thesis
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(B.Sc.2005)

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Table of symbols

a, b and c   = lattice parameters (constants).

α, β and γ = the axial angles.

λ =   wavelength.

d_{hkl} =   Interplanar distance.

θ =   Bragg's angle

AGS   =   Average Grain Size

FF   =   Filling Factor

ε =   Elastic Strain.

الخلاصة

البرنامج الحسابي crystal-2 المصمم بلغة فيجول بيسك ٦ صمم وطبق لتعريف خصائص ثلاثة انواع من البناء البلوري يتضمن قياس الابعاد البلورية (a, b, c) , الزوايا المحورية (α, β, γ) ,متوسط حجم الحبيبة (AGS) , نسبة الملئ (FF) والاجهاد المرن (ε) .

هذا البرنامج سوف يعطينا وصف كامل عن البناء البلوري لثلاثة انواع من البناء البلوري للمواد المستخدمة بواسطة ادخال المعلومات من البيانات التي تتضمن زاوية الحيود (2θ) ومعاملات ميلر hkl للمواد المستخدمة مثل كبريتيد الكادميوم (CdS) والبريليوم (Be) ومقارنة القيم المحسوبة مع القيم النظرية للبيانات المدخلة للمواد المستخدمة.

كما انه تم قياس (AGS) بواسطة استخدام نظرية شيرر وعامل المرونة بواسطة استخدام نظرية هول ويليامسون للمواد المستخدمة مثل كبريتيد الكادميوم .

جمهورية العراق

وزارة التعليم العالي والبحث العلمي

جامعة النهرين

كلية العلوم

برنامج حسابي لحساب بعض خواص التراكيب البلورية

رسالة

مقدمة إلى كلية العلوم في جامعة النهرين كجزء من متطلبات نيل شهادة الماجستير

في الفيزياء

من قبل

لينا حسين علي

بكالوريوس ٢٠٠٥

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