# INTRODUCTION

Continuing interest in the study of semiconductor materials since the early nineteenth century, in 1889 alternating Current with the low-frequency, and then introduced semiconductor (Rectifier) the use of selenium rectifier Conductors in the areas of practical applications, as copper oxide used in 1927 is widely Rectifier and low capacity of the battery chargers, so rolled female students to know the properties of material as it occupied a prominent place in the theoretical and applied research for the Solid State Physics[1,2].

Semiconductors are materials that have properties intermediate between conductors (materials that allow electric current to pass) and insulator (which block electric) [9].

Semiconductors fall into two broad categories .First, there are semiconductors. These are composed of only one kind of material. Silicon and germanium are two examples; they are also calling" untapped semiconductor "or intrinsic-type semiconductors. Other with impurities is call extrinsic (doped semiconductors). It is significant that the conductivities of this material can be varied over orders by changes in temperature, optical excitation, electrical field and impurity content. thus semiconductor can display arrange of useful electric and optical properties: electric properties such as passing current more easily in one direction than other this makes semiconductor material natural choices for device, thus semiconductors are foundation of modern electronics including radio, computer and telephone, Optical properties semiconductor material emitted range of spectrum thus used to detect photon[7].

(1-1) Cdmium sulfide (CdS) as Semiconductor:

Cadmium Sulfide (CdS), is a (II–VI) compound can be classified as semiconductor , because of its wide and direct band gap (2.42-3.3eV) at room temperature $300^{°}$k, which is insoluble in water, but soluble in dilute mineral acids ,good optical transmittance, low ohmic resistivity and easy contact it has found potential applications.[7]
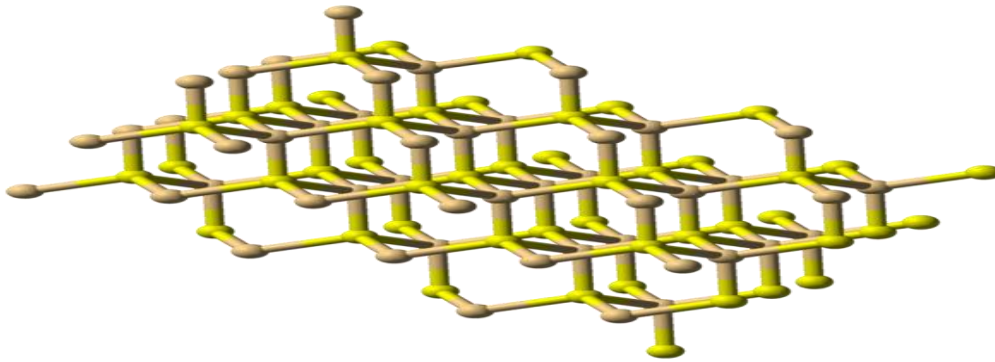
Fig(1-1) 3D model of the structure of CdS[12]

(1-2) Advantages of (CdS):

high stability, excellent physical, chemical and structural properties, availability, ease of preparation and handling, CdS nanomaterials can be exploited in various fields of life.

(1-3)Applications of (CdS):

CdS have received considerable attention during recent years because of their numerous excellent properties in optoelectronic fields. CdS has a broad range of application in important technical fields such as heterojunction solar cells , light emitting diodes , large screen liquid crystal devices, gas sensors and field effect

transistors, detectors for laser and infrared , nonlinear optical materials, various luminescence devices, optoelectronic devices etc[9].

CdS belongs to Cadmium Chalcogenide in particular, n-type CdS are widely used as a window layer in heterojunction realization of p-type CdTe and CuInSe solar cells.

Hence, a large number of studies have been carried in order to produce CdS thin films of this material with suitable optoelectronic properties for photovoltaic applications. For this purpose several properties are required of the CdS films:

(1) Relatively high transparency.

(2) Too thin to avoid the short current circuiting.

(3) Relatively large conductivity to reduce the electrical solar cells losses and higher photoconductivity to not alter the solar cell spectral response [7, 8, 9].

CdS is predominantly used as a pigment. About 2000 tons are produced annually.

CdS and cadmium Selenide are used in manufacturing of photo resistors (light dependent resistors) sensitive to visible and near infrared light.

CdS can be combined with other layers for use in certain types of solar cells. CdS was also one of the first semiconductor materials to be used CdS transistors (TFTs)[9].

However interest in compound semiconductors for TFTs largely waned after the emergence of amorphous silicon technology in the late 1970s. Thin films of Cadmium Sulfide can be piezoelectric and have been used as transducers which can operate at frequencies in the GHz region, such as low temperature operation

and economic. Many authors have also obtained highest efficiency using this method to grow buffer layer for solar cell [8].

(1-4) (CdS) Nano-particles:

(CdS) are particles between 1 and 100 nanometers in size. In nano-technology, a particle is defined as a small object that behaves as a whole unit with respect to its transport and properties. Particles are further classified according to diameter [20].

(1-5) The Objective of the study:

In this study, (CdS) is characterized by several techniques such as:

Preparation of Cadmium Sulfide(CdS), the UV-visible absorption spectrum and calculation of the Energy gap and absorption coefficient to the study optical properties, and other technique has been used is X-ray diffraction (XRD) spectrometer method in order to study characterized the structural of CdS .

(1-6) Previous studies:

1- Researchers (AMercy ,R.Samuel Selvaraj , B Milton Boaz AJesper Anandhi and Rkanagadurai,) were studied synthesis, structural and optical characterization of cadmium sulfide nanoparticles, and they were found good quality CdS nanoparticles of size ranging from(13-17)nm by using synthesized chemical precipitation method followed by heat treatment .The prepared CdS nanoparticles have characterized by XRD,HRSEM,UV-visible spectra and photoluminescence studies the presence of both cubic and hexagonal phases and calculated from the scherrers equation the average particle size and SEM micrographs show uniform orientation of low dimensional. [7].

2- Ashok Ch., Venkateswara Rao K.and Shilpa Chakra C studied the structural properties of CdS nanoparticles prepared in the presence of organic solvent , CdS nanoparticles which prepared by chemical precipitation technique in the presence of organic solvent. The obtained results of CdS nanoparticles were characterized by (XRD),(PSA),(SEM),(EDX),(TEM) and (FTIR) for average particle size, morphology, elemental composition, shape and bond analysis respectively .After analyzing the results, and these nanoparticles have been used in various applications[15].

3- Ch.ashok, K.venketesware ,Ch.shipa chakra and V.Rajender, they used XRD, SEM and EDX to determine the structural properties of CdS nanoparticles for solar cell applications. The XRD results indicated the presence of hexagonal phase in the sample and the crystallite size 35 nm was calculated with Debye-Scherrer's formula, particle size histogram showed the particle size as 39 nm. The SEM images showed spherical granules like structure. EDX pattern inferred, determined the presence of elements Cd, S and O. Depends upon the above properties these nano size particles are used in solar cell applications[8].

(1-7) Outline of this thesis:

This research consists of four chapters:

Chapter one: Is introduction the (CdS) of semiconductor materials, Physical and chemical properties of Cadmium Sulfide, advantages and application and objectives, Previous studies and outline of Research are presented.

 Chapter two: Explain the basic concepts used in the research

Chapter three: Is the methodology, materials preparation of CdS and the Device which used in the experiment.

Chapter four: results which obtained tram that measures the CdS nanparticles are characterized by using XRD for the study of average crystallite size and determine value of E_g for CdS from its UV absorption spectrum and conclusion.

Theoretical Background

The measurement of the band gap of materials is important in the Semiconductor, nano material and solar industries, demonstrates how the band gap of a material can be determined from its UV absorption spectrum. For this reason this chapter explains the Principles of spectroscopy and more details about UV and X- rays which are used in this research.

(2-1) spectroscopy:

When a beam of light is allowed to pass through a prism or grating, it will dispersed into seven colors from red to violet and the set of colors or band produced is called spectrum , Spectroscopy is the branch of the science dealt with the study of interaction of **E**lectro **M**agnetic **R**adiation (EMR) with matter[21].

So the spectroscopy means examination of spectrum. From the type of radiation, which is absorbed, we can get idea about the nature (type) of the compound and from the amount of the radiation, which is absorbed; we can get idea about the concentration (amount) of the substance. So the spectroscopy is used for qualitative and quantitative analysis [20].

(2-1-1) Classification of Spectroscopy:

1) **Absorption Spectroscopy**:

The type and amount of the radiation, which is absorbed, depend upon the structure of the molecules and the numbers of molecules interacting with the radiation. The study of these dependencies is called absorption spectroscopy (UV, IR, NMR, X-Ray, and ESR).

2) **Emission spectroscopy**:

  If sufficient energy gets impinged upon a sample, the outer electrons in the species will be raised from their stable ground state to higher energy level (unstable in nature). These excited species rapidly emits a photon and return to their ground stable energy level. The type and amount of radiation, which is emitted, is studied, this type of spectroscopy is called emission spectroscopy (AES, MES, Fluorimetry).

3) **Scattering spectroscopy**:

 if the incoming radiation strikes with the solid particles suspended in the solution, the light transmitted at an angle other than 180^0 from the incident light. This spectroscopy is called scattering spectroscopy. (turbidimetry, nephelometry)[21].

(2-2)Ultraviolet–visible spectroscopy:

Ultraviolet–visible spectroscopy or ultraviolet-visible pectro-photometry (UV-Vis or UV/Vis) refers to absorption spectroscopy or reflectance spectroscopy in the ultraviolet-visible spectral region. This means it uses light in the visible and adjacent (near-UV and near-infrared [NIR]) ranges. The absorption or reflectance in the visible range directly affects the perceived color of the chemicals involved. In this region of the electromagnetic spectrum, molecules undergo electronic transitions. This technique is complementary to fluorescence spectroscopy, in that fluorescence deals with transitions from the excited state to the ground state, while absorption measures transitions from the ground state to the excited state [13].

(2-3) optical properties:

The study properties of optical semiconductor very important sources to give information about the installation of the electronic package and disadvantages and non order (Disorder) and gap energy and frequency of visual styles and permittivity and other optical properties of the semiconductor and as a result lead Knowing this information to industrial and laboratory applications. In general, the optic properties of thin films differ from their properties optic (bulk) difference resulting from (Microstructure), optical properties of semiconductor dependent to facilitate the gaps in the valence band and the electron in connection band , and talked optical properties of absorption or emission of electromagnetic energy because of the free carriers passing between the package (Inter band) and valence between the package and the package conduction or transfer between the lowest package (Inter sub band) and between small packets (Mini bands)[1,2,9].

The item is addressed to the optical behavior, the phenomenon of optical absorption, optical constants.

(2-4)Interaction of light with semiconductors:

When the fall of the beam of monochromatic light on section of vertically from the surface of the semiconductor part this beam will be reflected and part of it will be implemented and another part of it is absorbed within the crystal, because energy sufficient to stir up electrons and converted from the low-lying energy levels to the levels of occupancy high is busy, and since there are a large number of electrons in the occupied levels pack valence and a large number of it also empty levels in the conduction package separated from each gap forbidden the probability absorbance be very large when energy photons are of the incident light Semiconductor. The absorption of light inside the proportion of fit (E_g) is greater

than banned energy gap Proportional to intensity of incident light (photons flow) when the length of a given wavelength and this phenomenon Physical are common and lead to the decay of the light intensity monochromatic exponential when it passed through the semiconductor and expressed mathematically according to the law of Lambert (the Beer-Lambert law) as follows [4]:

$$I = I_0 e^{-\alpha t} \quad \text{(2-1)}$$

I_0 = intensity of light incident upon sample cell

I = intensity of light leaving sample cell

t = thickness

α = is a function of wavelength incident known absorption coefficient

The equation can be written as:

$$\alpha t = 2.303 \log\left(\frac{I_0}{I}\right) \quad \text{(2-2)}$$

As the amount represents $A = \log\left(\frac{I_0}{I}\right)$ absorbance, and that the intensity of radiology, which represents (α) the absorption coefficient through the material, and ($e^{-\alpha t}$) incident decreases exponentially the proportion of decrease in the radiation energy through the material.

(2-5) Absorption coefficient:

The absorption coefficient has been calculated from the following equation

$$\alpha = \frac{2.303\ A}{t} \quad \text{(2-3)}$$

t is thickness

A is a constant of the material (absorbance).

Absorption coefficient is defined as the proportion of decrease in winning the iceberg radiation energy per unit directed toward the distance inside the center spread, and absorption depends on the photon energy (hυ) incident coefficient and on the properties of the semiconductor

The direct band gap of the semiconductor, the absorption coefficient (α) obeys the following relation for high photon energies (hv):

$$\alpha = \frac{A\left(hv - E_g\right)^{\frac{1}{2}}}{hv} \qquad (2-4)$$

Where

E_g is the optical band gap of the material

A is a constant of the material (absorbance).

*r =1/2 because the direct allowed transition

(2-6)Optical Energy Gap:

The band gap of a semiconductor is the minimum energy required to excite an electron that is stuck in its bound state into a free state where it can participate in conduction. The band structure of a semiconductor gives the energy of the electrons on the y-axis and is called a "band diagram", the lower energy level of a semiconductor is called the "valence band" (E_v) and the energy level at which an electron can be considered free is called the "conduction band" (E_c), the band gap (E_g) is the gap in energy between the bound state and the free state, between the valence band and conduction band, therefore, the band gap is the minimum change in energy required to excite the electron so that it can participate in conduction. other definition can be The term "band gap" refers to the energy difference between the top of the valence band to the bottom of the conduction another.

In order for an electron to jump from a valence band to a conduction band, it requires a specific minimum amount of energy for the transition equal to the band gap energy.

A diagram illustrating the band gap is shown in Figure (2-1).

Measuring the band gap is important in the semiconductor and nanomaterial industries, the band gap energy of insulators is large (>4eV), but lower for semiconductors (< 3eV). The band gap properties of a semiconductor can be controlled.
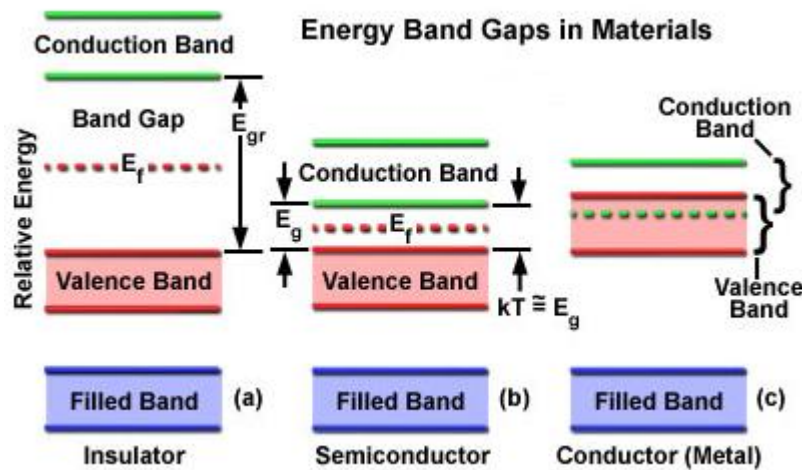
Figure (2-1). Show the illustration the band gap diagram

The measurement of the band gap of materials is important in the semiconductor, nonmaterial and solar industries. Demonstrates how the band gap of a material can be determined from its UV absorption spectrum [19].

The energy gap of the optical constants is important, and is a function of temperature(T), as the value of change of the energy gap increases in some

semiconductor, with little temperature change while less in others, it can calculate the energy gap by different models which :

1- Model (Tauc): graphs is plotted which explain the relationship between the $(h\upsilon)$ and $(\alpha h\upsilon)^2$ and extending the best line straight extension be conclusive to the axis of the photon energy $(h\upsilon)$. It is determined by the value of the energy gap for the intersection point is that he has $(\alpha h\upsilon)^2= 0$[5].

2- It can calculate the energy gap of taking the first derivative of the absorbance as a function of photon energy as representing the highest peak photon energy axis value calculated energy gap[6].

(2-7)Structural Properties of Semiconductors:

Contribute to the study of structural characteristics of the semiconductor by identifying components that have been obtained, the nature and type of systems and levels of crystal paved contained element. And help study the characteristics of many different structural interpretations of the results and to be attached to change the electrical properties of semiconductor.

(2-8)X-rays:

X-rays is the wavelength of electromagnetic radiation between 10 and 0.01 nm, i.e. the energy rays between 12 and 120 thousand electron volts, is widely used in many technical and scientific fields.

X-rays are produced when rapidly moving electrons that have been accelerated through a potential difference of order kV(s) to MV(s) strikes a metal target

X-rays released in two ways:

1-By acceleration of charged particles and electrons are usually used to product and this is bremsstrahlungs which form a continuous spectrum (i.e. a mixture of

electromagnetic waves of short and very short).

2- When electron transition in an atom or molecule from the shell of a very high level of energy to a low level. This is the X-ray distinct certain wavelength, and have a specific energy.

The discovery of X-rays in 1895 enabled scientists to probe crystalline structure at the atomic level [22].

(2-8-1)Interaction of X-ray with Matter:

It includes for three types

1-Fluorescence:

Fluorescence can be more simply defined as "the molecular absorption of light energy (photon) at one wavelength and its re-emission at another, usually longer, wavelength" [21].
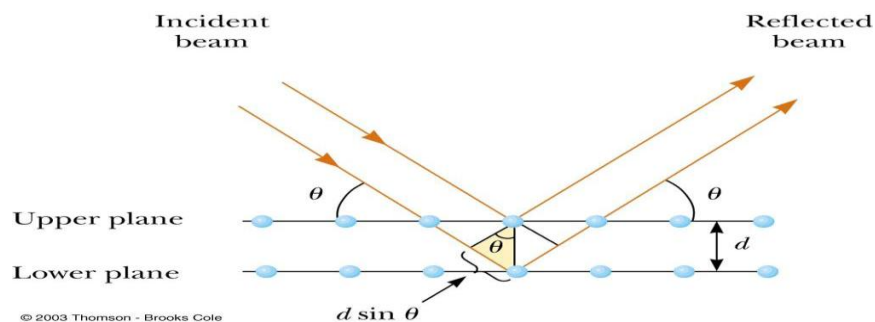
2-Ioniztion:

Ionizing radiations carry enough energy to break chemical bonds and separate electrons from the parent atoms and molecules, thereby creating ions in the irradiated material.

•Diffraction:

Coherent scattering of X-ray by crystalline substance.

(2-8-2)Bragg's law:

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Fig (2-2) Diffraction (scattering of 2 rays)

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William Lawrence Bragg discovered (1912) law relating the spacing between atoms in a crystal to the angle at which X-rays are scattered when they strike the crystal.

$$n\lambda = 2d \sin \theta \quad (2\text{-}5)$$

In-phase scattering of 2 rays depends on the distance (d) and the wavelength (λ) of the incident radiation. The distance is equal to $d \sin \theta$. For the 2 rays to scatter in phase, $\lambda = 2d \sin \theta$. This is Bragg's law in its simplest form X-Ray Diffraction

**(2-8-3)X-ray spectroscopy:**

X-ray spectroscopy is a gathering name for several spectroscopic techniques for characterization of materials by using x-ray excitation, using crystal as a wavelength selector, and the intensity of different wavelengths of X-rays can be measured.

(2-8-4)X-ray Diffraction (XRD):

X-ray diffraction has been in use in two main areas, for ngerprint characterization of crystalline materials and the determination of their structure. Each crystalline solid has its unique characteristic X-ray powder pattern which may be used as a "fingerprint" for its identification. Once the material has been identified, X-ray crystallography may be used to determine its structure, i.e how the atoms pack together in the crystalline state and what the inter-atomic distance and angle are etc. X-ray diffraction is one of the most important characterization tools used in solid state chemistry and materials science we can determine the size and the shape of the unit cell for any compound most[22].

(2-9) XRD:

Easily using X-ray diffraction Structural Analysis X-ray diffraction provides most definitive structural information measure the average spacing between layers or rows of atoms determine the orientation of a single crystal or grain find the crystal structure of an unknown material measure the size, shape and internal stress of small crystalline regions.
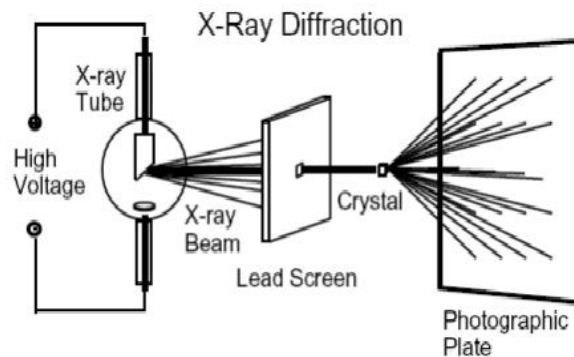
(2-10)Structural parameters:

(2-10-1)Lattice Constant (a):

The lattice constant for the installation of the cube is calculated under the following relationship:

$$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}} \qquad (2\text{-}6)$$

The lattice parameters of the hexagonal phase were measured using the formula

$$\frac{1}{a^2} = \frac{4(h^2+hk+k^2)}{3a^2} + \frac{1}{c^2} \qquad (2\text{-}7)$$

(h k l) represent Miller factors

(2-10-2)Average grain size (D):

The crystallite size was calculated using Debye – Scherrer's formula[8]

$$D = \frac{K\lambda}{\beta.\cos\theta} \qquad \text{(2-8)}$$

Where:

K is Debye-Scherer's constant

D is the average crystallite size of the particle

λ is the wavelength of the radiation

β is the Full Width Half Maximum (FWHM) of the peak

θ is the Bragg's angle.

(2-10-3)Dislocation density and number of grains:

Represents the density of dislocations number of dislocations lines that cut unit area in that the crystal, It represents the ratio between the total length of all dislocations lines and the size of the crystal, and the calculated density dislocations using the relationship (Williamson and Stallman's)[3]:

$$\delta = \frac{1}{D^2} \qquad \text{(2-9)}$$

Can calculate the number of grains per unit area of the following relationship[3]:

$$N = \frac{t}{D^2} \qquad \text{(2-10)}$$

N= Number of crystals per unit area   t = think

The strain and crystallite size of the sample were measured from the Williamson Hall equation[8]:

$$\beta \cos \theta = \frac{K.\lambda}{\tau} + 2\varepsilon \sin \theta \quad \text{(2-11)}$$

where :

β = is the Full Width Half Maximum (FWHM) of the XRD corresponding peaks

k =is Debye-Scherer's constant

τ =is the crystallite size

λ= is the wave length of the X-ray radiation

ε =is the lattice strain

θ is the Bragg angle.

MATERIALS AND METHODS

This chapter presents the preparation of CdS and the devices used in the practical work of this research.

(3-1) materials:

(3-1-1)Cadmium Sulfide Preparation:

We used a chemical method for the preparation of cadmium sulfide, in Sudan University chemistry laboratory and the resulting interaction of cadmium sulfide in room temperature in the form of powder.

To prepare the CdS the below steps has been followed:

$$Cd\ Cl_2 + Na_2S \rightarrow 2Na_2\ Cl + CdS$$
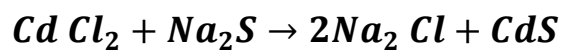
(1 ML) of an aqueous 0.012 mole of $Cd\ cl_2$ solution has been placed in a test tube , Was added drop also (1 ML) of an aqueous 0.012 mole Na_2S solution to the test tube. Note the color change upon mixing, after Stirring the mixture with a stir rod for half hour the bulk of the CdS crystals the formation of precipitate immediately ,the final yellow color of the crystals and solution which keep this CdS as a reference, will be observed, to measure the absorbance spectrum mixture of solution of ammonium hydroxide and CdS have been prepared, X-Ray Diffraction (XRD)Spectrometer has been used to study the structure the sample CdS powder solid .

After finishing from the preparing the sample the UV spectrometer used to achieve the absorbance spectrum between 190- 700 nm, and obtain the absorption

coefficient and energy gap from this spectrum, also the size of the nano particle has been obtain using XRD.

(3-2)Devices:

(3-2-1)UV spectrometers

Absorption measures device was used in the University of Khartoum in Central Laboratory **(Shimadzu** UV-1800 UV/Visible Scanning Spectrophotometer; 115 VAC).
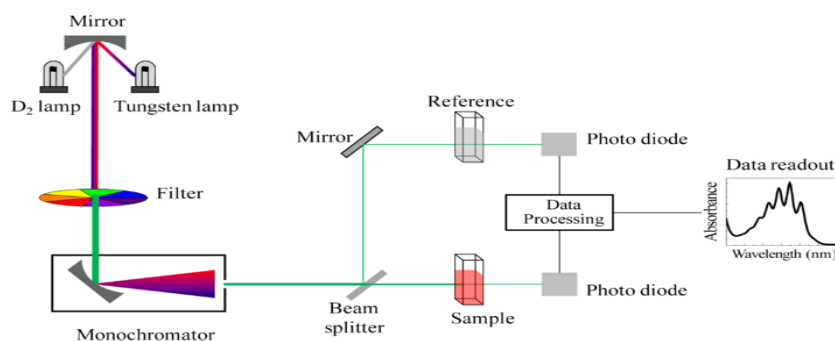
Fig. (3-1) the UV absorption spectrum composed spectrometer

1. Light Source
2. Monochromator
3. Sample and reference cells
4. Detector
5. Amplifier
6. Recording devices

Specifications :

Product Type	Spectrophotometer
Optics	Double-beam
Bandwidth	1 nm
Wavelength range	190 to 1100 nm
Wavelength accuracy	±0.1 nm
Wavelength reproducibility	±0.1 nm
Photometric range	0.0 to 400% T -4.0 to 4.0 A
Photometric noise	<0.00005 A at 700 nm
Photometric drift	<0.0003 A/hour
Detector	Silicon photodiode
Output	USB
Beam Type	Double
Stray light	<0.02% at 340 and 400 nm <1.0% at 198 nm
Source lamp	Tungsten-halogen and deuterium
Lamp life	2000 hours (tungsten-halogen)
Display	4.75" x 3.5" (12.1 x 8.9 cm) graphical LCD
Dimensions (cm)	45 x 27 x 49 cm
Brand	Shimadzu

(3-3)Structural Measurements:

in order to know the nature of the crystal structure used X-ray diffraction device in (P LRS).it is the following specifications:
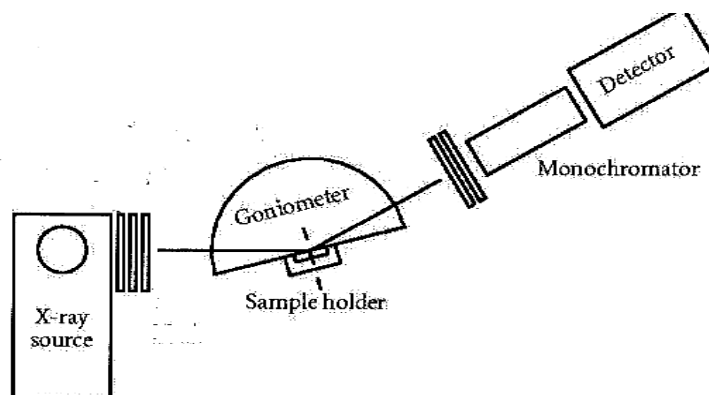
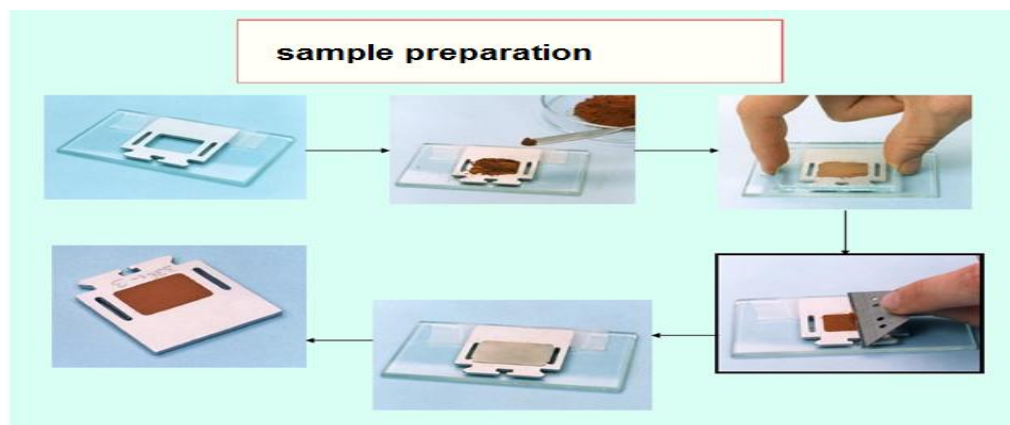TYPE**:** XRD-6000, SHIMADZU, JAPANESE ORIGIN

TARGET: Cu Kα

(3-3-1)X-ray Powder Diffract meter:

Components:

1. X-ray tube
2. Goniometer and optical path
3. Sample holder
4. Detector

Fig(3-2) the basic of Components XRD

Fig.(3-3) sample preparation

General Scan Condition

Generator Settings: 50mA, 40 kV

Step Size [°2Th.]: 0.02

Scan Step Time [s]:0.5

Scan range [°2Th.]: 2.0-80.00

* Specifications of the rest of the device in the fourth part of the research page (37).

Results and Discussion

In this chapter presents results details and discussion which obtained from measures the CdS nanoparticles by UV absorption spectrum to determine value of E_g and using X-Ray Diffraction (XRD) to characterized the sample and calculate the average crystallite and the conclusions.

(4-1)UV-visible spectroscopic analysis:

1. Band gap energy:

The measurement of the band gap of materials is important in the semiconductor, demonstrates how the band gap of a material can be determined from its UV absorption spectrum. The optoelectronic properties have been studied by UV-VIS absorption spectra the range in 190-700 nm and recording the spectra of (CdS) .
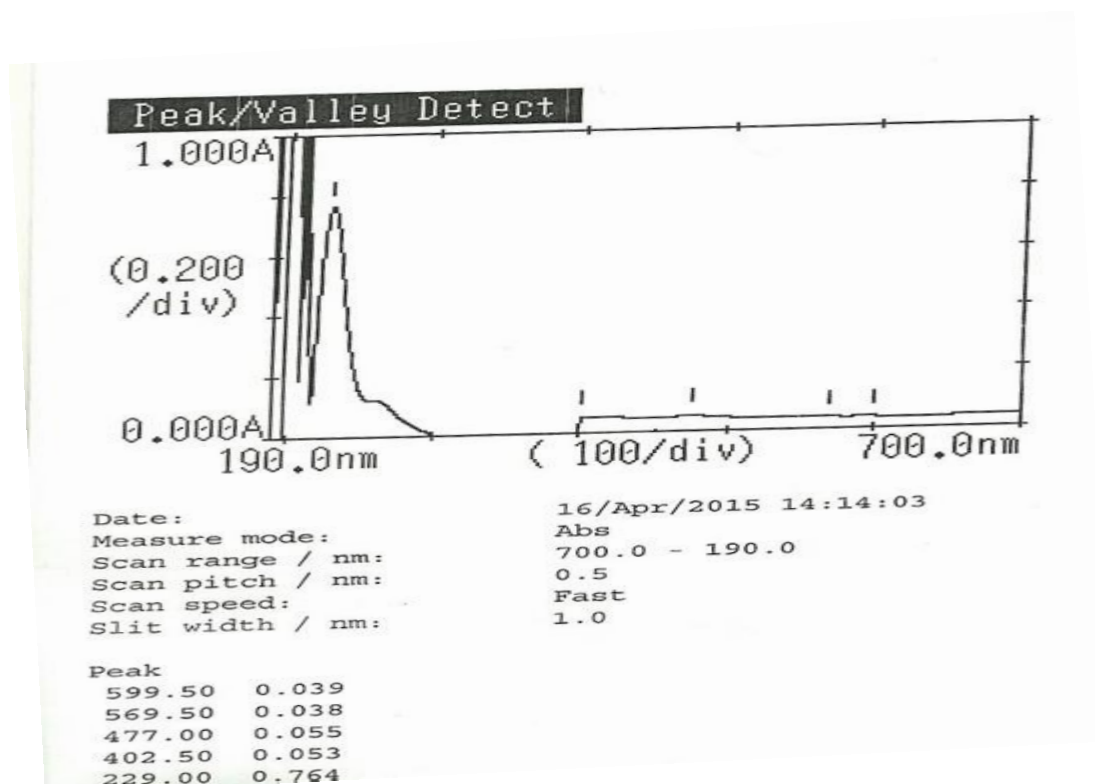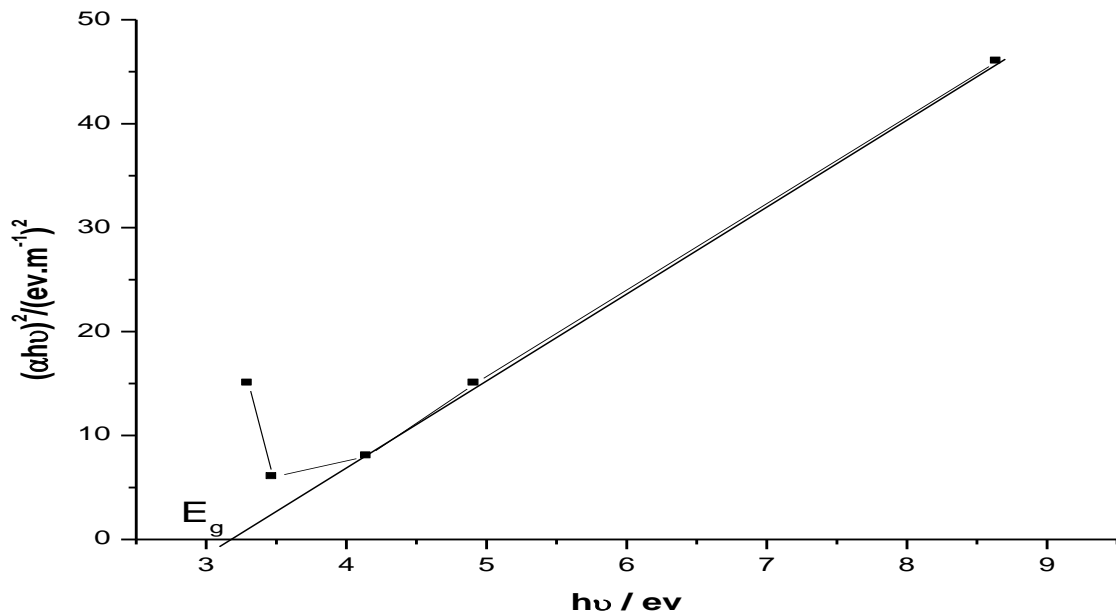

Fig.(4-1) the absorption spectra   in range 190-700 nm

The Result:

Table (4-1) show the result peak in the UV absorption spectrum:

λ/nm	hν/ ev	$(\alpha h\nu)^2/(ev.m^{-1})^2$
599.5	3.30275	14.9609
569.5	3.4767	5.90188
477.0	4.1509	8.41312
402.5	4.919	14.7656
229.0	8.6463	45.625

Fig. (4-2) the plot explain the relationship between the (hυ) and $(\alpha h\upsilon)^2$

Calculations:

Used the eq. (2-3) the absorber confection equal $\alpha=1.49$ m^{-1} at $300k°$.

$C=3\times10^8$m/s

$h=6.6\times10^{-34}$

$1ev =1.6\times10^{-19}$ j

$A=1.25$

The band gap energy for Cadmium Sulfide is **3.1783** ev.

Discussion:

The optical absorption spectrum of CdS nano particles recoded between 190 to 700 nm is orientation of the CdS nano particles is shown in Fig. (4-1) the high absorption is to be found in the lower wavelength corresponding to 299 nm indicating the blue shift in absorption edge.

Used the peaks in the spectrum and using (Tauc) model was calculated absorption coefficient and band gap energy.

(4-2)Results of Structural Measurements:

(4-2-1)X-Ray Diffraction (XRD):

     The Diffraction Studies were carried out using X-Ray Diffraction (XRD) Spectrometer powder with Cu K_α radiation (λ=1.54A°) with 2θ ranging from 0°to80°at the scanning speed 10° per minute .peak was also observed and Calculated from the FWHM, d-spacing, the average crystallite size.
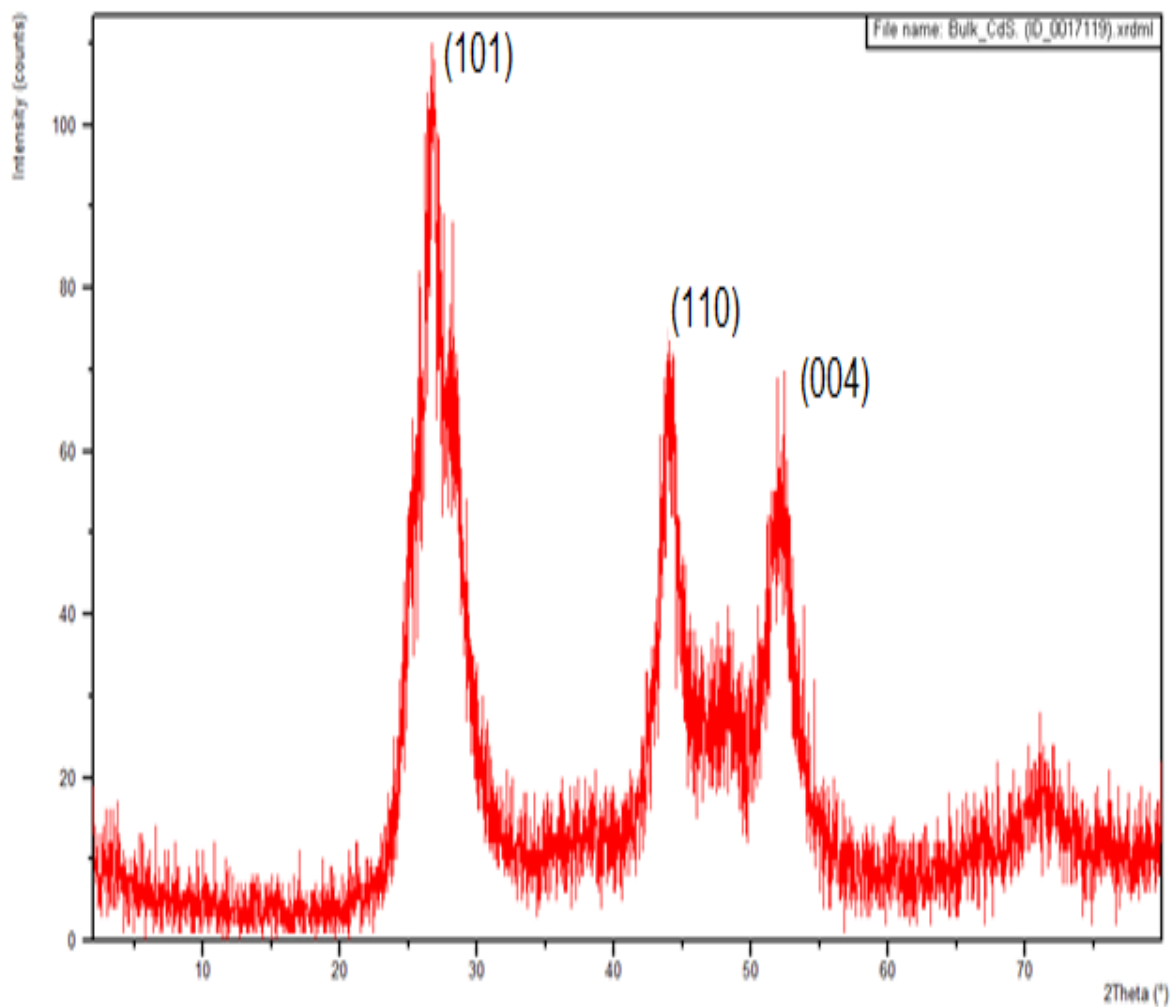
Fig. (4-3): XRD pattern of CdS nanoparticles

The Result:

Table(4-2) show Results obtained from X-ray diffraction:

NO.	Sample	Observed (2θ) Degree	d-spacing	Relative Intensity	D nm	FWHM deg	(h k l)
1	CdS	26.6769	3.34169	100.00	2.463710	0.6298	(101)
2	CdS	44.0660	2.05336	84.09	1.413835	1.1520	(110)
3	CdS	52.0375	1.75746	50.03	38.622	0.0435	(004)

Calculations:

1- The distance between the crystalline levels (d-spacing): It was calculating in table (4-2) the distance between the intra-crystalline levels using the Bragg's law of the relationship (2-5) and it found to be worth close to the value in the references [8].

2- Lattice Constant: It was calculating by the eq. (2-6) to found And found that its value is equal a=b=4.83A°, c=6.63A° in all peaks there is a difference with a value in reference [8].

3- Calculated using The crystallite size was calculated using Debye –Scherrer's formula:

$$D = \frac{K.\lambda}{\beta.\cos\theta} \qquad \text{(2-8)}$$

$\lambda = 1.54 A°$

k=0.98 (const)

at $\beta = 0.6298, 2\theta = 26.676$

$D_1 = 2.463710$

at β=**1.1520**2θ =44.066

D_2=1.413835

at β= **0.0435,**2θ =52.0375

D_3=38.622

The average crystallite size as **D=14.1665 nm** and It has been found that it varies within the range (13-17)nm[7].

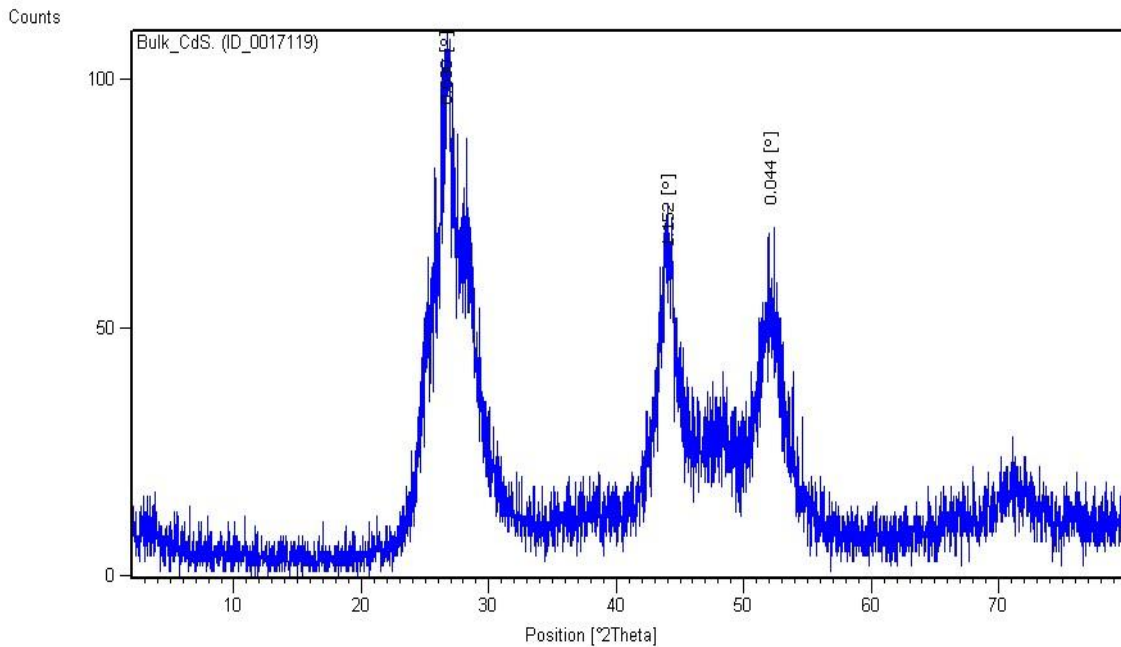**4-** The full width half maximum (FWHM) of the XRD corresponding peaks.

Fig.(4-4)

5- Dislocation density: It was calculating by the eq.(2- 9) to found 4.98×10^{-3}

Discussion:

Show in Fig.(4-3) that the structure of the CdS nanoparticles was in hexagonal phase. The peaks broadening represented the dimensions of CdS the nanoparticles. Peaks were observed at 26.677°, 44.066° and 52.0375° respectively which corresponded to (1 0 1), (1 1 0) and (0 0 4) planes Respectively, was Calculated the distance between the crystalline levels(d-spacing) not constent, lattice constant, calculated using The crystallite size was calculated using Debye –Scherrer's formula =14 nm , dislocation density $= 4.98 \times 10^{-3}$ found that some value consistent with previous studies.

(3-4)Conclusions:

It was prepared successfully compound the CdS nano particles and study its properties (structural and optical) as well as chemical process attended compound the Cadmium Sulfide at room temperature.

It has been studied optical properties of composite CdS through his studies using spectrometer used to achieve the absorbance spectrum between (190- 700) nm, and calculate the absorption coefficient =1.49 and energy gap=3.17 eV from this spectrum was consistent with previous.

studies from are characterized by using XRD Study the crystal structure revealed using X-ray diffraction that Cadmium Sulfide united peaks and half the width of the peaks and then found that for a hexagonal CdS type of installation wutzeile, are characterized by using XRD for the study was Calculated the distance between the crystalline levels(d-spacing), lattice constant, calculated using The crystallite size was calculated using Debye –Scherrer's formula , dislocation density found that some value consistent with previous studies.

And it found that good optical properties and structural can be used in many applications that the most important solar cells and resistors.

(4-4) Recommendation:

1-CdS Photo resistor and recording the current-voltage characteristics

2- Study of the electrical and optical properties of CdS Radiated by (He-Ne Laser).

3- synthesis and optical properties of CdS Different sizes.

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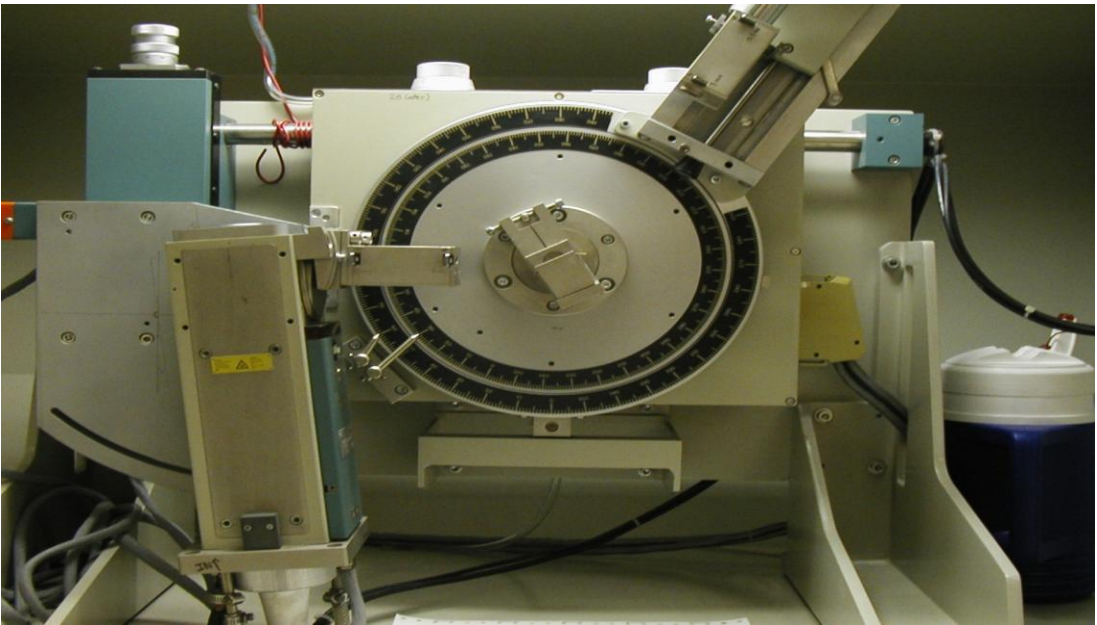
CONFIDENTIAL

SERVICE REPORT

Client: Student

X-ray Diffraction Analysis for one Sample

MINISTRY OF PETROLEUM
SUDANESE PETROLEUM CORPORATION
PETROLEUM LABORATORIES RESEARCH & STUDIES
(PLRS)
Date : 19-4-2015
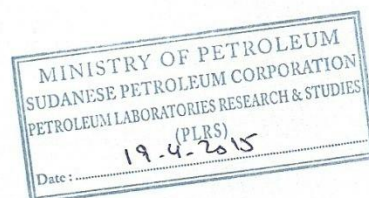
PLRS/GE 19 /04/2015
REPORT No.(0017119)

Towards Excellency

(F-13-02)

Report

Created on: 19/04/2015 12:00:01 ã
Operator: Administrator
File
File name: Z:\X'Pert Data\Bulk_CdS. (ID_0017119).xrdml
Checksum: 56b2d54be3faadcf1bff4ea6ac803776
File size (bytes):   14283
Time stamp
Started: 18/04/2015 08:34:38 ã
Finished: 18/04/2015 09:07:10 ã
Total time (h:m:s):   00:32:32
Comment
Configuration=CPL_Spinner, Owner=User-1, Creation date=1/30/2014 12:40:47 AM
Goniometer=PW3050/60 (Theta/Theta); Minimum step size 2Theta:0.001; Minimum step size
Omega:0.001
Sample stage=Spinner PW3064
Diffractometer system=XPERT-PRO
Measurement program=Bulk, Owner=User-1, Creation date=1/30/2014 12:58:16 AM
Status
Completed
Sample
Sample type: To be analyzed
Sample ID: CdS. (ID:0017119)
Measurement type
Single scan
Used wavelength
Intended wavelength type: $K\alpha_1$
$K\alpha_1$ (Å):   1.540598
$K\alpha_2$ (Å):   1.544426
$K\alpha_2/K\alpha_1$ intensity ratio: 0.50
$K\alpha$ (Å):   1.541874
$K\beta$ (Å):   1.392250
Incident beam path
Radius (mm):   240.0
X-ray tube
Name: PW3373/00 Cu LFF DK175087

Anode material:	Cu
Voltage (kV):	40
Current (mA):	50
Focus	
Focus type:	Line
Length (mm):	12.0
width (mm):	0.4
Take-off angle (°):	6.0
Soller slit	
Name:	Soller 0.04 rad.
Opening (rad.):	0.04
Divergence slit	
Name:	Prog. Div. Slit
Distance to sample (mm):	140
Type:	Automatic
Irradiated length (mm):	15.0
Offset (mm):	0.00
Sample movement	
Movement type:	Spinning
Rotation time (s):	16.0
Diffracted beam path	
Radius (mm):	240.0
Anti-scatter slit	
Name:	Prog. AS Slit
Type:	Fixed
Angle (°):	1
Soller slit	
Name:	Soller 0.04 rad.
Opening (rad.):	0.04
Monochromator	
Name:	Diffr. Beam Curved 1x graphite for Cu
Crystal:	
Name:	C
Type:	Symmetric
Shape:	Curved
No. of reflections:	1
hkl:	0 0 2
Receiving slit	

Name:	Prog. Rec. Slit
Height (mm):	0.10
Detector	
Name:	PW3011/20 (Miniprop. large window)
Type:	Point detector
PHD - Lower level (%):	35.0
PHD - Upper level (%):	80.0
Source	
Created by:	Xrd
Application SW:	X'Pert Data Collector vs. 2.1
Instrument control SW:	XPERT-PRO vs. 1.6
Instrument ID:	0000000080961113
Scan	
Start time stamp:	18/04/2015 08:34:38 ã
End time stamp:	18/04/2015 09:07:10 ã
Scan axis:	Gonio
Scan range (°):	2.000 - 80.000
Step size (°):	0.020
No. of points:	3900
Scan mode:	Continuous
Counting time (s):	0.50

No.	Pos. [°2Th.]	d-spacing...	Rel. Int.	FWHM ['...	Matched by	Area [cts*°2Th	Backgr.[cts]	Height [cts]
1	26.6769	3.34169	100.00	0.6298	00-048-1945	26.32	55.00	42.37
2	44.0660	2.05336	84.09	1.1520		54.73	26.00	35.63
3	52.0375	1.75746	50.03	0.0435		0.92	49.00	21.20