ANALYSIS OF LATTICE PARAMETER, ERROR, AND ENERGY BAND GAP IN CADMIUM SULFIDE (CDS) SEMICONDUCTOR MATERIAL

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ABSTRACT

Has successfully analyzed the lattice parameter, error, and energy band gap of *Cadmium Sulfide* (CdS) material. CdS is a semiconductor material. In this study, the CdS used is a material with a cubic crystal structure using database from the International Center for Diffraction Data (ICDD), then the data is calculated using the Cramer-Cohen method. From these data the resulting lattice parameter of a = b = c = 5.823791777 Å with an average error of 0.00034%. The band gap energy calculation of CdS material is 2,477 eV.

Keywords: CdS, lattice parameter, error, energy band gap

INTRODUCTION

Research of analysis lattice parameter, error, and energy band gap in CdS are exciting to be reviewed, as did previous researchers [1-25]. Previous researchers have successfully developed the application of analysis lattice parameter, error, and energy band gap in CdS for daily life in all fields of scientific disciplines including: An overview of semiconductor photocatalysis. Journal of Photochemistry and Photobiology [1], Crystalline structures properties doped RuO_2 (0, 2, 4, 6%) of thin film $LiNbO_3$ [2], An EKF assimilation of AMSR-E soil moisture into the ISBA land surface scheme [3], Verification of existence of cubic zirconia at high temperature [4], Crystalline structure and optical properties of thin film $LiTaO_3$ [5], Photoelectrocatalytic reduction of carbon dioxide in aqueous suspensions of semiconductor powders [6], Resolution of the Band Gap Prediction Problem for Materials Design [7], Crystal structure of fast lithium-ion-conducting cubic $Li_7La_3Zr_2O_{12}$ [8], Effect of temperature on properties of cadmium sulfide nanostructures synthesized by solvothermal method [9], Improved optical and structural properties of cadmium sulfide nanostructures for optoelectronic applications [10], Tuning electrical and raman scattering properties of cadmium sulfide nanoribbons via surface charge transfer doping [11], Journal self-citation study for semiconductor literature: Synchronous and diachronous approach [12], Journal co-citation analysis of semiconductor literature [13], Modified eccentric descriptors of crystal cubic carbon [14], Molecular dynamics (MD) simulation of uniaxial tension of some single-crystal cubic metals at nanolevel [15], Chemically deposited CdS by an ammonia-free process for solar cells window layers [16], First-principles study of the effect of organic ligands on the crystal structure of CdS nanoparticles [17], Error analysis of continuous GPS position time series [18], The relationship between the distribution of electronic states and the optical absorption spectrum of an amorphous semiconductor: An empirical analysis [19], Analysis of students' errors in solving probability based on Newman's error analysis [20], A simple method for the determination of lattice parameters from powder X-Ray diffraction data [21], Topological Characterization of Carbon Graphite and Crystal Cubic Carbon Structures [22], Analysis of Students' Errors on the Fraction Calculation Operations Problem [23], Lattice constants analysis of baxsr1-xtio3 ceramic for x =0.3; 0.5 and 0.7 by visual basic program [24], Microstructure and nanoindentation behavior of Cu composites reinforced with graphene nanoplatelets by electroless co deposition technique [25].

The purpose of this experiment is to analyzed the lattice parameter, error, and energy band gap of *Cadmium Sulfide* (CdS) material.

METHOD

This study uses Excel software with calculations using the cramer method. In this method, determine the matrix from the ICCD data calculation and find the determinant of the matrix. So that the lattice parameter value obtained from the calculation results. The difference between the calculated lattice parameter and the theoretical lattice parameter is the error value of the method.

Find the lattice parameter (a=b=c) of the cube for the vertex of many distance between fields, d [26] (Kurniawan 2021):

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

According to Bragg's law :

$$\lambda = 2d \sin\theta$$

$$\lambda^2 = 4d^2\sin^2\theta \text{ atau } \frac{1}{d^2} = \frac{4\sin^2\theta}{\lambda^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

Combining equations (1) and (2) results in:

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2} = \frac{4\sin^2\theta}{\lambda^2}$$

$$\sin^2\theta = \frac{\lambda^2(h^2 + k^2 + l^2)}{4a^2}$$

To obtain the lattice parameter value (a = b = c) using the relationship,

$$\sin^2\theta = \frac{\lambda^2(h^2 + k^2 + l^2)}{4a^2}, \text{ and}$$

$$\sin^2\theta - \frac{\lambda^2}{4a^2}(h^2 + k^2 + l^2) = D\sin^2 2\theta$$

$D\sin^2 2\theta \lll 0$ is the smallest measuring error

$$\sin^2\theta = \frac{\lambda^2}{4a^2}(h^2 + k^2 + l^2) + D\sin^2 2\theta$$

Finally obtained the form:

$$\sin^2\theta = B\alpha + A\delta$$

Where,

$$B = \frac{\lambda^2}{4a^2} , \alpha = h^2 + k^2 + l^2, A = \frac{D}{10} , \text{ dan } \delta = 10\sin^2 2\theta$$

Arrange according to the order 2 x 2 matrix and find the values of B and A using the Cramer method.

$$\begin{pmatrix} B\sum\alpha^2 & A\sum\alpha\delta \\ B\sum\alpha\delta & A\sum\delta^2 \end{pmatrix} \begin{pmatrix} B \\ A \end{pmatrix} = \begin{pmatrix} \sum\alpha\sin^2\theta \\ \sum\delta\sin^2\theta \end{pmatrix}$$

RESULT AND DISCUSSION

Analysis of the carbon crystal structure

Analysis of the carbon crystal structure that has been characterized using XRD (X-Ray Diffraction) produces data in the form of a difragtogram, which is a graph of the relationship between the intensity (I) of the crystal spectrum peak and the scattering angle (2θ). The

diffragtogram shows the spectral peaks that appear in the sample. Intensity diffraction results using XRD can be expressed in ICDD (FIGURE 1).
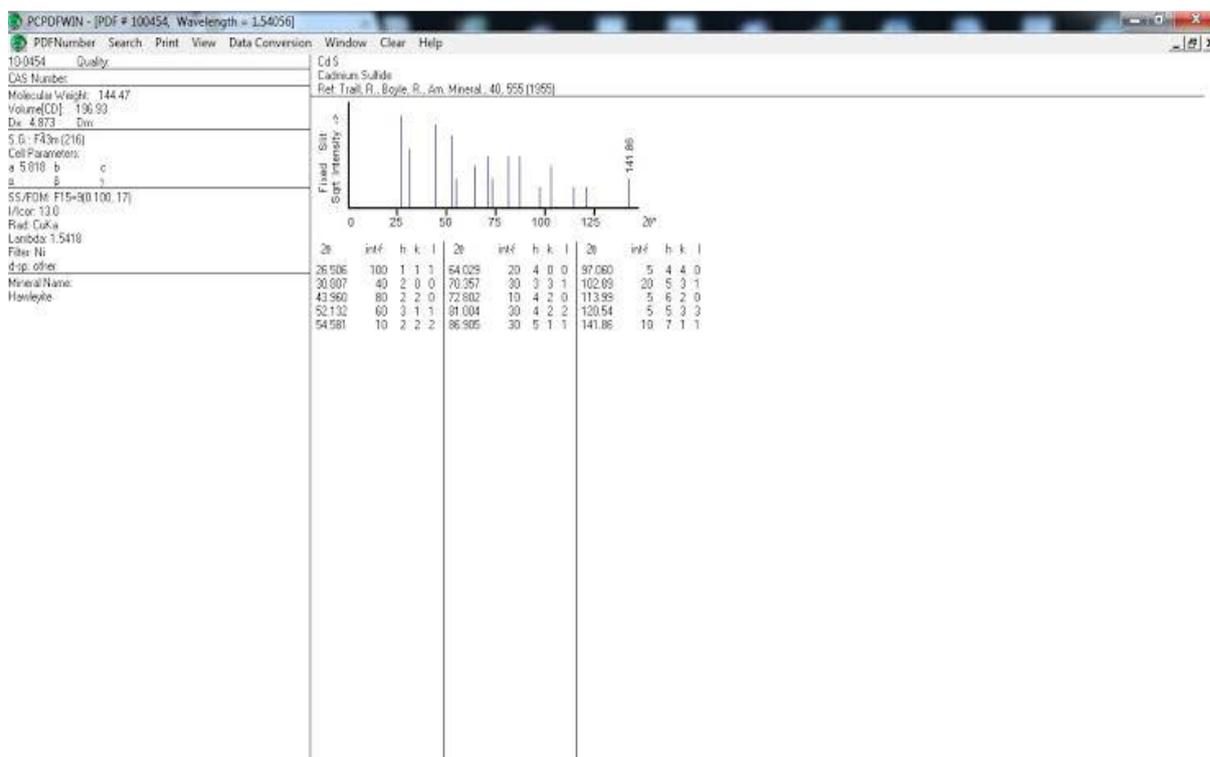

FIGURE 1. Database ICDD Cadmium Sulfide (CdS)

From the data, identified 16 diffraction peaks using excel formula and Cramer-Cohen method. Through the Cramer-Cohen method the following is obtained:

$$\begin{pmatrix} 10975 & 2682,085048 \\ 2682,085048 & 865,4161341 \end{pmatrix} \begin{pmatrix} B \\ A \end{pmatrix} = \begin{pmatrix} 192,4311078 \\ 47,03649806 \end{pmatrix}$$

The results above it's solved by a matrix determinant from excel formula. So we can get the lattice parameter of CdS of a = b = c = 5.82379177 Å. CdS is a crystal, where the crystal is a material that has a regular and periodic arrangement of atoms in a three-dimensional structure. The CdS semicondutor material has a cubic crystal structure. The experimental results lattice parameters are closed to the literature on the ICDD database. The percentage of errors from the experimental calculation of the CdS lattice parameter is 0.00034%. This indicate that the percentage of calculation error is very small.

Analysis bandgap of the carbon semiconductor

Conductivity is a measure of ability of a material to conduct electric current. From this definition, it can be categorized according to their conductivity into conductors, semiconductors, and insulators. A semiconductor is a material with an electrical conductivity that is between an insulator and a conductor. To explain the conductivity of a material, the concept of energy bands is often used. There are two energy bands, namely the valence band and the conduction band. The electrons from the valence band must have a minimum energy

equal to the energy gap to get to the conduction band. The energy gap calculation can use the equation as follows [13] (Sze 1981) :

$$E_g = -\ln\left(\frac{n_i{}^2}{N_c\,N_v}\right)kT$$

Where:

Eg = energy gap in electron volt (eV)

n_i = intrinsic carrier concentration (cm^{-3})

N_c = effective conduction bamd density of states (cm^{-3})

N_v = effective valence band density of states in (cm^{-3})

k = Boltzmann constant is $1{,}38 \times 10^{-23}$ J.K^{-1}

T = temperature (Kelvin)

With the value of the intrinsic carrier concentration (n_i) in CdS of 0.012 cm^{-3}, the value of the carrier electron concentration in the conduction band N_c is 2.41×10^{18} cm^{-3}, the concentration value the carrier hole in valence band (N_v) is 25.7×10^{18} cm^{-3} and temperatur (T) = 300 K. Based on the energy gap analysis E_g at CdS is 2.477 eV. The CdS energy gap in literature is 2.48 as can be seen in FIGURE 2 [27] (Gildenblat and Schmidt 1992). This indicate that the energy gap in the analysis is close to the true value.

Parameter Unit	E_g (eV)	m_c (m_0)	m_v (m_0)	N_c (10^{18} cm^{-3})	N_v (10^{18} cm^{-3})	n_i (cm^{-3})
Si (X)	1.12	1.18	0.55	32.2	10.2	7×10^9
Ge (L)	0.66	0.22	0.34	2.6	5.0	1×10^{13}
GaAs (Γ)	1.42	0.063	0.52	0.40	9.41	2×10^6
InP (Γ)	1.34	0.079	0.60	0.56	11.6	1×10^7
AlAs (X)	2.15	0.79	0.80	17.6	18.1	15.
GaSb (Γ)	0.75	0.041	0.82	0.21	18.6	1×10^{12}
AlSb (X)	1.63	0.92	0.98	22.1	24.2	5×10^5
InAs (Γ)	0.36	0.023	0.57	0.09	10.9	9×10^{14}
GaP (X)	2.27	0.79	0.83	17.6	18.9	1.6
AlP (X)	2.45	0.83	0.70	20.0	14.8	0.044
InSb (Γ)	0.17	0.014	0.43	0.04	7.13	2×10^{16}
ZnS (Γ)	3.68	0.34	1.79	4.97	60.3	2×10^{-12}
ZnSe (Γ)	2.71	0.16	0.65	1.61	13.1	8×10^{-5}
CdS (Γ)	2.48	0.21	1.02	2.41	25.7	0.012
CdSe (Γ)	1.75	0.112	1.51	0.94	46.5	1×10^4
CdTe (Γ)	1.43	0.096	0.76	0.75	16.5	3×10^6

FIGURE 2. Band Gap Energy Cadmium Sulfide (CdS)

CONCLUSION

Has successfully analyzed the lattice parameter, error, and energy band gap of *Cadmium sulfide* (CdS) material. Based on the results of data processing, it can be concluded that the results of calculating the lattice parameter value with the Crammer Cohen method on CdS material are close to the lattice parameter value in the existing literature. The lattice parameter

of ICDD of CdS are a = b = c = 5.818 Å, while with the Cramer Cohen method the lattice parameter values a = b = c = 5.82379177. It can be concluded that the calculation of lattice parameters using the Crammer Cohen method is considered accurate because the error value obtained is very small. The percentage of errors from the experimental calculation of the CdS lattice parameter is 0.00034%. Then, the band gap energy calculation of CdS material are close too with value on literature, where in literature the band gap energy is 2.48 eV, while the band gap energy from calculation is 2.477 eV.

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