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THE PARAMETER ANALYSIS IN CUBICAL STRUCTURED *CADMIUM TELLURIDE* (CDTE) SEMICONDUCTOR MATERIALS

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ABSTRACT

Cadmium telluride (CdTe) semiconductor materials will be used to analyze the energy gap, lattice parameters, and error value of these cubical structured crystal materials. The data that we used to be analyzed is using data from the *International Center for Diffraction Data (ICDD)* that used the *X-ray Diffraction* (XRD) method. This research has been successfully analyzing energy gap, lattice parameters, and the error value of *Cadmium telluride* (CdTe) materials which have a cube-shaped crystal structure. The result of the gap energy analysis of *Cadmium telluride* (CdTe) with a cubical structure yields a value of 1.43 eV. The lattice parameters of *Cadmium telluride* (CdTe) with a cubical structure analyzed by the Cramer-Cohen method yields a value of a = b = c = 9.922 Å. The error value of *Cadmium telluride* (CdTe) with a cubical stcucture yields a value of 6.75 x 10^{-4} %.

Keywords: *Cadmium Telluride* (CdTe), energy gap, lattice parameter, Cramer-Cohen method, analysis of errors

INTRODUCTION

The purpose of this research is to analyze the energy gap, lattice parameters, and the error value of the semiconductor materials called Cadmium telluride (CdTe) with a cube structure. The analysis of the error value is intended to find out how accurate the calculation results of the lattice parameter of semiconductor materials, especially Cadmium telluride. This research is also analyze the energy gap of the Cadmium telluride material. The energy gap can indicate whether the material is a conductor, semiconductor, or isolator.

Research on stable crystalline compounds formed on Cadmium and Telluride which are used as material of thin film solar cells [1], metal interfaces for high performance solar cells [2], development of ZnTe as a back contact material for thin film Cadmium Telluride solar cells [3], thin film used as back contact for CdTe solar cells [4], determination of the extinction coefficient of CdTe, CdSe, and CdS nanocrystals [6]. Research related to energy gap [7], electron pumping and spectral density dynamics [8], energy gap at low density [10], energy gap-refractive index relations in semiconductors [11], semiconductor optoelectronic devices [12], semiconductor devices [13]. Research related to lattice parameters, strain state and composition in semipolar III-nitrides [14], CdTe thermal parameters studied by single-crystal x-ray diffraction [15]. Research method Cramers rule for quaternionic systems of linear equation [17], application of the cramer rule in the solution of sparse systems of linear algebraic equations [19], data analysis software design for cube crystal structure with analytic and cohen methods [20].

Experiments related to error analysis for the optimal control of magneto-static fields [22], a posteriori error analysis for a viscous flow-transport problem [23], analysis of errors of derived slope and aspect related to DEM data properties [24], measurement errors and their consequences in protein crystallography [25], the analysis of errors of omission in english narrative composition made by EFL students [27], error analysis in writing discussion text [28]. Research on Bragg's law on electrons [29]. Research on semiconductor materials based on energy gap [30].

METHOD

The research method is carried out by inputting the results of XRD analysis data for Cadmium Telluride (CdTe) contained in the ICDD literature (FIGURE 1), then inputting the scattering angle data and field dimensions on each x, y, and z axes. After that, input data obtained into Microsoft Excel and processed using the Cramer-Cohen method, so that the lattice parameter values will be obtained from Cadmium Telluride (CdTe). Compare the calculated lattice parameter values with the lattice parameter values in the literature obtained from ICDD and get the error value for the material. Determination of bandgap energy of Cadmium Telluride by inputting intrinsic carrier concentration (ni) values, effective conduction of the state density band (Nc), effective valence band density of the state (Nv), Boltzmann constant (k), and temperature (T) at the equation [9], then obtained the value of the bandgap energy calculation results. Then, compare the calculated band gap energy value of Cadmium Telluride with literature that we get before [10].

RESULT AND DISCUSSION

Semiconductor material

The Semiconductor material is a material that is semi-conductor because the energy gap formed by the structure of this material is smaller than the energy gap of the insulating material but larger than the energy gap of the conductor material, thus allowing electrons to move from one constituent atom to another constituent atom with the certain treatment of the material. such as the provision of voltage, temperature changes, and so on. Therefore, semiconductors can be semi-conducting. Semiconductors can be semi-conductive [24].

Bragg's law

Bragg's law states that the surface plane of atoms in a crystal that acts as a mirror on X-rays is able to reflect incoming rays at the same angle as the angle they reflect. Mathematically, Bragg's Law is formulated as follows [1]

$$2d \sin\theta = n\lambda \quad (1)$$

where d is the plane distance between parallel lattices [23].

Lattice parameter

The crystal structure in each shape has different lattice parameter values. The lattice parameter describes the unit cell size in each material [13]. The lattice parameters have constants denoted as *"a", "b", "c", "α","β"* and *"γ". "a", "b"* and *"c"* describe a distance between atoms in the *x, y,* and *z* axis unit cell. Meanwhile *"α","β"* and *"γ"* explains the angle between each axis, namely between *y* and *z* axis, *x* and *z* axis, *x* and *y* axis.

XRD data analysis Cadmium Telluride (CdTe)

Analysis of the crystal structure of Cadmium Telluride which has been characterized by using the X-Ray Diffraction (XRD) method produces data in which the detector records and processes the x-ray signal and processes it in the form of a graph called a diffractogram. The diffractogram states the relationship between the intensity [1] and the diffraction angle (2θ). The results of the intensity diffraction using the X-Ray Diffraction (XRD) method can be expressed in the form of the International Center for Diffraction Data (ICDD).

Cadmium Telluride (CdTe) has a unique crystal structure, one of which is a cube. The cube crystal structure has the same lattice parameter value, namely a = b = c, and the same value of the angle between the axes, namely $\alpha = \beta = \gamma = 90°$. The crystal structure only requires 1 lattice parameter value to describe the characteristics of the crystal structure, which is denoted by "a". Then, the distance between the lattice parameters in the crystal structure is denoted by "d", which is formulated mathematically as follows (2) [16],

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \tag{1}$$

where h, k, and l are the dimensions of the planes on the x, y, and z axes, respectively. Then the equation (1) substituted in the equation (2), so that the equation (3),

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

$$\sin^2\theta - \frac{\lambda^2}{4a^2}\left(h^2 + k^2 + l^2\right) = 0 \tag{3}$$

By substituting zeros in the equation (4) with the aim of the smallest instrument measurement error or error, which is described by $D\sin^2 2\theta$, so that the equation (5),

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

$$\sin^2\theta = \frac{\lambda^2}{4a^2}\left(h^2 + k^2 + l^2\right) + D\sin^2 2\theta \tag{5}$$

$$\sin^2\theta = \mathrm{X}\psi + Y\chi \tag{6}$$

with $X = \frac{\lambda^2}{4a^2}$, $Y = \frac{D}{10}$, $\psi = h^2 + k^2 + l^2$, and $\chi = 10\sin^2 2\theta$. Then change the equation (7) into the form of a linear matrix shown in equation (8),

$$\begin{pmatrix} \Sigma\psi\sin^2\theta \\ \Sigma\chi\sin^2\theta \end{pmatrix} = \begin{pmatrix} \Sigma\psi^2 & \Sigma\psi\chi \\ \Sigma\psi\chi & \Sigma\chi^2 \end{pmatrix}\begin{pmatrix} X \\ Y \end{pmatrix} \tag{8}$$

Equation solution (8) demonstrated the Cramer-Cohen method for cubic crystal structures. Cadmium Telluride (CdTe) is a type of semiconductor that has a cubic crystal structure. Based on data obtained from the International Center for Diffraction Data (ICDD) in FIGURE 1, Cadmium Telluride (CdTe) has a lattice parameter literature value of a = b = c = 6,481 Å. Then by calculation using the Cramer-Cohen method, Cadmium Telluride (CdTe) has a lattice parameter value of a = b = c = 6.482 and with an average error analysis of 9.22 x 10^{-3} %.

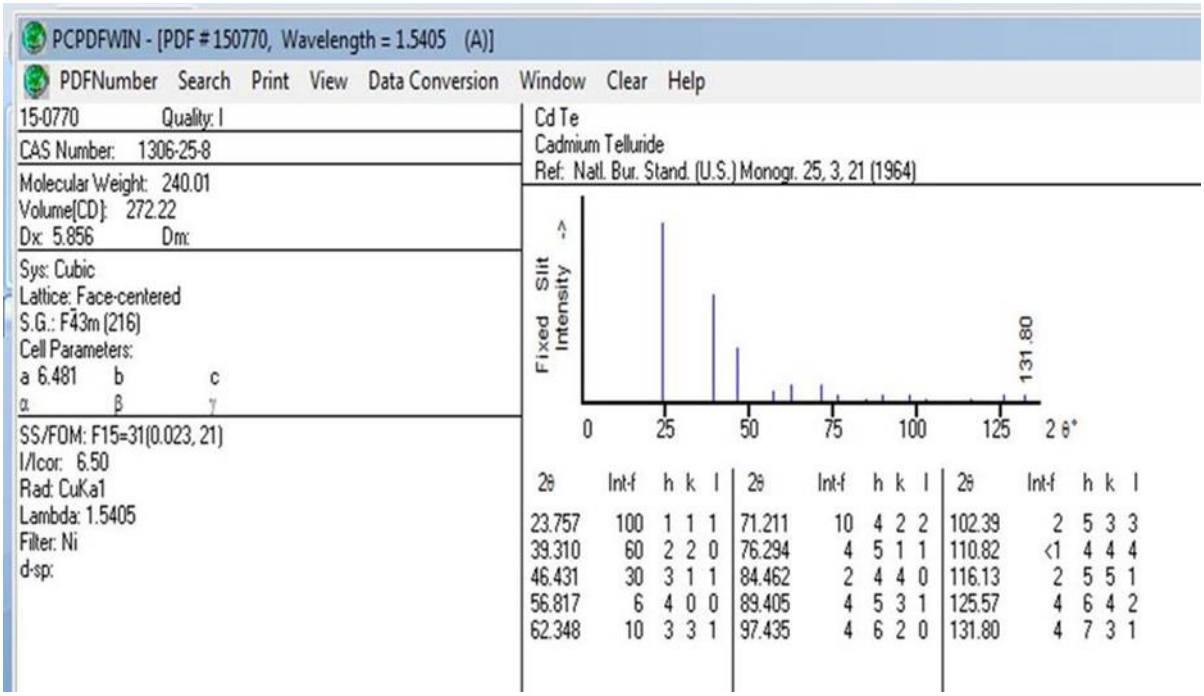

FIGURE 1. ICDD *Cadmium Telluride* (CdTe)

Band gap energy Cadmium Telluride (CdTe)

An insulator is the basic structure of a semiconductor material that has an energy gap of less than 1 electron volt (eV). Because the energy gap is not too large, then the thermal excitation is very possible for electrons to move from the valence band to the conduction band through the energy gap [6]. The calculation of the energy gap for each material can use the equation (9) [11],

$$Eg = -\ln\left(\frac{ni^2}{NcNv}\right)kT \tag{9}$$

Where :

- Eg is the energy gap in electron volts (eV)
- ni is the intrinsic carrier concentration in cm^{-3}
- Nc is the effective conduction of the state density band in cm^{-3}
- Nv is the effective valence band density of the state in cm^{-3}
- k is the Boltzmann constant of JK-11,38×10^{-23}
- T is the temperature in Kelvin

TABLE 1. Database band gap energy Cadmium Telluride (CdTe)

Parameter Unit	Eg (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 x 10^9
Ge (L	0.66	0.22	0.34	2.6	5.0	1 x 10^{13}
GaAs (***Γ***)	1.42	0.063	0.52	0.40	9.41	2 x 10^6
InP (***Γ***)	1.34	0.079	0.60	0.56	11.6	1 x 10^7
AlAs(X)	2.15	0.79	0.80	17.6	18.1	1.5 x 10
GaSb (***Γ***)	0.75	0.041	0.82	0.21	18.6	1 x 10^{12}
AlSb (X)	1.63	0.92	0.98	22.1	24.2	5 x 10^5
InAs (***Γ***)	0.36	0.023	0.57	0.09	10.9	9 x 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	4.4 x 10^{-2}
InSb (***Γ***)	0.17	0.014	0.43	0.04	7.13	2 x 10^{16}
ZnS (***Γ***)	3.68	0.34	1.79	4.97	60.3	2 x 10^{-12}
ZnSe (***Γ***)	2.71	0.16	0.65	1.61	13.1	8 x 10^{-5}
CdS (***Γ***)	2.48	0.21	1.02	2.41	25.7	1.2 x 10^{-2}
CdSe (***Γ***)	1.75	0.112	1.51	0.94	46.5	1 x 10^4
CdTe (***Γ***)	1.43	0.096	0.76	0.75	16.5	3 x 10^6

Based on the energy gap analysis on Cadmium Telluride (CdTe) in TABLE 1 is 1.43 eV with an intrinsic carrier concentration value (ni) of 3 x 106 cm^{-3}, the value of the concentration of electron carriers in the conduction band (Nc) is equal to 7.5 x 10^{17} cm^{-3}, the value of the carrier concentration in the velocity band (Nv) equal to 1.65 x 10^{19} cm^{-3}, and a temperature of 300 K. The energy gap of Cadmium Telluride (CdTe) in the literature is 1.43 eV [10]. This shows that the calculation of the energy gap analysis is following the literature value (true value) of the energy gap in the Cadmium Telluride (CdTe) material, which is 1.43 eV.

CONCLUSION

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 Cadmium telluride material are close to the lattice parameter value in the existing literature with an average error value of 9.22 x 10^{-3} %. The lattice parameter values obtained from the International Center for Diffraction Data (ICDD) of Cadmium telluride material are a = b = c = 6,481 Å, while with the Cramer Cohen method the lattice parameter values are a = b = c = 6,482 Å. Therefore, 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.

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