The Characterization of Semiconductor Crystal Sn(Se_{0.8}Te_{0.2}) Prepared by Bridgman Technique for Solar Cell

ANGGRAENI Kumala Dewi¹,a and Dr. ARISWAN²,b

¹Gadjah Mada University, Indonesia
²Yogyakarta State University, Indonesia

aanggraenikumala@gmail.com, bariswan@uny.ac.id

Keywords: Semiconductor, Crystal Sn(Se_{0.8}Te_{0.2}), Bridgman Technique

Abstract. These study aims determine the characterization of structure and chemical composition of crystal Sn(Se_{0.8}Te_{0.2}). The growth of crystal Sn(Se_{0.8}Te_{0.2}) is obtained by preparation outcome through Bridgman Technique. Hence, characterized by using the XRD (X-Ray Diffraction) for to determine the crystal structure, SEM (Scanning Electron Microscopy) to determine the surface morphology, and EDAX (Energy Dispersive Analysis of X-ray) to determine the chemical composition. The four samples are characterized results indicate that crystal Sn(Se_{0.8}Te_{0.2}) has orthorhombic structure with the results of the samples I and III have the highest intensity. SEM characterization result for sample I and III indicate that the formation of crystal Sn(Se_{0.8}Te_{0.2}) is characterized by the presence of grains. Based on the results of EDAX, it is known that the crystal Sn(Se_{0.8}Te_{0.2}) contains elements of Sn, Se, and Te with a percentage of the chemical composition of the sample I is Sn = 39.85%, Se = 36.09%, and Te = 2.57 %. Comparison the molarity of the sample I is Sn: Se: Te is 1: 0.90: 0.10.

Introduction

Solar energy can be utilized as a thermal or even converted into electrical energy directly [1]. Rahmat Adiprasetya Al Hasibi (2011) said that the technology can be used directly to convert solar energy into electrical energy is photovoltaic technology (PV) or commonly called solar technology. Photovoltaic (PV) technology has low CO2 emissions as well as flexible modular structures [2,3]. Photovoltaic (PV) technology consisting of photovoltaic cells or solar cells is a semiconductor consisting of a p-n connection. When exposed to sunlight, it will create electrical energy. The change of solar energy into electrical energy is called as the photovoltaic effect [4].

Tin Selenide (SnSe) is a p-type semiconductor of a mixture of elements of Group IV (Sn) and Group VI (Se), with high power factor and ultralow (very low) thermal conductivity makes the crystal structure is orthorhombic and highly suitable for materials high efficiency [5]. Based on research conducted by Kumar et al (2012), he notes SnSe has a energy gap of 1.3 eV. It further demonstrates that SnSe is suitable for use as semiconductor materials for solar cell materials [6]. Therefore, for this research about the semiconductor Sn(Se_{0.8}Te_{0.2}) should be studied to know its application to photovoltaic technology or solar cell. In addition, there is still minimum research on semiconductor Sn(Se_{0.8}Te_{0.2}) [7].

Research on the characterization of structure and chemical composition of Sn(Se_{0.8}Te_{0.2}) result of preparation with Bridgman Technique is conducted to the growth of the crystal which then will be given treatment to the crystal to know the quality of crystal produced. Sn(Se_{0.8}Te_{0.2}) has a tendency towards the nature of the SnSe semiconductor because the magnitude of the Se content is compared to Te. SnSe is a compound which composed of abundant elements on earth and this is shown intrinsically with ultralow (very low) thermal conductivity. In addition, the multi-layered SnSe and anisotropic crystal structure with the space group of JCPDS data is Pnma (62). SnSe adopts a layered orthorhombic crystal structure at room temperature which can be derived from three-dimensional distortion of NaCl structure [8].

After crystallization process, the characterization of crystal Sn(Se_{0.8}Te_{0.2}) using the XRD (X-Ray Diffraction), SEM (Scanning Electron Microscopy), and EDAX (Energy Dispersive Analysis X-
Ray) is done. The purpose of using the XRD is to know the parameters of the crystal lattice. SEM is used to determine the structure and morphology of the crystal surface, and EDAX is used to determine the chemical composition quantitatively by utilizing the interaction of electron collisions with the material. The results of this study are expected to be used as a reference and provide information on research in the field of solar technology, especially understanding of the preparation and characterization of semiconductor materials Sn(Se\textsubscript{0.8}Te\textsubscript{0.2}) by using Bridgman Technique.

Theory

**Crystal.** The crystals are composed of solid, regular, geometric, solid atoms so that they are repeatedly arranged in all directions in the crystal arrangement [9]. According to Malvino, crystals are the joined atoms that then form into a solid and the atoms regulate themselves in a particular order pattern [10].

Crystals are divided into three in terms of their structure, namely monocrystal, polycrystal, and amorphous. In monocrystal or commonly referred to as single crystals have atoms or constituents fixed structure. This is because the atom or molecule compilers are arranged regularly in a three dimensional pattern. In addition, the patterns are arranged repeatedly (periodically) within an infinite long range. Polycrystal is a collection of single crystals that have very small size and accumulate to form solid objects. In the amorphous formed by the process of rapid cooling has a pattern of irregular and irregular arrangement of atoms or molecules repeatedly. An excessive cooling process causes the atoms to not properly occupy the lattice [11].

**Lattice parameters.** The lattice parameters are the length of each cell space in the direction of the crystallographic axis. Usually called the lattice constant and is also called the axis lattice parameters a, b, and c. The angles formed by the lines bc, ac, and ab are referred to as α, β, and γ [12].

If a crystal has orthorhombic symmetry (α = β = γ= 90) with the size of the lattice parameter (a ≠ b ≠ c), so the diffraction angle of the crystal plane (hkl) can be calculated by the Bragg equation of the relation between the fields, as follows:

\[
n\lambda = 2d \sin\theta \tag{1}
\]

\[
\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \tag{2}
\]

Then substituting the Bragg equation (1), to obtain the equation:

\[
\frac{4\sin^2 \theta}{d^2} = \left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right) \tag{3}
\]

\[
sin^2 \theta = \frac{A}{4} \left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right) \tag{4}
\]

Based on the above equation it can calculate the lattice parameter values a, b, and c with the equation:

\[
sin^2 \theta = Ah^2 + Bk^2 + Cl^2 \tag{5}
\]

Then the lattice parameters a, b, and c can be written as follows [13]:

\[A = \frac{\lambda^2}{4d^2}, \text{ then } a = \frac{\lambda}{2\sqrt{A}}\] \tag{6}

\[B = \frac{\lambda^2}{4b^2}, \text{ then } b = \frac{\lambda}{2\sqrt{B}}\] \tag{7}

\[C = \frac{\lambda^2}{4c^2}, \text{ then } c = \frac{\lambda}{2\sqrt{C}}\] \tag{8}
Crystal Sn(Se0.8Te0.2). Crystal Sn(Se0.8Te0.2) is a combined semiconductor or alloy of an SnSe semiconductor that is doped with the element Te. Semiconductor SnSe has a p-type conductivity because of its high coefficient of absorption and it is quite high, which is $10^5$ cm$^{-1}$. In semiconductors SnTe has an n-type conductivity because of the increase of temperature in the furnace process and the material composition at SnTe sources causes the carrier concentration to decrease.

The purpose of combining the semiconductor Sn(Se0.8Te0.2) in this research is to produce an energy gap corresponding to the solar energy spectrum. The semiconductor Sn(Se Te) has an orthorhombic structure for ratio Sn(Se0.8Te0.2). This is because the amount of Se material is more dominating than the Te material, also due to the replacement of the composition of several Se atoms with Te [14].

The Group IV - VI on the periodic table is a chalcogenide semiconductor material that has a variable energy gap band, so it is enabling the chalcogenide semiconductor material to utilize various regions of the solar spectrum. The groups of compounds belonging to the IV - VI groups in the form of binary compounds are SnS, SnSe, SnTe, PbS, PbSe, and PbTe. In ternary compounds are Sn (Se S), Sn (Se Te), Sn (S Te), Pb (Se S), Pb (Se Te), Pb (S Te), Sn (Pb S), Sn (Pb Se), and Sn (Pb Te).

Based on research on Sn(S Te) conducted by Anshori (2016) with Sn(S0.8Te0.2) and Nuril (2016) with Sn(S0.6Te0.4) is semiconductor material in the group IV - VI. Semiconductor materials Sn(S0.8Te0.2) and Sn(S0.6Te0.4) are alloys of SnS and SnTe. Then, for the semiconductor Sn(S0.8Te0.2) has been heated in the furnace and it is treated in the form of heating flow variation. While for the semiconductor Sn(S0.6Te0.2) is treated with mass variation. Furthermore, characterization of the XRD and SEM-EDAX is done for both of the semiconductors [15,16].

The result of the XRD characterization obtained that Sn(S0.8Te0.2) and Sn(S0.6Te0.4) crystals are more directed to SnS. It can be shown from the diffraction angle data and the peak intensity Sn(S0.8Te0.2) and Sn(S0.6Te0.4). Also, both of the data on Sn(S0.8Te0.2) and Sn(S0.6Te0.4) crystals were compared with the same standard data (JCPDS NO.39-0354). The standard data (JCPDS NO.39-0354) leads to the SnS material, so from their comparison known that there is a shift in the diffraction angle. The diffraction angle shift can affect the value of lattice parameters obtained with standard data. The values of SnS crystal lattice parameters in standard data (JCPDS NO.39-0354) are $a = 4.329$ Å, $b = 11.19$ Å, and $c = 3.983$ Å. The parameters of Sn grid parameters Sn(S0.8Te0.2) in sample III are the best samples from other samples, namely $a = 4.3154$ Å, $b = 11.2509$ Å, and $c = 3.9637$ Å. The value of the lattice parameter is less than the price of the standard SnS data lattice parameter (JCPDS NO.39-0354). In the Sn(S0.6Te0.4) crystals, the lattice parameter values for sample I which are the best samples are $a = 4.426$ Å, $b = 11.151$ Å, and $c = 3.959$ Å. This shows the value of the lattice parameter of the research result is greater than the value of SNS lattice parameter of the standard data. This difference of lattice parameter values can be due to the presence of the material on Sn(S0.8Te0.2) and Sn(S0.6Te0.4), so that it can affect the price-quantity of the second lattice parameter of the crystal.

The results of the characteristics crystal Sn(S0.8Te0.2) by Anshori and Sn(S0.6Te0.4) by Nuril using SEM shows that the crystals formed are polycrystal with orthorhombic structure. Based on the results of EDAX characterization, it is known that the preparations performed have been successful, so the formation of Sn(S0.8Te0.2) and Sn(S0.6Te0.4) consists of elements Sn, S, and Te. However, from the data obtained that there is little difference of mol comparison Sn, S, and Te between the results of research and theory. The result showed that the mole ratio for Sn(S0.8Te0.2) is Sn: S: Te is 1: 0.71: 0.17. The result of the mole ratio is theoretically 1: 0.8: 0.2. The difference in the mole ratio can be due to the oxidation of the sample during the cooling process after the sample is heated. In addition, there have not been mixed elements Sn, S, and Te into semiconductors Sn(S0.8Te0.2).

Temperature temperatures that are too high can also cause the S and Te elements to be slightly lost in the semiconductor Sn(S0.8Te0.2). In the Sn(S0.6Te0.4) the mol ratio Sn: S: Te is 1: 0.57: 0.42. When compared with the mole yield theoretically is 1: 0.6: 0.4. Based on these comparisons, the results appear to be similar between the mole ratio of the theoretical and the research results. The difference in the difference in the mole ratio can be due to the probability of particles being
dissipated unequally between other materials depending on the binding energy as well as the term. In addition, the lack of maximum mixing that occurs during the preparation process can have an effect.

Based on research that has been done by Anshori (2016) and Nuril (2016) it can be a reference in analyzing research on this crystal Sn(Se₀.₈Te₀.₂). This is because the semiconductor materials of Sn (Se Te) and Sn (S Te) semiconductors belong to the same semiconductor group, the semiconductor group of semiconductor alloys of class IV-VI [15,16].

**Crystal Sn (Se Te) for Solar Cell Application.** The ingredients Sn, Se, Te belong to chalcogenide. The chalcogenide semiconductor material is included in Group IV-VI, where it has a variable energy band gap allowing the chalcogenide semiconductor material to utilize various regions of the solar spectrum. In addition, chalcogenide Sn(Se Te) semiconductor materials have suitable optical and electrical properties in solar cell applications [14].

The Tin Selenide (SnSe) material exhibits high chemical stability and attractive physical properties, which is an energy band gap of about 1.3 eV with a high absorption coefficient of 10⁵ cm⁻¹ and is included in p-type conductivity. This property shows that SnSe as a suitable semiconductor material in solar cell applications [7]. In addition, SnSe material is a semiconductor material with a narrow band IV-VI band gap energy. Thus capable of absorbing most of the solar energy, thus reinforcing that the semiconductor material is appropriately used in the fabrication of solar cells [17].

**Result and Discussion**

**The Characterization of Structure on Crystal Sn(Se₀.₈Te₀.₂).** Based on the results analysis from the XRD characteristics (shown in table 1), it can be seen that for the four samples of crystals Sn(Se₀.₈Te₀.₂) have the same crystal structure form as orthorhombic structured polycrystal. It is also seen that the crystals Sn(Se₀.₈Te₀.₂) are more directed toward the data (JCPDS NO.48-1224) are JCPDS data for SnSe. According to Nares Padha et al (2015), this can be due to the number of Se materials that are more dominating materials Te. Therefore, there was a change of composition of several Te atoms replaced by Se. The grid parameter values of the four samples can be obtained from the analysis using the analytic method. The results can then be compared with standard data (JCPDS NO.48-1224) and the following results are obtained:

<table>
<thead>
<tr>
<th>Table 1. Comparison of standard lattice parameter data values (JCPDS NO.48-1224) with analytic method result data.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Comparison of Grid Parameters</strong></td>
</tr>
<tr>
<td><strong>A</strong></td>
</tr>
<tr>
<td>JCPDS SnSe</td>
</tr>
<tr>
<td>Sample I</td>
</tr>
<tr>
<td>Sample II</td>
</tr>
<tr>
<td>Sample III</td>
</tr>
<tr>
<td>Sample IV</td>
</tr>
</tbody>
</table>

Based on the data of analytical method, it can be appreciated that there are differences of lattice parameters values of I, II, III, and IV with standard lattice parameter data values (JCPDS NO.48-1224). This can be due to the semiconductor crystal Sn(Se₀.₈Te₀.₂)is an off the SnSe semiconductor which is doped with the element Te. In the analysis and discussion in the researches of Anshori (2016) on Sn(S₀.₈Te₀.₂) and Nuril (2016) on Sn(S₀.₆Te₀.₄), where there is a difference of grating parameter of research result with JCPDS data caused because the material has an effect as well as a diffraction angle shift. Therefore, previous research can be used as a reference source in analyzing and discussing the structure and value of the lattice parameter of crystal Sn(Se₀.₈Te₀.₂) from the XRD characteristic result. Therefore, the crystal Sn(Se₀.₈Te₀.₂)in this study belongs to the group IV-
VI which is a chalcogenide semiconductor. This further illuminates that the material of Te seems to have an effect on the value of the crystal lattice parameter Sn(Se_{0.8}Te_{0.2}). In addition, the diffraction angle shift also affects the values of lattice parameters obtained with standard data so that there are differences.

**The Characterization on Surface Morphology and Chemical Composition of Crystal Sn(Se_{0.8}Te_{0.2}).** In this study, we choose the samples arbitrarily. Then, samples I and III were characterized using SEM as both samples had the highest intensity compared to the other samples. The result of SEM characteristic in the form of the photo shown at Fig. 1 and Fig. 2. Based on the photographs of samples I and III, it appears that the morphology of the crystalline surface Sn(Se_{0.8}Te_{0.2}) is an orthorhombic polycrystal structure and has a homogeneous surface visible from uniform shapes and colors of the crystals. According to Nares Padha et al (2015), the semiconductor Sn(Se Te) has an orthorhombic structure for ratio Sn(Se_{0.8}Te_{0.2}) because the amount of Se material is more dominating than the Te material, resulting in the replacement of some Se with atoms. Also, in the photograph of SEM characteristic results in both samples (I and III) it can be seen the grain. At 40000x magnification for sample III the grain is larger than the sample I, this shows that the regularity of the atoms in sample III is better than the sample I.

Based on the photographs of samples I and III, it appears that the morphology of the crystalline surface Sn(Se_{0.8}Te_{0.2}) is an orthorhombic polycrystal structure and has a homogeneous surface visible from uniform shapes and colors of the crystals. According to Nares Padha et al (2015), the semiconductor Sn(Se Te) has an orthorhombic structure for ratio Sn(Se_{0.8}Te_{0.2}) because the amount of Se material is more dominating than the Te material, resulting in the replacement of some Se with atoms. Also, in the photograph of SEM characteristic results in both samples (I and III) it can be seen the grain. At 40000x magnification for sample III the grain is larger than the sample I, this shows that the regularity of the atoms in sample III is better than the sample I.

**Figure 1.** Photograph of surface morphology of I sample crystal Sn(Se_{0.8} Te_{0.2}) with (a) 1000x magnification, (b) magnification 10000x, (c) 20000x magnification, and (d) magnification 40000x.
Figure 2. Photograph of surface morphology of III sample crystal Sn(Se0.8 Te0.2) with (a) 1000x magnification, (b) magnification 10000x, (c) 20000x magnification, and (d) magnification 40000x.

But, for the EDAX characteristics, the only sample I is characterized. Results from EDAX characteristics of both samples:

Figure 3. The graph of energy relation resulted from characterization using EDAX with intensity on crystal I sample Sn(Se0.8 Te0.2).

Based on the result of the EDAX characteristic in sample I shows the comparison of the chemical composition in percentage, that is Sn equal to 39.85%, Se equal to 36.09%, and Te equal to 2.57%. It can be known that the difference in comparison of chemical composition between the results of research with the theory. The theoretical mole ratio for Sn: Se: Te is 1: 0.8: 0.2. The existence of another phase indicated by the angular deviation of the XRD characteristic results causes the EDAX results to differ significantly from the theory. The EDAX result also proves that the crystal Sn(Se0.8 Te0.2) has orthorhombic structure. It is because of Se in the experiment is 90% and the theoretical is 80% is higher than Te in experiment is 10% and the theoretical is 20%. It produces that the crystal Sn(Se0.8 Te0.2) is chalcogenide SnSe which is doped by Te.
In another hand, the EDAX characterization is performed on a massive sample. Table 2 shows the chemical composition of massive materials of Sn(S$_{1-x}$Te$_x$) solid. The EDAX results show the compatibility of chemical composition on the massive material. This shows the superiority of vacuum evaporation techniques [18].

**Table 2.** The chemical composition of Sn(S$_{1-x}$Te$_x$) massive materials.

<table>
<thead>
<tr>
<th>Solid Solutions Expected</th>
<th>Chemical Composition (wt %)</th>
<th>Solid Solutions Obtained</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Sn (%)</td>
<td>S (%)</td>
</tr>
<tr>
<td>SnS</td>
<td>52.79</td>
<td>47.15</td>
</tr>
<tr>
<td>Sn(S$<em>{0.80}$Te$</em>{0.20}$)</td>
<td>53.27</td>
<td>37.67</td>
</tr>
<tr>
<td>Sn(S$<em>{0.60}$Te$</em>{0.40}$)</td>
<td>50.26</td>
<td>28.26</td>
</tr>
<tr>
<td>Sn(S$<em>{0.40}$Te$</em>{0.60}$)</td>
<td>50.86</td>
<td>11.94</td>
</tr>
<tr>
<td>Sn(Se$<em>{0.80}$Te$</em>{0.20}$)</td>
<td>46.86</td>
<td>9.08</td>
</tr>
<tr>
<td>SnTe</td>
<td>53.6</td>
<td>-</td>
</tr>
</tbody>
</table>

The EDAX table shows that the surface structures of massive material with sulfur and tellurium dominant are significantly different. The chemical composition of Table 2 in row(a), (b), and (c) related to the orthorhombic structures. The chemical composition of Table 2 in row(d), (e) and (f) looks related to the cubic structures. Crystals Sn(S$_{1-x}$Te$_x$) and Sn(Se$_{0.8}$Te$_{0.2}$) are included in the semiconductor chalcogenide, then the EDAX of Sn(S$_{1-x}$Te$_x$) table is further reinforces the assumption that in crystals Sn(Se$_{0.8}$Te$_{0.2}$), it is dominated by Se. Because of that the crystal Sn(Se$_{0.8}$Te$_{0.2}$) structure is orthorhombic. While the crystalline Sn(Se$_{0.8}$Te$_{0.2}$) will be cubic structure and it is dominated by Te.

**Summary**

The characterization of structure and chemical composition of crystal Sn(Se$_{0.8}$Te$_{0.2}$) between experiment and theoretical did not seem to have significant effect and differences on the structure and parameters of the crystal lattice Sn(Se$_{0.8}$Te$_{0.2}$) by using the XRD and the SEM-EDAX characteristics for surface morphology and chemical composition. The four samples have the same structure of orthorhombic structure. The lattice parameters in the four samples were in sample I of $a = 11.51$ Å, $b = 4.14$ Å, and $c = 4.28$ Å. Sample II is $a = 11.53$ Å, $b = 4.04$ Å, and $c = 4.41$ Å. Sample III is $a = 11.52$ Å, $b = 4.04$ Å, and $c = 4.41$ Å. Sample IV is $a = 11.51$ Å, $b = 4.07$ Å, and $c = 4.42$ Å. Based on the result of SEM characteristics in samples I and III further strengthen the assumption that the morphology of the crystalline surface Sn(Se$_{0.8}$Te$_{0.2}$) is polycrystalline with orthorhombic structure. Also, the EDAX characterization results in sample I show that the Sn(Se$_{0.8}$Te$_{0.2}$) contains elements Sn, Se, and Te. The percentage of chemical composition of sample I, namely Sn = 39.85%, Se = 36.09%, and Te = 2.57%. Comparison of molarity in sample I Sn: Se: Te is 1: 0.90: 0.10. The existence of another phase indicated by the angular deviation of the XRD characteristic results cause the EDAX results to differ significantly from the theory. The EDAX result also proves that the crystal Sn(Se$_{0.8}$Te$_{0.2}$) has an orthorhombic structure. It is because of crystals Sn(Se$_{0.8}$Te$_{0.2}$), it is dominated by Se. From the information that we get about the characterization of structure and chemical composition of crystal Sn(Se$_{0.8}$ Te$_{0.2}$), we can use that information as a data to make semiconductor for the solar cell. We hope for the next research can make the semiconductor of crystal Sn(Se$_{0.8}$ Te$_{0.2}$) as a thin film, so we can identify the energy gap for the solar cell.
References