Intrinsic thin film properties study of hydrogenated silicon using the method of RF-PECVD

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Abstract. Effect of hydrogen dilution on deposition rate, energy band gap, localized state defect - through observation of energy absorption Urbach, and surface roughness of intrinsic thin film was investigated using RF-PECVD. Films were grown on ITO glass substrate. Analysis of energy band gap was conducted to determine changes in the structure of a thin film of a-Si:H. Energy band gap is important to determine the portion of the spectrum of sunlight that is absorbed solar cells. The sun's rays with energy greater than the energy band gap will be absorbed by the solar cell, but the rest will be the thermal energy which results in low efficiency. Characterization using UV-Vis spectrometer and Tauc's plot methods showed that wide energy band gap was greater for larger hydrogen dilution. Moreover, the increase of the hydrogen dilution will decrease the rate of deposition and the Urbach energy. It is estimated that with an increased dilution of hydrogen will be obtained μc-Si:H film structure. This structure is more conductive due to the reduction of residual bandtail defect or dangling bond defects.

1. Introduction
The study of a-Si: H in the growth process is continuing, in order to optimize the performance of this material-based device. The research of this material is very interesting to be further developed, due to the existence of several advantages of a-Si: H material compared to silicon crystals. These advantages include a wide band of energy gap (1.70 - 2.0 eV), the relatively low growth temperature of ~200°C (for crystal growth > 1000 °C), and high light absorption coefficient of 10⁶ cm⁻¹. Low temperatures and substrate preferences are factors that make the growth process relatively inexpensive [1].

One of the major problems found in hydrogenated amorphous silicon-based solar cells (a-Si:H) is its efficiency instability after being exposed to high intensity for extended periods of time. This phenomenon is known as the Staebler-Wronski effect (SWE). High hydrogen content is then known to be one of the causes of SWE, where the bond between silicon-hydrogen is easily released by the effects of irradiation with high intensity leaving the defects in the solar cell material [2]. Therefore, some researchers then developed a PECVD technique to solve this problem.

The optical and electrical properties of a-Si:H thin films grown using PECVD method are strongly determined by the radicals of the hydrogen and SiHₙ atoms (n = 1,2,3) in the plasma, generated by silane gas (SiH₄) dissociation by the collision of electrons and the interaction between the radical and the growth surface [3]. Mechanisms in the PECVD method involved complex chemical-physics processes.
Many factors in the deposition process affect the quality of the resulting thin film. Among them are chamber pressure, substrate temperature, RF power, excitation frequency, and gas flow rate. To optimize the parameters of a-Si:H, such as electrical conductivity and absorption coefficients, it is necessary to know the structure and its properties, in particular its structural defects.

One drawback of a-Si:H material is the low of long-range order and midgap state density, resulting in low electron drift density. This parameter has a strong influence on the PV efficiency of a-Si:H material. To improve the performance of solar cells based on the a-Si:H material, several studies have been conducted by the Solar Cell Materials Research Group, Department of Physics, Sepuluh Nopember Institute of Technology (ITS) Surabaya, Indonesia [4-6]. In this paper, the study focused on the influence of the hydrogen dilution ratio on the quality of the structure through the analysis of energy bandgap and its defect of the resulting layer.

2. Methods of Activities

ITO glass (Indium Tin Oxide) is used as the substrate for depositing the thin film of a-Si:H. To avoid the dirt on the surface of the sample, the substrate was cleaned with alcohol and then rinsed with water both in an ultrasonic cleaner for 15 minutes. After that, the sample was dried or rinsed with nitrogen. The thin film deposition process of a-Si:H was carried out by using Radio Frequency - Plasma Enhanced Chemical Vapor Deposition (RF-PECVD). Phase or energy bandgap engineering process was carried out by varying the hydrogen dilution (R= H2/SiH4), i.e. R = 0, 16, and 36. The conditions of the deposition included 5 watt RF power, 2 torr chamber pressure, 270 °C substrate temperature, and 30 minute deposition time.

The thin film deposition was followed by physical characterization to determine its properties. Properties such as transmittance (absorptivity), energy bandgap, deposition rate, Urbach absorption energy, and particle size, are determined by using the UV-Vis spectrometer. The width of energy band gap is determined using Tauc's Plot method.

3. Results and Discussion

3.1. Transmittance

Figure 1 shows the transmittance shift for the intrinsic thin layer of a-Si:H deposited with different hydrogen dilutions, i.e. R = 0, 16, and 36. Larger hydrogen dilutions will make the film transmit more visible light. This means that as R increases, the transparency of the layer will be greater. Larger transparency can be due to the reduction in localized state or energy band gap defects. High transparency nature of solar cell material is highly desirable, including in the intrinsic thin film of a-Si:H. The thin film optical performance can be obtained from the optical transmittance information.

It is also shown by Figure 1 that the greater dilution of hydrogen will cause thinner film deposition. This is indicated by presence of interference fringe that occurs as a result of a thick change of film. More interference fringe at the same wavelength interval indicates the presence of a thicker film.

3.2. Energy Band Gap (Eg)

Figure 2 shows the results of energy bandgap calculation for R= 36. Energy bandgap calculation using Tauc's Plot method, which is an extrapolation of function [7],

$$[a h \nu]^2 = B (h \nu - E_g)$$  

(1)

where \(a\) is absorption coefficient, \(h \nu\) is the energy of the photon, and \(B\) is the constant showing sharpness (width) of the side of energy bandgap. Intercept on the horizontal axis is obtained by extrapolating linear part of the graph plot to produce energy bandgap. Corrugated part as the result of the interference effect is not included in this calculation.
Results of energy gap calculations for hydrogen dilution variations are shown in Table 1. It appears that the energy bandgap increases with the dilution of hydrogen. The increase is caused by the increase of hydrogen bonding concentrations or the increased degradation passivation process, and the reduced tail defects.

**Table 1** Energy bandgap for several variations of hydrogen dilution.

| No | \(R=\text{H}_2/\text{SiH}_4\) | \(E_g\) (eV) |
|----|------------------|----------|
| 1. | 0                | 1.65     |
| 2. | 16               | 1.70     |
| 3. | 36               | 1.80     |
3.3. Deposition Rate

The rate of thin film deposition is determined using the thickness data of thin film and measurement deposition time. The thickness of the thin film \( (d) \) is calculated by [8]

\[
d = \frac{1}{2n_1(1/\lambda_1 - 1/\lambda_2)}
\]  

(2)

where \( \lambda_1 \) and \( \lambda_2 \) are the wavelengths at the top of first and second spectra, whereas \( n_1 \) is the refractive index of the thin film formulated by the equation

\[
n_1 = \frac{(1 + n_0) + \sqrt{(1 + n_0)^2 - 4n_0T_0}}{2T_0}
\]  

(3)

where \( n_0 \) is the refractive index of glass (1.5) and \( T_0 \) is the minimum transmittance (%).

Figure 3 shows the calculation results of the deposition rate as a function of hydrogen dilution. It appears that there is a decrease in the deposition rate when the hydrogen dilution is increased. This decrease is possibly due to the reduction in dominance by SiH\(_3\) radicals. Increasing hydrogen dilution causes H atoms generated by dissociation process to be reduced since given RF power is set constant. As a result, SiH\(_3\) is generated by the reaction of H atoms and silane becomes reduced.

![Figure 3. Energy bandgap and deposition rate as a function of hydrogen dilution.](image)

The decrease in deposition rate is thought to lead to defect reduction that forms on growth surface during the deposition process for higher dilution of hydrogen. As a result, the irregularities of bonds formed and dangling bond defects reduced. Such defects are more likely to result in band tail defect and midgap defects that causes inhibition of charge carrier mobility in energy band. Hence increasing hydrogen dilution will reduce bandgap defect or will increase the conductivity value of the formed thin film.

The indication of a decrease in bandgap defect is reinforced by the calculation resulted from the energy bandgap above. From Figure 3, it is clear that greater hydrogen dilution causes larger energy bandgap.

3.4. Urbach Absorption Energy \( (E_u) \)

The tail absorption coefficient indicates that there is a concentration of impurities (state defect) which causes band structure to be interrupted, resulting in the tail of band entering energy band. Absorption coefficient \( \alpha \) in this section is characterized by exponential dependence of the absorption coefficient on photon energy [9].
\[ \alpha = \alpha_0 \exp \left( \frac{h \nu}{E_U} \right) \]  

(4)

where \( \alpha_0 \) is thin film characteristic parameter, and \( E_U \) is the Urbach absorption energy, which is used as an indicator of the presence of structural defects. This section, which is called Urbach edge, describes the transition between valence band state and conduction band state. Linear relationship in Equation (4) is used to determine the magnitude of Urbach energy as shown in Figure 4. The magnitude of \( E_U \) decreases with increasing dilution of hydrogen. The decline of this \( E_U \) indicates a decrease in density of state on band tail. It is believed that the exponential dependence of photon energy may arise from the random fluctuations of the internal plane associated with structural disturbances in many amorphous materials. It means that film thickness increases the Urbach energy which may be due to structural disturbances in the sample.

![Figure 4](image)

**Figure 4.** The Urbach energy for R= 0, 16, and 36.

Figure 5 shows that energy bandgap decreases when the Urbach energy increases. Supposedly, energy bandgap increases when the Urbach energy increases to form an amorphous structure. The increase indicates that there has been a material change towards nanostructures forming a microcrystalline film (μc-Si:H). The decrease in energy bandgap is thought to be due to a small effect of increased defect concentration compared with the effect of particle size change [6].

![Figure 5](image)

**Figure 5.** Relationship between Energy bandgap and Urbach energy.
4. Conclusions
A thin film deposition of hydrogenated silicon without doping (Si:H) by varying hydrogen dilution has been performed. UV-Vis spectroscopy data and the associated Tauc's Plot showed an increased energy bandgap with increasing hydrogen dilution. It was also shown that increasing dilution of hydrogen decreases deposition rate and Urbach absorption energy. Moreover, the increased dilution of hydrogen will give μc-Si:H film structure. This structure is more conductive than the other structures due to the reduction of the residual bandtail defect.

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