

# Physical Structure Analysis and Optical Properties of Sudan III Thin Film

Heindrich Taunamang, Djeli Tuladi, Prisilia Wakary

Physics Department, Mathematics and Natural Sciences Faculty, Manado State University, Tondano, Indonesia

Email: hein.taunamang@yahoo.com

**How to cite this paper:** Taunamang, H., Tuladi, D. and Wakary, P. (2021) Physical Structure Analysis and Optical Properties of Sudan III Thin Film. *Advances in Materials Physics and Chemistry*, 11, 101-110. <https://doi.org/10.4236/ampc.2021.116010>

**Received:** January 17, 2021

**Accepted:** June 14, 2021

**Published:** June 17, 2021

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## Abstract

**Background:** Sudan III is known red disazo dye possess a hydroxyl group which is sensitively to interact with others molecules such as CO<sub>2</sub>, O<sub>2</sub>, SO<sub>2</sub> through hydrogen bonding. **Methods:** Fabrication of Sudan III thin film for sensor technology application has been carried out by using PVD method. The physical structure that is crystallinity of this film has been investigated by using XRD method. **Results:** The XRD spectra of powder Sudan III shows crystalline structure while the XRD spectra of thin film results of the PVD method, which is deposited on substrate glass slide shows amorphous structure. There are no differences in the crystallinity content of Sudan III thin film that exposure to acetone and alcohol vapor. The interplanar distance of crystals plane is about 28.47 nm, the average crystallite size is about 35.6 nm and the average molecular chain separation is about 37.9 nm. Sudan III thin film result of the PVD method shows an interesting optical characteristic (absorption). There are significantly different between UV-VIS spectra Sudan III thin film compared to the UV-VIS spectra of Sudan III solution. The UV-VIS spectra of the Sudan III thin film shows a decreasing of peak intensity in visible wavelength which indication of orientation effect of molecule on substrate surface. The absorption peak at UV region for Sudan III thin film shows a shifting to the long wavelength compared to the Sudan III in form of solution.

## Keywords

Sudan III, Thin Film, Crystallinity, PVD

## 1. Introduction

Organic molecules azobenzene based such as Disperse Red 1 (DR1), Disperse Red 19 (DR 19) and Sudan III have been known as interesting researches object

due to their potential applications for optical sensor or fotonic sensor [1] [2]. For optical sensor technology application basis on optical fibre resulting in lightweight sensor, and also without using electrical power at sensing point and easily produced and low cost [3].

For this research, Sudan III molecule was chosen because of this molecule possesses azobenzene group which is sensitive to environmental especially in presence of another molecules such as ethanol, acetone vapor. Sudan III molecule has been used as a chromophore in polymer matrix for design of optical sensor applications [4]. Furthermore this molecule contains of OH group which is able to interact with another molecules through hydrogen bonding.

An investigation of physical structural of Sudan III molecule such as crystallinity content of material is important because of the molecular structure strongly influences the material properties. In this article were discussed the crystallinity content involving the distance of crystals plane, the average crystalline size and the average molecular chain separation within Sudan III for pristine Sudan III powder and Sudan III thin film which was fabricated using Physical Vacuum Deposition (PVD) method.

## 2. Methods

### Materials

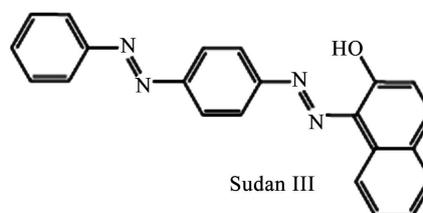
Material used in this research was Sudan III molecule. Sudan III is known red disazo dye which consists of hydroxyl group. Sudan III molecules possess one OH group. The structure of Sudan III molecule is shown in **Figure 1**.

### Sample preparation of Sudan III Solution.

Sudan III solution was prepared by solving the Sudan III pristine powder (0.1 mg) into 10 ml Cloroform ( $\text{CHCl}_3$ ) and then stirred for about 12 hours in room temperature in order to get a homogeneous solution.

### Sample preparation of Sudan III thin film.

Sample preparation of Sudan III thin film was carried out by using vacuum evaporation method (PVD). Fabrication of Sudan III thin film fabrication should be able to obtain a good quality thin films which were smoothly and homogeneous film surface. In this experiment Sudan III thin film was fabricated using a simple equipment system vacuum chamber evaporation was built in Physics Laboratory Manado State University as shown in **Figure 2**. For this experiment, the ivacuum chamber was equipped with vacuum pump of type MZ 2C NT at vacuum level of about  $10^{-3}$  Torr.



**Figure 1.** Chemical structure of Sudan III [5].



**Figure 2.** Thin film fabrication of Sudan III molecule by using physical vapor deposition method.

In terms of future work especially for gas sensor application, the Sudan III thin film which was deposited on the glass slide would be exposed to acetone or alcohol vapor. The thin film sample on the substrate was put on the vessel which is containing of about 5 ml acetone or alcohol solvent and then it was exposed to acetone or alcohol vapors at room temperature of about 23°C for 12 hours as shown in **Figure 3**. The distance between the surfaces of acetone or alcohol solvent and the film is about 10 cm.

#### **X-Ray Diffraction (XRD) Measurement**

The molecular structure of Sudan III in form of powder and Sudan III in form of thin film results of vacuum evaporation were characterized by using XRD measurement method. The aims of this XRD measurements were to investigate the crystal structure or crystalline content that are the interplanar distance of crystals plane, the average crystallite size and the average molecular chain separation within the Sudan III thin film and also for pristine Sudan III in powder form as comparison.

The XRD measurement was carried out by using diffractometer which is based on reflection method. From this measurement can be obtained the XRD spectra.

The width of XRD spectra indicates the crystal size of the sample. The sample that possesses small crystal size shows wider XRD spectra because of a small plane diffraction. The XRD measurement of pristine powder was carried out in ranges of angle diffraction of 3.5° - 75° by using Philips Diffractometer. In this measurement the XRD diffraction pattern was scanning  $2\theta$  at 30 kV, 30 mA with radiation source of  $\text{CuK}\alpha$  ( $\lambda = 1.5406$  Angstrom).

For the sample of Sudan III film which is deposited on glass slide was then exposed to acetone or alcohol vapor and then characterized using Rigaku Miniflex 600 (600 W, 30 kV, 10 mA dengan X-Ray tube Cu).



**Figure 3.** The experimental setting of Sudan III thin film exposed to acetone vapor or alcohol vapor.

### UV-VIS Measurement

The Ultraviolet and Visible (UV-VIS) measurement has been done for characterization of optical properties (absorbance or optical transparencies) of Sudan III molecule in form of solution and films. This method is a sensitively method for detecting a changing of molecular structure/deformation or molecular orientation [6]. The UV-VIS light is absorbed by atomic/molecules dependent on the electronics structure of atoms/molecules so that the relationship between the electronic spectra and the molecular structure as the whole can be studied. In fact, that the absorbance from the UV-VIS spectra for polarized light parallel to molecular orientation is more higher than for polarised light to perpendicular molecular orientation [7].

The optical properties (absorbance or transparencies) of the Sudan III film in form of solution and film were characterized using *Beckman DU-7000 Single Beam Spectrophotometer*. The measurement was obtained absorption UV-VIS spectra in range of wavelength 250 - 800 nm. For each, the UV-VIS measurement of the sample was initially by measurement of the background of the sample.

## 3. Results

The results preparation of Sudan III solution is shown in **Figure 4**.

The Sudan III thin film result of vacuum evaporation deposition is shown in **Figure 5**.

The XRD measurement of pristine Sudan III in powder form is shown in **Figure 6**.

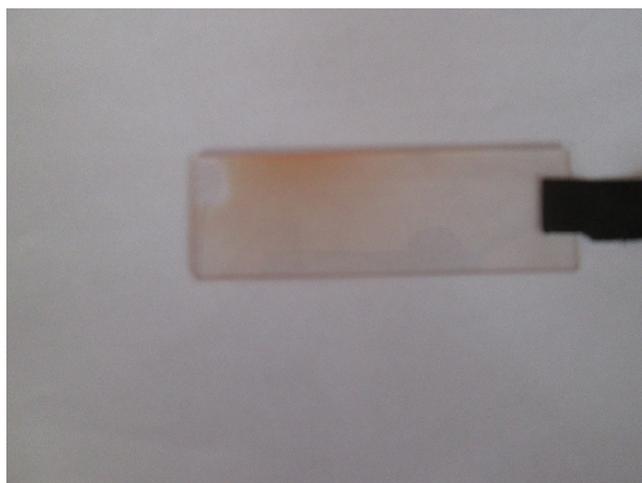
The results of the XRD measurement of Sudan III thin films were obtained from vacuum evaporation deposition on glass slide substrate which was then exposed to acetone or alcohol vapor are shown in **Figure 7** and **Figure 8** respectively.

The results of UV-VIS measurement of Sudan III solution are shown in **Figure 9**.

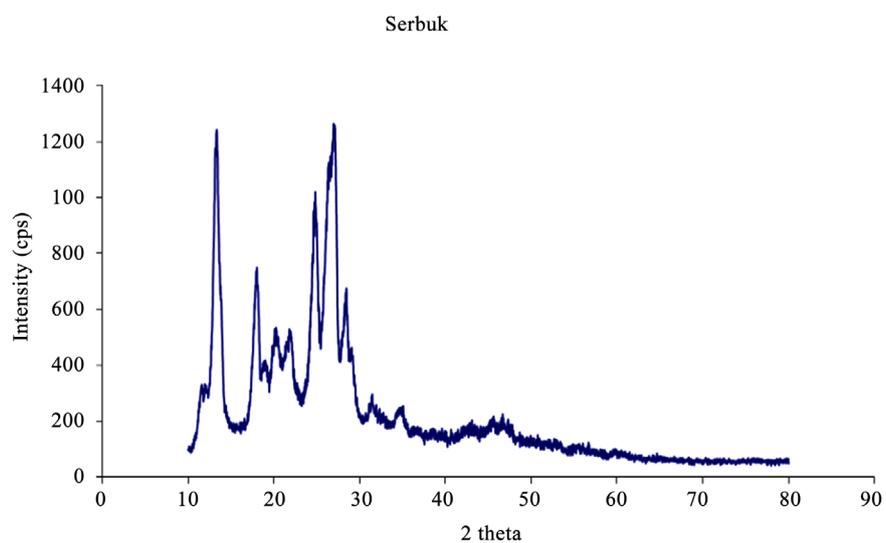
**Figure 10** shows the UV-VIS spectra of Sudan III thin film results of vacuum evaporation deposition.



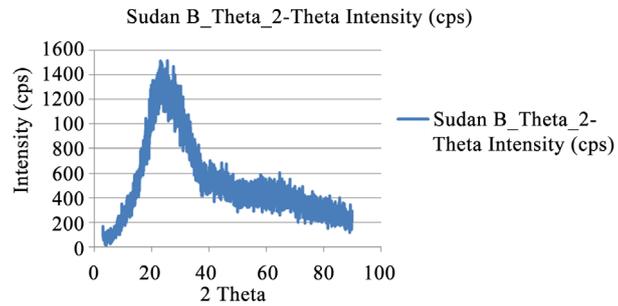
**Figure 4.** Sudan III solution.



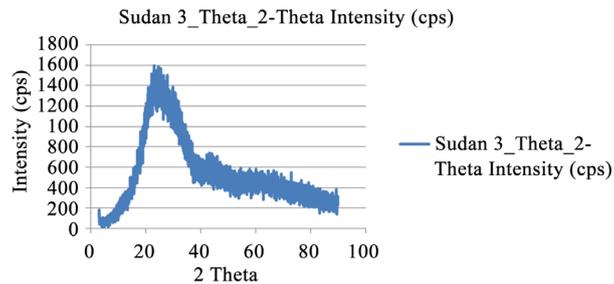
**Figure 5.** The Sudan III thin film result of the PVD method on the glass slide substrate.



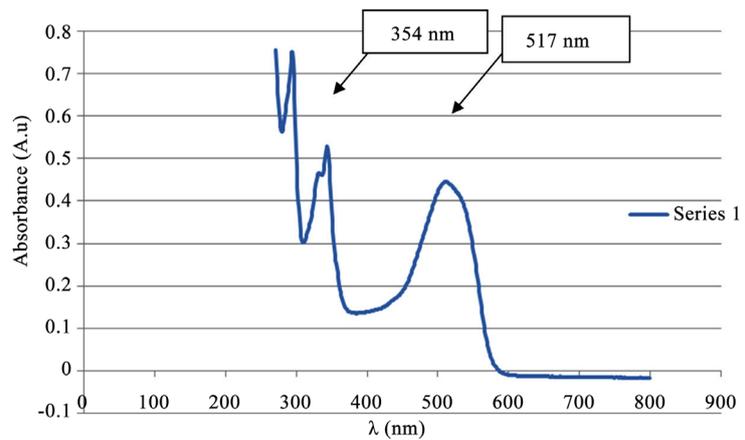
**Figure 6.** XRD spectra of pristine powder of Sudan III.



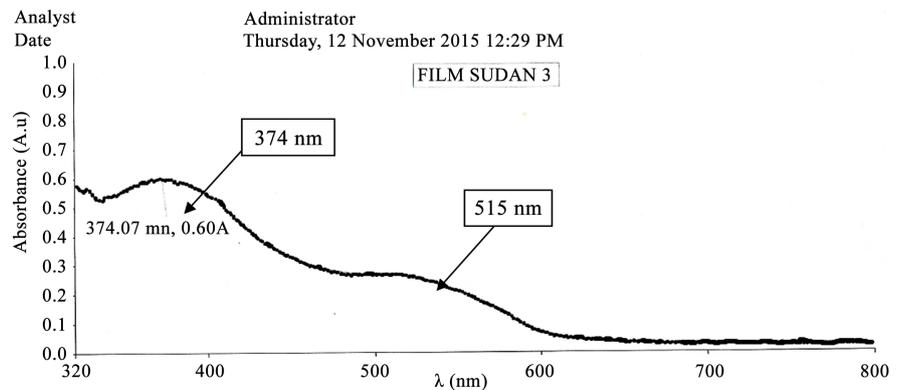
**Figure 7.** The XRD spectra of Sudan III thin film exposed to acetone vapor.



**Figure 8.** The XRD spectra of Sudan III film exposed to alcohol vapor.



**Figure 9.** UV-VIS spectra of Sudan III solution (Cloroform Solvent).



**Figure 10.** UV-VIS spectra of Sudan III thin film results of vacuum evaporation deposition.

## 4. Discussion

The XRD spectra of Sudan III in powder form indicates as a crystalline structure. From the XRD spectra (**Figure 6**) can be determined the interplanar distance of crystals plane ( $d_{(hkl)}$ ) by using Bragg equation [8] as follows:

$$d_{hkl} = \frac{\lambda}{2 \sin \theta} \quad (1)$$

( $d_{(hkl)}$ ) in Angstrom unit.

The results of calculation of the interplanar distance of crystals plane ( $d_{(hkl)}$ ) is presented in **Table 1**.

The average crystallite size of Sudan III thin film was estimated from a sharp peak at 22.42° by using Scherrer's formula [9] [10] that is:

$$D = K\lambda/\beta \cos \theta \quad (2)$$

With  $D$  is crystallite size (diameter of crystallite).  $K$  is shape factor of about 0.89 if the unknown shape, and  $\theta$  is diffraction angle at maximum intensity and  $\beta$  is Full Width at Half Maximum (FWHM) in radian (1 degree = 0.0174 radian). The results of crystallite size calculation using the Equation (3.3) for Sudan III thin film exposed to acetone or alcohol vapor are same that is about 37.19 nm as shown in **Table 2** and **Table 3** respectively.

**Table 1.** The Bragg angle ( $2\theta$ ) in degree unit and the interplanar distance of crystals ( $d_{(hkl)}$ ) in Angstrom unit.

Sample	$2\theta$ (degree)	$d_{(hkl)}$ (Å)
Sudan III pristine powder	13.3	6.64
	17.94	4.94
	18.36	4.81
	20.12	4.40
	21.7	4.05
	24.84	3.58
	26.96	3.31
	27.4	3.25
	31.36	2.85
	34.26	2.62
	42.08	2.14
	45.2	2.01
45.38	2.00	

**Table 2.** The characteristics of Sudan III thin film were exposed to acetone vapor.

Variables	Characteristics of Sudan III thin film were exposed to acetone vapor
$2\theta$ (degree)	21.4
$d_{(hkl)}$ (nm)	28.47
$S$ (nm)	35.6
$D$ (nm)	37.19

**Table 3.** Characteristics of Sudan III thin film were exposed to alcohol vapor.

Variables	Characteristics of Sudan III thin film were exposed to alcohol vapor
$2\theta$ (degree)	21.4
$d_{(hkl)}$ (Å)	28.47
$S$ (nm)	35.6
$D$ (nm)	37.19

Next, from XRD spectra can be calculated the average molecular chain separation within the Sudan III thin film and also for pure Sudan III in powder form by using equation

$$S = 5\lambda/8\sin\theta \quad [11] \quad (3)$$

With  $\lambda = 1.5406$  Angstrom.  $\theta$  is diffraction angle at maximum intensity of halow amorphous. The average molecular chain separation ( $S$ ) within pure Sudan III in powder form which is calculated from maximum peak intensity that is,  $2\theta = 26.96$  ( $d_{hkl} = 3.31$  Angstrom), was obtained that  $S = 57.44$  nm.

From the XRD spectra as shown in **Figure 7** and **Figure 8** above can be calculated the average molecular chain separation ( $S$ ) within the Sudan III thin film results of vacuum evaporation exposure to acetone or alcohol vapor is the same to be 35.6 nm.

The characteristics of Sudan III thin film was exposed to acetone and alcohol vapor respectively were shown in **Table 2** and **Table 3** respectively.

From the XRD spectra reveal that there are no differences in characteristics between Sudan III thin film exposed to acetone and alcohol vapor.

**Figure 9** shows the UV-VIS spectra of Sudan III solution (chloroform solvent). From this figure shows that the maximum absorption peak ( $\lambda_{\max}$ ) is about 517 nm (visible region) which is corresponding to electronic transition energy (band gap energy)  $E$ , where  $E = hc / \lambda = 2.4$  eV .

This absorption is identified as  $\pi$ - $\pi^*$  electronic transition from OH through azobenzne group. And the absorption peak at wavelength of 354 nm (UV region) is corresponding to electronic transition energy  $E = 3.6$  eV. And the absorption peak at wavelength of 299 nm (UV region) is corresponding to electronic transition energy  $E = 4.2$  eV. This UV-VIS spectra (**Figure 9**) shows a broad absorption band and also strong intensity in a visibel region. This absorption is corresponding to the electronics transition of  $\pi$ - $\pi^*$  in azobenzene group.

**Figure 10** shows UV-VIS spectra of Sudan III thin film results of vacuum evaporation deposition on glass slide substrate. It appears that the maximum peak intensity ( $\lambda_{\max}$ ) in visible region to be 515 nm which is corresponding to electronic transition energy or gab energy,  $E_{\text{vis}} = 2.4$  eV. This absorption peak is corresponding to  $\pi$ - $\pi^*$  from OH group through azobenzene group.

Absorption peak at wavelength of 374 nm is corresponding to energy electronic transition,  $E_{\text{uv}} = 3.6$  eV. This spectra shows a broad absorption band with strong intensity which is corresponding to electronic transition of  $\pi$ - $\pi^*$  in azo-

benzene group. The UV absorption peak at 354 nm of Sudan III in form of solution (**Figure 9**) is shifting to 374 nm in form of the thin film (**Figure 10**) is probably due to conformation effect (trans-cis) of the molecule.

It appears that there are significant differences between the UV-VIS absorption band pattern especially in the visible region of Sudan III thin film (**Figure 10**) compared to the UV-VIS absorption band pattern of Sudan III solution (**Figure 9**). There is decreasing intensity in the visible region due to molecular orientation effect. Whether parallel or antiparallel molecular arrangement in the Sudan III thin film would be subjected to further work.

## 5. Conclusions

The XRD spectra of powder Sudan III shows crystalline structure while the XRD spectra of thin film results of the PVD method, which is deposited on substrate glass slide shows amorphous structure. The crystallinity content such as the interplanar distance of crystals plane, the average crystallite size and the average molecular chain separation within the Sudan III thin film and also for pure Sudan III in powder form could be determined.

Sudan III thin film result of the PVD method shows an interesting optical characteristic (absorption). There are significant differences between UV-VIS spectra Sudan III thin film compared to the UV-VIS spectra of Sudan III solution. The UV-VIS spectra of the Sudan III thin film shows a decreasing of peak intensity in visible wavelength which indicates an orientation effect of molecule on substrate surface. The absorption peak at UV region for Sudan III thin film shows a shifting to the long wavelength compared to the Sudan III in form of solution.

## Acknowledgements

The authors would like to acknowledge the financial support for this research from Rector Unima through LPPM Unima for funding this research.

## Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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