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Estimation Crystal Size and Lattice Strain of Nanocrystal Bi_2O_3 using the Scherrer and Size-Strain Plot Method

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ABSTRACT
Crystal size is an important parameter that affects the physical properties of nanocrystals that are correlated in determining the characteristics of crystal structure. This study aimed to estimate the crystal size and view the Bi_2O_3 nanoparticle lattice stretching. Synthesized nanoparticles Bi_2O_3 using the precipitation method assisted by microwave with variations in microwave power 100 W, 300 W, 450 W, 600 W, and 850 W, respectively. Bi_2O_3 with crystal structures identified through X-ray diffraction peak profiles. The size of the crystal and lattice stretch obtained through the size-strain plot method is more accurate than the Scherrer method, as seen from the correlation coefficient value ($R^2 > 0.9$).

Keywords: Bi_2O_3, Precipitation assisted by microwave, Size-Strain Plot

I. INTRODUCTION

Bismuth Oxide (Bi_2O_3) is the simplest Bismuth-based material. Bismuth has good optical and electric properties such as photoluminescence, good photoconductive responses, high refractive index, high dielectric permittivity, high chemical thermal stability, and non-toxic [1]. Besides that, Bi_2O_3 also has a narrow energy band gap, a low valence band position, and is responsive to visible light [2]. The characteristics possessed by Bi_2O_3 make it a suitable material for various applications such as photocatalyst, gas sensors, superconductors, and photographic [3]. Bi_2O_3 has six forms of polymorphic, namely: α-Bi_2O_3 (monoclinic), β-Bi_2O_3 (tetragonal), γ- Bi_2O_3 (FCC), δ-Bi_2O_3 (cubic), ε-Bi_2O_3 (tetragonal), and ω-Bi_2O_3 (triclinic). Among the six phases, α-Bi_2O_3 is the most stable at room temperature, while the γ-Bi_2O_3 phase is stable at high temperatures (730-825 °C). The other four phases are metastable. In addition, different crystal structures result in different photocatalytic performances [4].

In this study, nanocrystal Bi_2O_3 was prepared by microwave-assisted precipitation method. This method is chosen because it is simpler, low cost, and has high purity. In addition, this method can control particles' morphology, shape, and size at low temperatures [5]. The calcination process in the precipitation method generally uses furnaces that require a relatively long time to form nanoparticles Bi_2O_3, because the heat transfer process occurs in conduction, so the heating process starts from the surface to the nucleus of the material. The use of a microwave is an alternative to shortening calcination time because the heating process occurs

volumetrically. This results in a shorter heating time and impacts energy efficiency [6]. The amount of energy emitted by microwaves depends on the power used. The greater the energy emitted by microwave, the higher the heat produced [7].

Physical properties in nanocrystal depend on the crystal's size, which correlates with determining the characteristics of the crystal [8]. The crystal size is important in determining nanomaterial properties such as electrical, optical, and chemical properties. Perfect crystals are composed of regular atoms, in reality no perfect crystal is found due to small material size. This imperfection affects the expansion of the peak diffraction. The size of the crystal and lattice strain are two properties that can be analyzed through the X-ray diffraction profile (XRD). The crystal size can be defined as a coherent domain size. The crystal size is not the same as the particle size due to the formation of polycrystalline aggregates [9]. Lattice strain is a lattice constant obtained from crystal defects such as dislocation, point defect, and contact voltage [10]. In this study, the size of the crystal and lattice strain can be predicted through an analysis of X-ray diffraction spectrum profiles. The method commonly used to predict crystal size is the Scherrer method, where the prediction of crystal size is based on the width of the diffraction peak. However, this method does not consider the existence of the strain's inhomogeneity. The Size-Strain Plot (SSP) method is one method that is often used in predicting two parameters at once. First, there are the size of the crystal and lattice strain.

II. METHODS AND MATERIAL

Powder of Bi_2O_3 was synthesized using a microwave precipitation method with $Bi(NO_3)_3.5H_2O$ as precursors, ammonia solutions, and NaOH. The synthesis procedure is carried out by dissolving 0.5 gr $Bi(NO_3)_3.5H_2O$ into a 5% ammonia solution. Then proceed with homogenization for 5 minutes. After that, 250 ml of NaOH (1 M) is added to the solution and followed by stirring for 2 hours until the precipitate is produced. Next, the precipitate is separated from the solution and heated using a hotplate at 120^{oC} so that Bi_2O_3 powder is produced. The last stage of Bi_2O_3 powder is heated using a microwave with a variation of 100 W, 300 W, 450 W, 600 W, and 850 W for 1 hour.

Nanocrystal Bi_2O_3 formed was analyzed using XRD (Shimadzu XRD 6100/7000). The X-ray wavelength used is 1.54016 Å. Data collection 2θ is done in the angle range of 20^{o}-80^{o}. XRD produces diffraction patterns that will be processed using Match and Highscore Plus software to see the Bi_2O_3 crystal structure. The SSP (Size-Strain Plot) method analyzes crystal size estimates and lattice strain from X-ray diffraction data.

III. RESULTS AND DISCUSSION

Crystal structure of Bi_2O_3

X-ray diffraction spectrum profiles from Bi_2O_3 with power variations show different diffraction peaks, as seen in Table 1. The peaks indicate compatibility with data (COD #96-901-257) for all samples. These matching results indicate that all samples have the same crystal structure, monoclinic with lattice parameters a = 5.849, b = 8.166, c = 7.510, and angular parameters α = 90^{o}, β = 113^{o}, Υ = 90^{o}. However, the X-ray diffraction spectrum profile also shows the existence of the secondary phase of Bi_2O_4 monoclinic (COD #96-900-9766) in 2θ = 29.50^{o} and 30.34^{o} with respective crystal orientations (311) and (400).

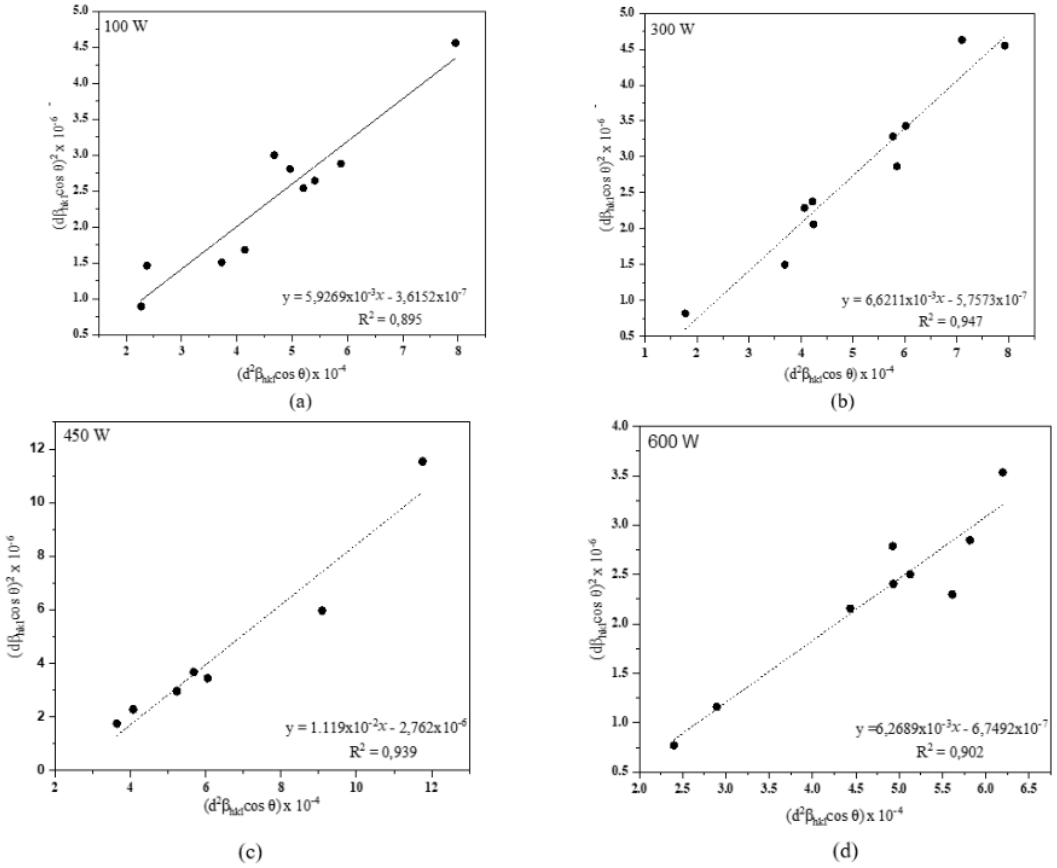
Crystal size and lattice strain

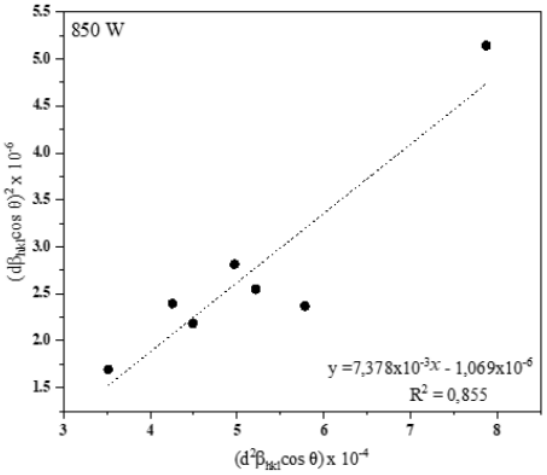
The crystal size and lattice strain are obtained by identifying X-ray diffraction spectrum profiles. The crystal and lattice strain size is calculated using the Scherrer equation and the Size-Strain Plot (SSP) method. In the Scherrer equation, the effect of the lattice strain on the peak widening of the X-ray

spectrum is not calculated, so it can be assumed that the profile widening is diffraction as a total contribution of the crystal size. The SSP method assumes a link between the widening of the peak diffraction with the crystal size and the lattice strain. This method assumes that the diffraction peak profile is a combination of Lorentzian and Gaussian functions, where this function is each describing the size of the crystal and lattice stretch [11]. The merging of the two functions can be expressed through Eq.1 [12].

$$(d_{hkl}\beta_{hkl}\cos\theta)^2 = \frac{K}{D}\left(d_{hkl}^2\beta_{hkl}\cos\theta\right) + \left(\frac{\varepsilon}{2}\right)^2 \quad (1)$$

With K is a constant that depends on the shape of the particle (3/4 for a spherical particle), βhkl is FWHM related to the size of the crystal and lattice strain. In the SSP method, the crystal size is obtained through the intersection point on the X-axis, while the lattice strain is determined from the slope of the graph. Figure 1 shows the SSP graph from Bi_2O_3 which is calculated using power of microwave with 100 W, 300W, 450 W, 600 W, and 850 W.





(e)

Figure 1. Graph of Bi_2O_3 with SSP method: (a) 100 W, (b) 300 W, (c) 450 W, (d) 600, (e) 850

The crystal size and lattice strain of Bi_2O_3 using a different approach can be seen in Table 1. Based on Table 1. it can be seen that the crystal size obtained using the SSP method is greater than the crystal size using the Scherrer equation. This phenomenon indicates the influence of the lattice strain on the accuracy of the size of the Bi_2O_3 crystal. Furthermore, the accuracy of the SSP method can be seen from the correlation coefficient value (R^2> 0.9). Therefore, the sample synthesized by microwave with a 100 W power has a larger crystal size than other samples.

This indicates the occurrence of crystal growth and increased crystallinity. This statement is strengthened through the XRD pattern, where samples have a higher peak intensity and narrower peak width. The greater crystal size shows the smaller percentage of lattice strain. The lattice strain value shows a change in lattice length [13].

Table 1. Crystal size and lattice strain with the Scherrer equation and the SSP method

Sample	Scherrer		SSP Method		
	D (nm)	ε (%)	R^2	D (nm)	ε (%)
100 Watt	28,11	0,492	0,895	126,54	0,120
300 Watt	26,46	0,528	0,947	113,27	0,152
450 Watt	22,70	0,657	0,939	67,02	0,332
600 Watt	30,44	0,480	0,902	119,64	0,164
850 Watt	27,12	0,529	0,855	101,65	0,207

The lattice parameter for the monoclinic crystal structure is calculated using the Eq.2 (Gbashi, et al., 2018)

$$\frac{1}{d^2}=\left(\frac{h^2}{a^2}+\frac{k^2\sin^2\beta}{b^2}+\frac{2lh\cos\beta}{ac}\right)\csc^2\beta \quad (2)$$

Equation 2 can be further elaborated to obtain lattice parameters a, b and c through the peak fields (200), (120), and (002) (Eq.3-5)

$$a=\frac{\lambda\csc\beta}{\sin\theta_{(200)}} \quad (3)$$

$$b = \frac{\lambda}{\sqrt{\sin^2\theta_{(120)} - \frac{\sin^2\theta_{(200)}}{4}}} \quad (4)$$

$$c = \frac{\lambda \, csc \, \beta}{sin \, \theta_{(002)}} \quad (5)$$

Unit volume cells for monoclinic structures are calculated using Eq.6:

$$V = a\, b\, c \sin\beta \quad (6)$$

The results of the calculation of the lattice parameter and the unit volume cells using Eq.3-6 are shown by Table 2. Based on the table, there are no significant differences in each sample. So it still shows a match with a lattice parameter of the monoclinic crystal structure.

Table 2. Results of lattice parameter and unit volume cells of Bi_2O_3

Sample	Lattice Parameter			Unit Volume Cells $(Å)^3$
	$a\,(Å)$	$b\,(Å)$	$c\,(Å)$	
JCPDS	5.849	8.166	7.510	330.18
100 Watt	5.862	8.195	7.528	332.89
300 Watt	5.847	8.157	7.508	329.62
450 Watt	5.845	8.188	7.526	331.55
600 Watt	5.835	8.124	7.486	326.65
850 Watt	5.868	8.207	7.540	334.25

IV. CONCLUSION

Nanocrystal Bi_2O_3 has been successfully synthesized using a microwave-assisted precipitation method with power variations. Analysis of X-ray diffraction shows that nanocrystal Bi_2O_3 has a monoclinic crystal structure. Power variations in microwaves did not change the structure crystals of Bi_2O_3. The crystal size of the Bi_2O_3 obtained by the Scherrer equation is greater than the size-strain plot (SSP) method. The level of measurement accuracy can be seen from the correlation coefficient, where the size-strain plot (SSP) method is more accurate because it has (R2> 0.9). Size-strain plot method is more effective for determining the size of the crystal and lattice strain with a higher level of accuracy.

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