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Sol-Gel $BaTiO_3$ Thin Films for Optical Application

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Abstract: A layer of $BaTiO_3$ thin films which is prepared using the sol-gel method are coated with different number of layers and has been annealed at 900°C. Every single layer has been baked for 20 min at 200°C. This studied about structural and optical properties through X-Ray Diffraction (XRD), UV-Vis spectrophotometer and FE-SEM. X-ray diffraction patterns of barium titanate samples show that the peaks of the diffractogram were successfully indexed with the cubic structure of $BaTiO_3$. The $BaTiO_3$ thin films have been analysed for optical application and it was suitable to apply as a bio-sensor, as an optical band gap calculated through UV Visible spectrophotometer even the surface are slightly rough compared to the other deposition technique.

Key words: $BaTiO_3$, thin film, optical, patterns, Malaysia

INTRODUCTION

Barium Titanate ($BaTiO_3$) has been investigated since 1940 because of their interesting characteristic (Wang *et al*., 2008; Ihlefeld *et al*., 2008; Kobayashi *et al*., 2008; Song *et al*., 2007). There are many methods to produce a $BaTiO_3$ such as electrochemical deposition (Wu and Lu, 2001) plasma evaporation (Huang and Yao, 2004) and sputtering. Compare to the other method, sol-gel is the most inexpensive and can be prepared easily. It can be prepared only by mixing some chemical such as acetic acid, 2-methoxyethanol, barium acetate and titanium (IV) Isopropoxide. Nowadays, there are many applications that are using $BaTiO_3$ as their dielectric material such as capacitor, thermistor, sensor and so on (Thomas *et al*., 1999; Zeng *et al*., 1999). The reason why $BaTiO_3$ received much attention are because it have a high refractive index compared to other lead-free material (NIIR Board of Consultants and Engineers, 2005). It also has the ability to change the polarization of the electric field when the annealing temperature are increased (Yuanbing *et al*., 2010). In terms of optical application, $BaTiO_3$ is suitable because it is a trans parent cmaterial which is applicable for most of optical applications.

MATERIALS AND METHODS

Sol-gel preparation: The materials used for sol-gel $BaTiO_3$ solution were barium acetate ($Ba(CH_3COO)_2$), titanium (IV) isopropoxide ($Ti\,[OCH\,(CH_3)_2]_4$), acetic acid as a solvent and 2-methoxyethanol as a stabilizer. Firstly, Barium acetate were dissolved by acetic acid at temperature of 80°C for one hour with stirring continuously. In the other hand, titanium (IV) isopropoxide and 2-methoxyethanol were mixed separately at room temperature with continuously stirred condition. Then the titanium mixture were drop added into the barium solution and continuously stirred for 1 h at room temperature. Finally, the solution was ready to be coated on the substrate.

Thin films preparation: Fuse silica glass and Si substrates were cleaned with IPA, acetone, deionized water and dried with a nitrogen stream. The substrates were then transferred to the spin coater. $BaTiO_3$ sol-gel was deposited by spin coating at spin speed of 4500rpm for 20 sc. The thin layer of $BaTiO_3$ was baked at 200°C for 20 min to remove the solvent and moisture. The $BaTiO_3$ thin films are then annealed at 900°C for 2 h by increasing the temperature rate at 10°C/min. The sample is then characterized using XRD, AFM, FE-SEM and UV-Vis.

Surface morphology and microstructure: The sample was characterized using the XRD, AFM and FE-SEM for the surface analysis. The sample size for XRD were prepared 1.5×1.5 cm to fit the sample holder. As for UV-Vis, the sample was prepared separately because it deposited on silica substrate.

RESULTS AND DISCUSSION

Surface morphology and microstructure: The result covered about BaTiO3 analysis on the Si and silica surface. AFM, FESEM and UV-Vis result and discussion.

X-ray diffraction: The result in Fig. 1 shows the XRD peaks of $BaTiO_3$ after annealing at 900°C for 2 h. The peaks at (21.9°), (31.2°), (38.6°) are the $BaTiO_3$ thin films

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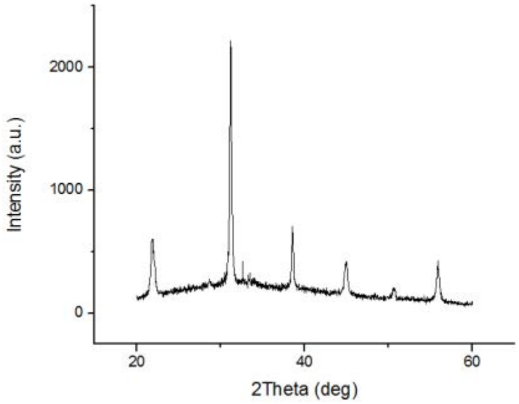

Fig. 1: The XRD diffractogram after annealing at 900°C for 2 h

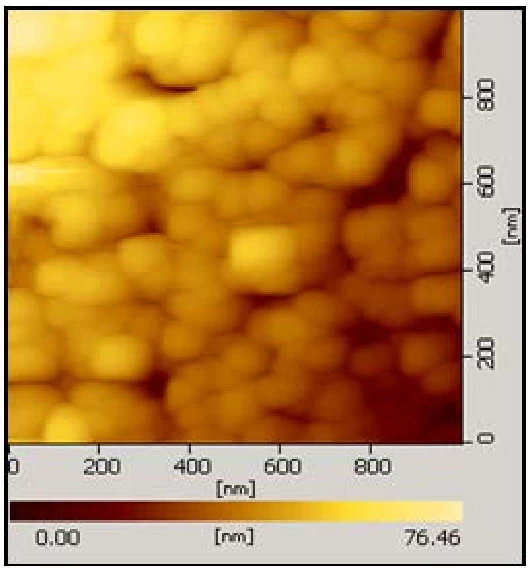

Fig. 2: The 2D structure of $BaTiO_3$ thin film

by referring to the PDF Card 01-078-2793. As for material analysis, it considered as $BaTiO_3$ material. However, the crystal structure of this result is considered as a cubic structure. The result shows a slightly different from using the sputtering method.

Atomic Force Microscopy (AFM): The surface morphology, such as the grain size, surface roughness smoothness and pinholes, is one of the key parameters in determining the electrical and optical properties of high dielectric constant thin films (Zeng *et al*., 1999). Figure 2 shows the surface morphology of the $BaTiO_3$ film where the grains are comparatively smaller. The value of peak to valley of the films is 53.45 nm while the roughness is 4.32 nm. By using AFM measurement, the thickness can be determined roughly. As for this result, the thickness can be assumed as around 40 nm as for roughly assumption. The RMS for this sample is 5.75 nm. The $BaTiO_3$ layers show uniform grain size because of the spin coating method used are made of film layering-where a layer is spun and baked before the next layer, then both are baked again and this process is repeated several times. Hence, the growth builds upon the previously built structure and the final annealing agglomerates these into bigger grains. Figure 3 shows 3the same resul but in a 3-D perspective where the layer grain growth is seen to produce rougher terrain due to the bigger and more uneven grains in the 10 layer film.

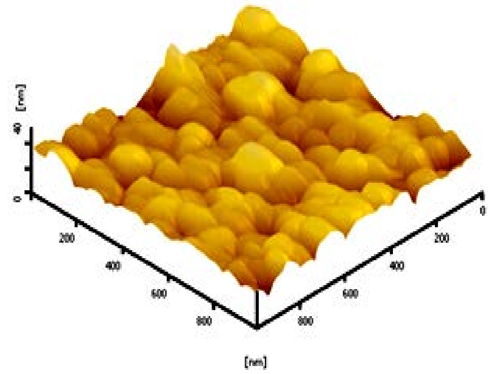

Fig. 3: The 3D structure of $BaTiO_3$ surface

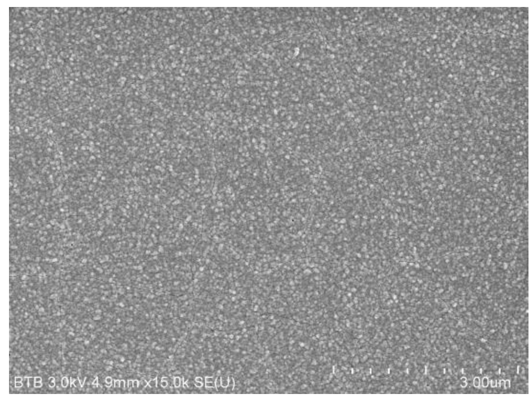

Fig. 4: Surface of $BaTiO_3$ thin film coated on Si wafer at x150 k magnification

FE-SEM: As for surface analysis, the image in Fig. 4 shows the surface of $BaTiO_3$ thin films at x15.0k magnification. The thin films can be clearly seen have a uniform surface area without any void or particle. After increasing the magnification up to x100 k (Fig. 5), the grains can be clearly seen and the size is about even with each other. By increasing the magnification up to x250 k (Fig. 6) and it seems that the average grains size is

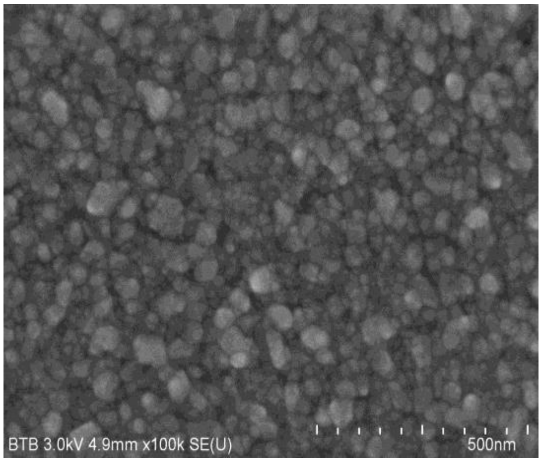

Fig. 5: Surface of $BaTIO_3$ thin film coated on Si wafer at x100 k magnification

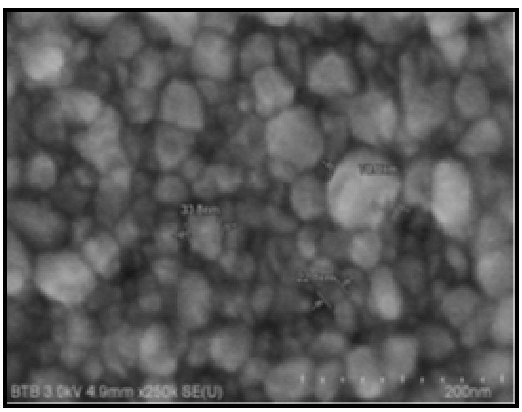

Fig. 6: Surface of $BaTiO_3$ thin film coated on Si wafer at x250 k, magnification

41.97 nm. The grain size were measured sort bythe largest grain, medium grain and smallest grain and divide by average.

Uv-visible spectrophotometer: For the optical studies, the $BaTiO_3$ film was deposited on fused silica substrate and annealed at 900°C for 2 h and then characterized by Perkin-Elmer Lambda 950 UV-Vis Spectrophotometer with an Integrating Sphere. An empty fused silica substrate was used as a reference in the baseline scan. The optical transmission spectra of the $BaTiO_3$ film is shown in Fig. 7. According to this spectrum, it shows high attenuation in the short wavelength region.

In contrast, the $BaTiO_3$ film was highly transparent in the wavelength region from 400-800 nm with an average transmission of >90%. A comparatively high transmission indicates that those films exhibit weak absorption in the visible region. It also revealed the high absorption in the short wavelength region. We understand that the incident light energy transmitting through a transparent material is divided into two parts. The light transmitted through the material is the first part and the other is the losses due to the reflection and absorption.

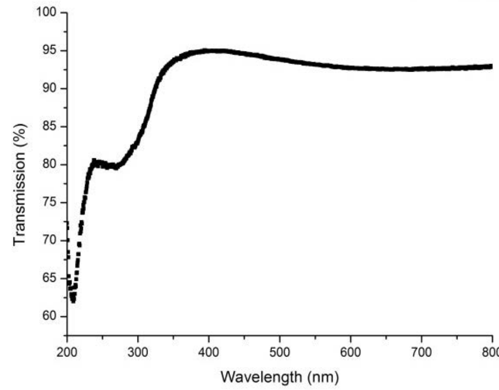

Fig. 7: Transmission Spectra (%T) of $BaTiO_3$ films deposited on fused silica substrate and annealed at 900°C for 2 h

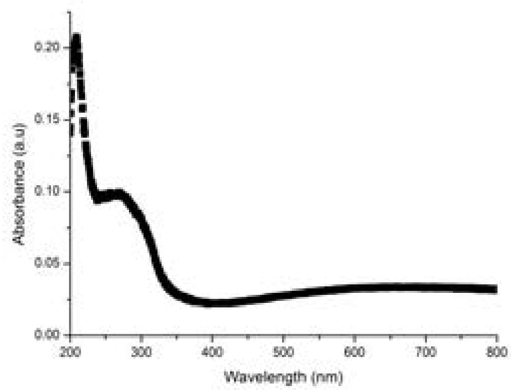

Fig. 8: Absorbance spectra of $BaTiO_3$ films deposited on fused silica substrate and annealed at 900°C for 2 h

Therefore, Fig. 8 and 9 shows the film exhibits high transparency and low energy losses in visible and near infrared region (Ashiri *et al* ., 2009). The transmission of the films drops drastically when the wavelength was reduced to about 330 nm, this could be explained by the fundamental of light absorption and occurrence of inter-band transitions as mentioned earlier (Ashiri *et al*., 2009; Zhang *et al*., 2000; Xu *et al*., 2006). The absorption of the photons may occur by exciting an electron from the almost occupied valence band, across the band gap into an empty state of the conduction band. The absorption

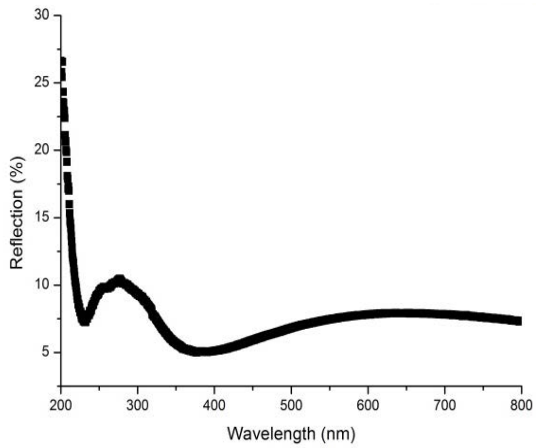

Fig. 9: Reflection spectra (%R) of $BaTiO_3$ films deposited on fused silica substrate and annealed at 900°C for 2 h

and excitation arise only if the photon energy is greater than the band gap energy. The band gap of the system could be determined based on this circumstance (Ashiri *et al*., 2009).

CONCLUSION

The sol-gel method is preferable in optical application. It is highly recommended since it requires lower cost compared to other methods (Brinker *et al*., 1991). As for conclusion, the optical properties of material such as $BaTiO_3$ even it prepared using different method also will give almost similar result in optical properties. A transparent thin films of $BaTiO_3$ have been prepared by using the spin coating technique. The transmission, reflectance and absorbance value was recorded. In conclusion, $BaTiO_3$ thin film of a material that is often studied its capabilities in the field of microelectronics. However, it has proved that it is also able to be used in optical applications.

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