Determining Optical Constants of Selenium Thin Films using the Envelope Method

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ABSTRACT

Two Selenium thin films were deposited on glass substrates using thermal evaporation technique. The optical constants (refractive index, absorption coefficient and extinction coefficient and energy gap) were calculated using the Transmittance (T) spectrums of the films in the spectral range of 500-900 nm. The envelope method was used to determine optical constants. The calculated refractive index was found to be in the range of 2.60 to 2.85 and the Energy gap (E_g) was found to be 1.8 eV which are in agreement with other studies made using other procedures. The films were found to be amorphous according to the results obtained by XRD technique. This method can be used to have a good results for many tranparent thin films with more mathematical tools.

Keywords: Refractive Index, Extinction Coefficient, Optical Constants, Absorption Coefficient, Amorphous Selenium, Envelope Method

1. INTRODUCTION

Selenium (Se) thin films and its other copounds such as CuInSe are used in many industrial applications such as photovoltaic cell and optical devices industry (Bhadra *et al*., 1999; Bindu *et al*., 2002). Recently, the optical and electrical properties of a-Se films have a substantial renewed interest due to its use as an ultra-sensitive photoconductor in newly developed flat panel x-ray image detector and high definition digital and video camera (Chong, 2006). Moreover, doping Se with other metals like Te will enhance its optical properties, such as decreasing the energy band gap, made it of much interest for applications in new technology (Zishan *et al*., 2012). The optical constants are of much importance for applications. These optical constants are the refractive index (n), the extinction coefficient (k) which is a measure of the energy loss in material and is related to the absorption coefficient (α) according to the relation Equation 1:

$$k = \frac{\alpha\lambda}{4\pi} \tag{1}$$

where, λ is the wavelength of the incident light (Marquez *et al*., 1992; Chavez-Rivas *et al*., 1982). The importance of the absorption coefficient is that it indicates how readily photons will be absorbed by the material.

In order to measure the optical constants, some experimental measurements and data must be known and measured. This can be accomplished by measuring the Reflectance (R) and/or Transmittance (T), of the film; then solving three non-linear equations can give the optical constants (Heavens, 1955). However, solving these equations for many semiconducting materials is not quite easy. Therefore, an other method based on the ability of the film to form an interference pattern on T spectrum and then using what is referred to as the envelope method is an alternative easy method which was proposed by (Swanepoel, 1983).

Optical constants of Se thin films have been investigated and calculated in many ways but not the envelope method. Therefore, this method will be used to measure the optical constants for two different Se thin film and comparing the results with what have been already published (Salwan *et al*., 1990; Bindu *et al*., 2002; Bhadra *et al*., 1999; Gross *et al*., 1977;

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Manifacier *et al.*, 1976; Kasasbeh, 2010; Streetman, 1995; Tashtoush, 2002).

This method depends on the transmittance curve of the sample. In films at which the thickness of the substrate is several orders of magnitude larger than the thickness *d* and the film is uniform, interference pattern could be seen in the VIS and IR region of the transmittance spectrum. This effect will give rise to an oscillating transmission curve. Such interference fringes will be used to determine the optical constants, as well as the film thickness. This method was completely described by Swanepoel (1983); Marquez *et al.* (1992) and Kasasbeh (2010).

2. MATERIALS AND METHODS

Selenium powder of 99.99% purity was used to prepare two samples of *a-Se* thin films using the thermal evaporation technique. This was achieved by using Edwards Coating System E306 A model. The samples were deposited on glass substrates (microscope slides) with a refractive index of about 1.52. The substrates were cleaned by the usual method of cleaning that is: using the ultrasound cleaner filled with acetone, then filled with distilled water. After this, all substrates were cleaned again with methanol and then with distilled water. Finally, a hot clean air was used to dry the substrates.

The base pressure inside the chamber was less than 10^{-5} mbar. The film thickness was controlled and monitored using a Quartz crystal thickness monitor of the type Edwards FTM5 model.

The Transmittances (T) of the films were measured over the range of 450-900 nm wavelength using a UV-VIS spectrophotometer, Specord M500 model.

3. RESULTS AND DISCUSSION

Many experiments have been conducted to study the optical properties of *a-Se* thin films. **Figure 1** shows a typical XRD pattern for one of the as deposited Se thin films. The pattern shows that the film was amorphous.

Figure 2 shows a typical transmittance spectrum (the solid line) of a-Se thin film of a thickness of 1580 nm. It seems that there is no transmission (high absorption) in the range of 300 nm to about 580 nm. The curve shows an interference fringes on the high transmittance (low absorption) region of wavelength. For measurements needs, the curve can be split into two regions; the first region is the strong and medium absorption region which appears in the interval 550-700 nm, the second region appears in the interval of 700-900 nm and known as the transparent region.

It is important to mention that the photons with energies less than band gap are transmitted, on the other hand the photons with energies greater than or equal to band gap can be absorbed, where a photon with energy less than E_g is unable to excite an electron from the valance band to the conduction band, thus in a pure semiconductor there is a negligible absorption of photons with $h\upsilon < E_g$. This explains why some materials are transparent, like our sample, in certain wavelength range (Streetman, 1995).

In order to determine the optical properties we have to build up two curves that are T_M curve which is related to the maximum points at which the interference took place and T_m curve which is related to the points at which minimum points at which the interference took place (dashed line on **Fig. 2**. T_M and T_m are considered to be continuous function of λ. Also, the refractive index is a function of λ, i.e., n (λ). The two curves of T_M and T_m formed the envelope of the T curve as shown in **Fig. 2**. These curves are constructed using three point extrapolation method. As it is indicated on **Fig. 2**, we see that at any λ, for any value of T_M there is a corresponding value of T_m.

One of the advantages of this method is that it can be used to measure the refractive index of the substrate (s). This is by using the maximum transmittance (T_M) value in the second region of spectrum in **Fig. 2**, then the equation (Swanepoel, 1983; Marquez *et al.*, 1992) Equation 2:

$$s = \frac{1}{T_M} + \sqrt{\frac{1}{T_M^2} - 1} \qquad (2)$$

The refractive index of the substrate was measured and found to be 1.52.

Using the data of the first region of the curve in **Fig. 2**, the refractive index can be calculated using the following equation (Equation 3 and 4) (Swanepoel, 1983; Marquez *et al.*, 1992):

$$n = \sqrt{N + \sqrt{N^2 - s^2}} \qquad (3)$$

Where:

$$N = 2s\left(\frac{T_M - T_m}{T_M T_m}\right) + \frac{s^2 + 1}{2} \qquad (4)$$

Figure 3 shows the calculated values of refractive index for the as deposited Se thin film as a function of wavelength. As **Fig. 3** shows, the refractive index decreases from 2.815-2.615 as λ increases from 632-890

nm (the dot points in the figure). The calculated values of $n(\lambda)$ can be fitted to a reasonable function such as the two-terms Cauchy dispersion relationship, $n(\lambda) = a + \dfrac{b}{\lambda^2}$, which can be used for extrapolation to shorter and longer wavelengths. The fit of the values of $n(\lambda)$ yields $n(\lambda) = 2.385 + \dfrac{168385}{\lambda^2}$. The full curve in **Fig. 3** represents the fitting curve while the dot points are the calculated ones.

In order to measure the absorption coefficient (α) of the sample the following equation was used (Equation 5) (Swanepoel, 1983; Marquez et al., 1992):

$$\alpha = \frac{-\ln[x]}{d} \tag{5}$$

where, d is the film thickness and x is given by Equation 6 and 7:

$$x = \frac{E_m - \sqrt{E_m{}^2 - (n^2-1)^3 \ (n^2-s^4)}}{(n-1)^3 \ (n-s^2)} \tag{6}$$

where E_m is given by:

$$E_m = \frac{8n^2 s}{T_M} + (n^2-1)(n^2-s^2) \tag{7}$$

The measured values of the absorption coefficient, (α), as a function of the wavelength is shown in **Fig. 4**
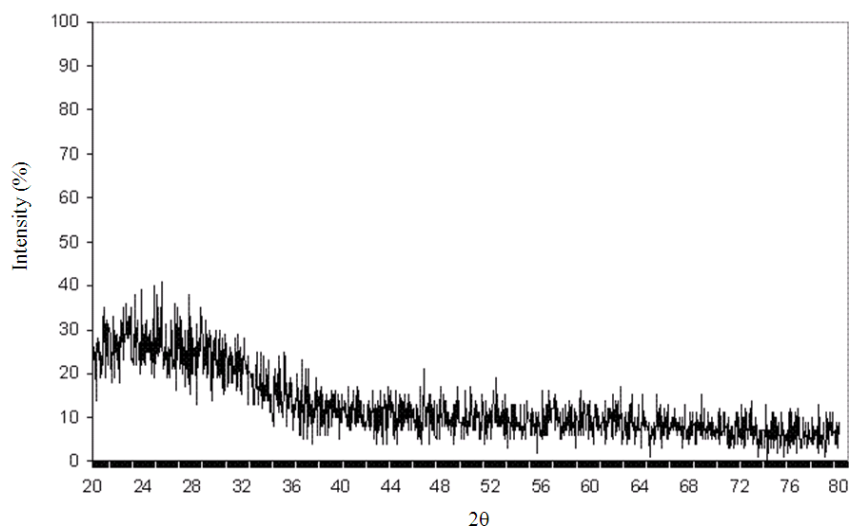

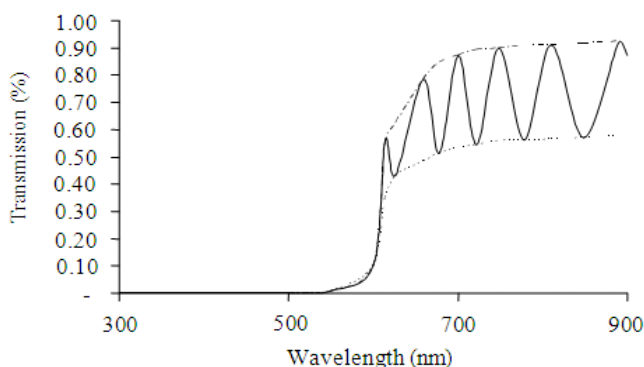**Fig. 1.** The X-ray diffraction pattern of as deposited Se thin film on glass substrate

Fig. 2. The transmission spectrum (full curve) for a 1580 nm a-Se thin film on a glass substrate
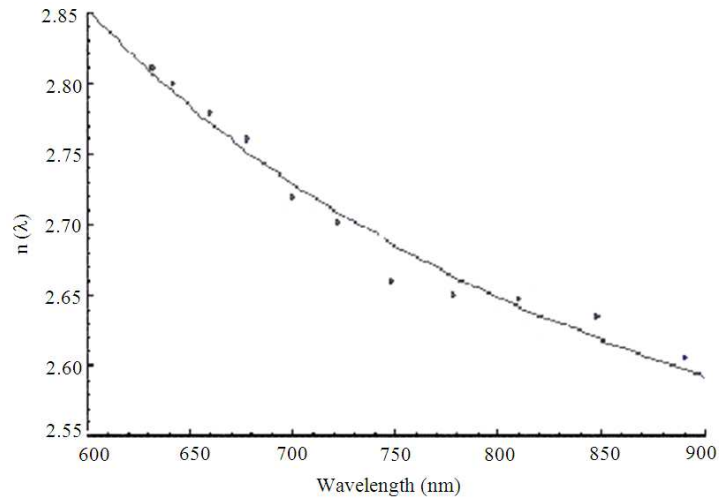
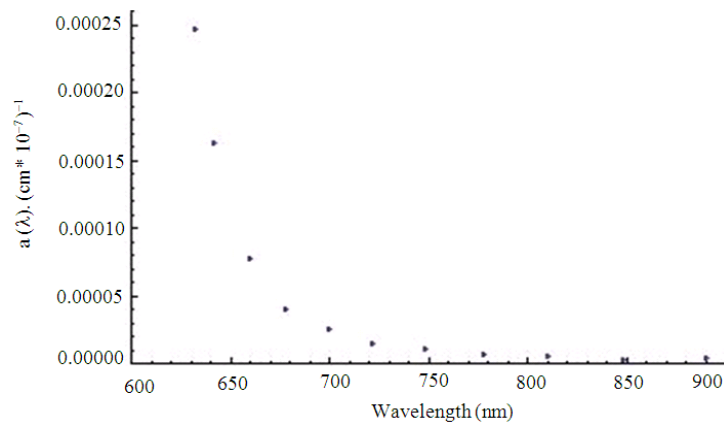**Fig. 3.** Refractive index of as deposited Se (1580 nm) film versus wavelength

Fig. 4. Absorption coefficient of the as deposited Se (1580 nm) thin film versus wavelength
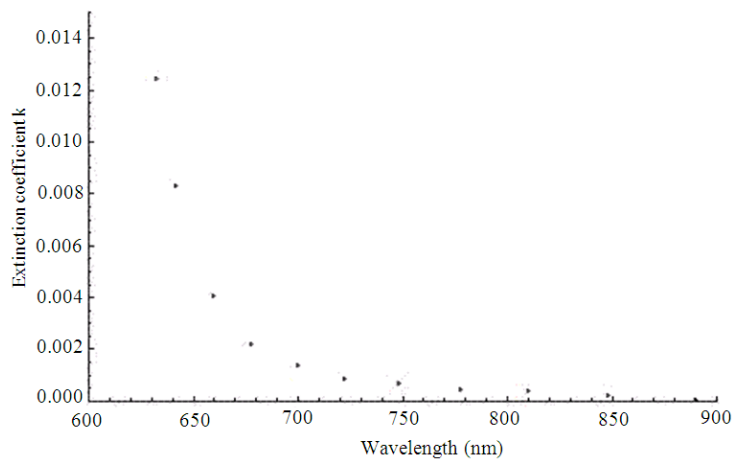

Fig. 5. Extinction coefficient of as deposited Se (1580 nm) thin film versus wavelength
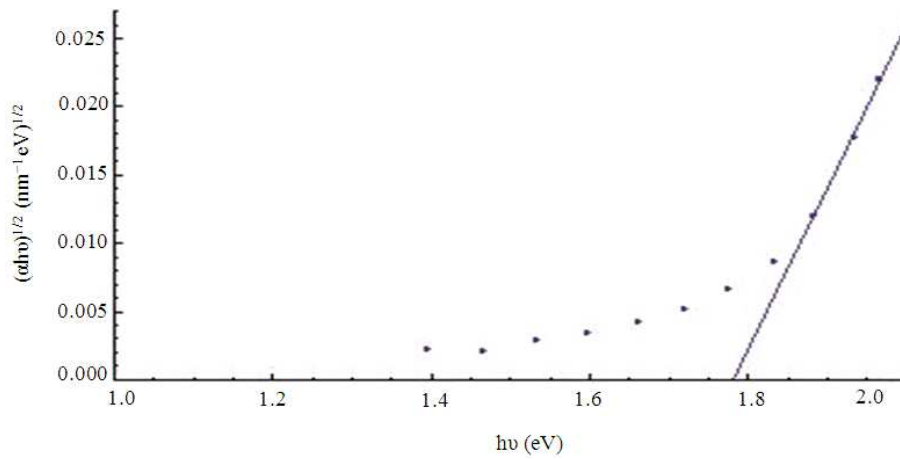
Fig. 6. $(\alpha h\upsilon)^{1/2}$ versus $(h\upsilon)$ plot for 1580 nm Se thin film
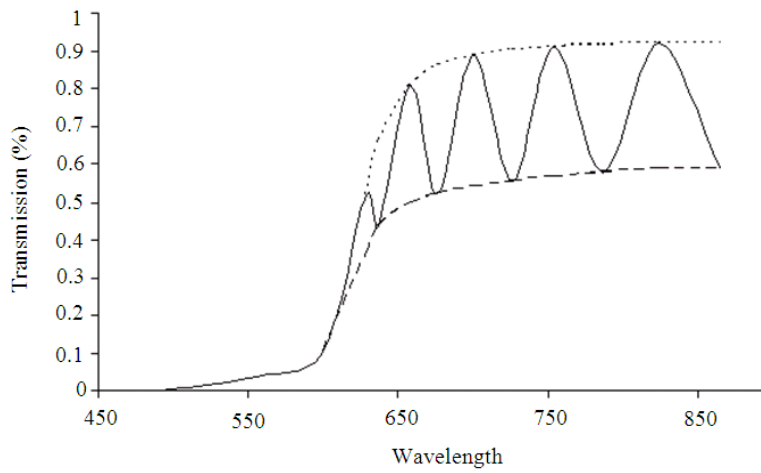

Fig. 7. The transmission spectrum (full curve) for a 1400 nm a-Se thin film on a glass substrate
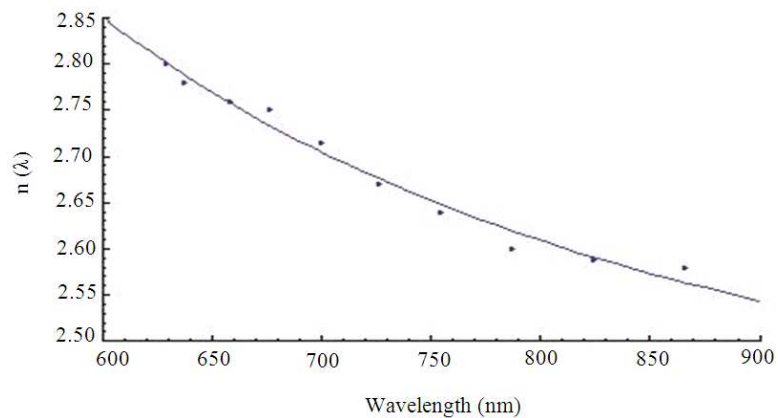

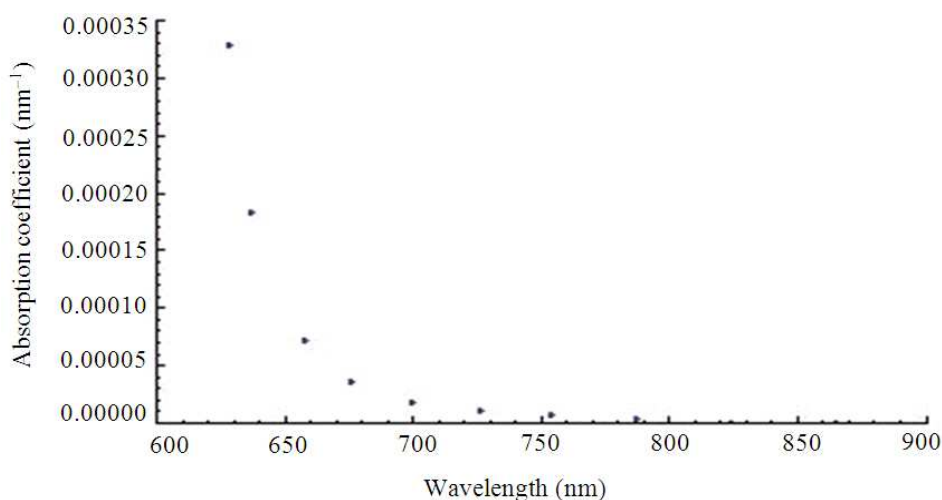**Fig. 8.** Refractive index of Se (1400 nm) film against wavelength

Fig. 9. Absorption coefficient of as deposited Se (1400 nm) thin film against wavelength

It appears that the absorption coefficient decreases from 0.00024712-0.00000379 $(cm*10^{-7})^{-1}$ as wavelength increases from 632-890 nm. Moreover, the absorption coefficient is high at the low region of wavelength while it becomes to zero (no absorption) at high wave lengths as shown on the T curve, i.e., **Fig. 2**.

Figure 5 shows the behavior of the extinction coefficient versus wavelength. The extension coefficient was calculated by using Equation 1. It appears that the extinction coefficient decreases from 0.01243-0.000026816 as wavelength increases from 632-890 nm.

The absorption coefficient is related to the direct allowed band gap energy (E_g) according to the relation (Tashtoush, 2002) Equation 8:

$$\alpha h\upsilon = B(h\upsilon - E_g)^N \tag{8}$$

where, N is an integer equals to 2 for amorphous Selenium.

Therefore, in order to measure the energy gap of the as deposited Se thin film, the relation between $(\alpha h\upsilon)^{1/2}$ and $(h\upsilon)$ was plotted and a linear behavior is expected. **Figure 6** shows this behavior. Using this curve, the energy gap of *a-Se* thin film was calculated and found to be approximately 1.783 eV. This value is consistent with previous studies (Chong, 2006).

Another sample of 1400 nm thickness was prepared and the optical constants were calculated. **Figure 7** shows the transmittance spectrum (solid line) as a function of wavelength. The three point extrapolation curve (dashed line) is also shown connecting between the maximum and the minimum points.

The spectrum on **Fig. 7** can be classified into two regions; first region is the strong and medium absorption region which appears in the interval 550-700 nm. The second region appears in the interval 700 nm to 850 nm which called the weak absorption region (i.e., the transparent region).

Using the same procedure used for the previous film (i.e., envelope method (Chavez-Rivas *et al*., 1982; Bindu *et al*., 2002), the refractive index was measured. The variation of refractive index as a function of wavelength is shown in **Fig. 8** as a dot points. It appears that the refractive index decreases from 2.8-2.58 as wavelength increases from 628.57-865.71 nm. The data were fitted to the two-term Cauchy dispersion relationship and the relation was found to be: $n(\lambda) = 2.29812 + \dfrac{199032}{\lambda^2}$. This is represented on **Fig. 8** by the solid line.

The absorption coefficient α (λ) versus wavelength for the 1400 nm as deposited *Se* thin film is shown in **Fig. 9.** As the Figure shows, $\alpha(\lambda)$ decreases from 0.000328-0.00000043 nm^{-1} as wavelength increases from 628-865 nm.

Figure 10 shows the behavior of the extinction coefficient as a function of wavelength. It appears that the extinction coefficient decreases from 0.01641-0.00003 as wavelength increases from 628 -865 nm.

In **Fig. 11**, $(\alpha h\upsilon)^{1/2}$ versus hυ was plotted to determine the energy gap of the film. It was found to be about 1.815.
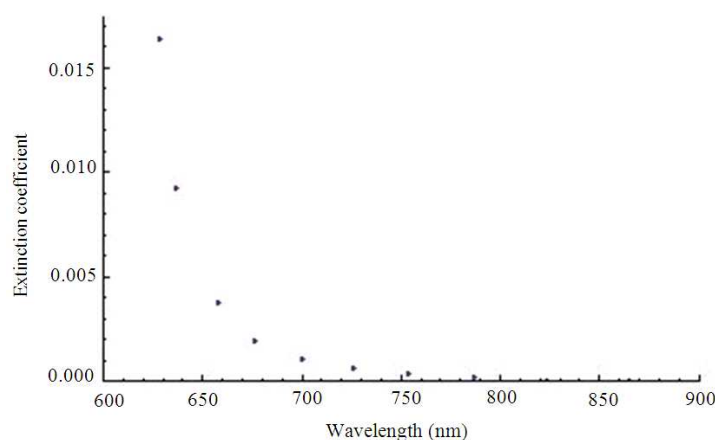
Fig. 10. Extinction coefficient of the as deposited Se (1400 nm) thin film against wavelength
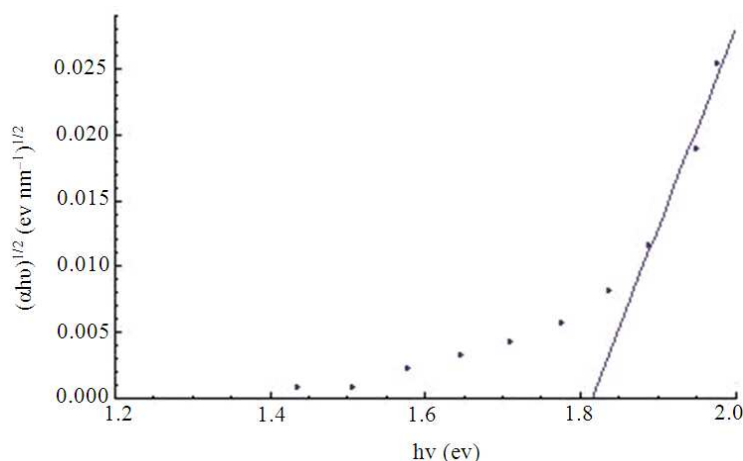

Fig. 11. $(\alpha h\upsilon)^{1/2}$ versus $(h\upsilon)$ plot for 1400 nm a-Se thin film

4. CONCLUSION

In this study, the envelope method which was proposed and used by Swanepoel (1983) was used to calculate the optical constants. The refractive index was found to be in the range of 2.60 to 2.85 and the energy gap (E_g) was found to be about 1.8 eV. The results were found to be in consistent with other studies that utilized other procedures. Also, the absorption coefficient and extension coefficient were found to be consistant with previous studies.

5. ACKNOWLEDGMENT

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