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Research Article

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Optical properties of silicon nano layers by using Kramers- Kronig method

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Abstract

Silicon thin layers are deposited on glass substrates with the thickness of 103 nm, 147 nm and 197 nm. The layers are produced with electron gun evaporation method under ultra-high vacuum condition. The optical Reflectance and the Transmittance of produced layers were measured by using spectrophotometer. The optical functions such as, real and imaginary part of refractive index, real and imaginary part of dielectric constant, real and imaginary part of conductivity, absorption coefficient and optical band gap energy are calculated basing on the Kramers-Kronig relations. The void fractions of the silicon films are calculated by using Aspnes theorem. The effect of layer thickness on optical properties of silicon thin films is investigated.

Keywords : Silicon; Optical properties; Kramers-Kronig relations; Thin films.

1 Introduction

It is well known that the optical parameters of thin-film materials are generally different from those of the same materials in bulk form. The differences in optical parameters depend very much on the conditions in which the deposition has been carried out [1], such as substrate temperature, angle of incidence, deposition rate and film thickness. The most significant properties of the most widespread layered film structures include the layer thickness and basic optical properties such as refractive index (n) and extinction coefficient (k) [2]. The basic thin film properties are well known to depend mainly on its microstructure [3] which is controllable by deposition method and parameters [4]. Refractive index of thin films is thickness dependent and the film thickness is responsible for the optical loss. Thus, the control of the refractive index and the thickness of the waveguide are very important to produce suitable materials for optical applications [5]. In recent years, there has been considerable interest in semiconductor nanocrystals, because of their novel optical or physical properties which can be conveniently tailored over a broad range simply by altering their size. Keeping in mind the technological importance of silicon, great interest was driven toward the Si nanostructures [6]. Silicon is non-toxic, relatively inexpensive, easy to process, and has quite good mechanical properties [7]. The aim of this work is to study the relation between optical properties of silicon thin films and their thicknesses. It has been proven that the film thickness represents very important factor that determines the optical constants.

2 Experimental details

Silicon nanolayers were prepared on glass substrates ($1 \times 20 \times 20 mm^3$) using an ETS160 sys-

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tem with a pressure of $2.9 \times 10 - 5$ mbar. The layers were deposited in ultra-high vacuum condition, using an electron gun evaporation method with the deposition rate of 2 A/s. The purity of Silicon was 98%. All substrates were cleaned with an ultrasonic-bath technique before the deposition process. The layers were produced at 300 K. The thicknesses of the layers were 103, 147 and 197 nm. Optical transmittance and reflectance of the films were measured by using UV-VIS spectrophotometer (Hitachi $U-3310$) instrument. The spectra of the layers were in the visible range. The optical constants of our samples were derived on the basis of standard Kramers-Kronig relations using computer techniques. Aspens and $Thee'ten's$ [8] data were added to calculated results for comparison.

2.1 Kramers-Kronig relations

The Kramers-Kronig relations were first derived by H. A. Kramers (1927) and R. de L. Kronig (1926) independently [9] .Kronig and Kramers showed that the real part of could be expressed as an integral of the imaginary part. The dispersion relations may be taken as a consequence of causality [10]. It is common knowledge that the Kramers-Kronig relations connect real and imaginary parts of an analytic function describing some causal physical process [10, 11].

$$f(x_0) = u(x_0) + v(x_0) \tag{2.1}$$

$$u(x_0) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{v(x)}{x - x_0} dx \tag{2.2}$$

$$v(x_0) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{u(x)}{x - x_0} dx \tag{2.3}$$

Where P denotes the Cauchy Principal value. In statistical physics and electrodynamics any material susceptibility satisfies these relations [11]. The electric susceptibility is $(\chi(\omega))$ [12]:

$$\chi(\omega) = \frac{i}{\pi} P \int_{-\infty}^{\infty} \frac{\chi(\omega')}{\omega - \omega'} d\omega' \tag{2.4}$$

Separating the real and imaginary parts, we obtain the result:

$$Rel(\chi(\omega)) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{Im\chi(\omega')}{\omega' - \omega} d\omega' \tag{2.5}$$

$$Im\chi(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{Rel\chi(\omega')}{\omega' - \omega} d\omega' \tag{2.6}$$

The most frequent expression of the dispersion relation in optics relates the refractive index , n, to the absorption coefficient , α , over all frequencies, ω' [13]:

$$n(\omega) - 1 = \frac{c}{\pi} P \int_{0}^{\infty} \frac{\alpha(\omega')}{\omega'^2 - \omega^2} d\omega' \tag{2.7}$$

When a plane wave is normally incident from vacuum on a medium, the reflectivity is given by [14]:

$$r = \frac{|1-\eta|^2}{|1+\eta|^2} = \frac{(1-n)^2 + k^2}{(1+n)^2 + k^2} \tag{2.8}$$

Where

$$\eta = \varepsilon^{1/2}, n = Rel\eta, k = Im\eta \tag{2.9}$$

n, k are related by the Kramers-Kronig relations:

$$n(\omega) = 1 + \frac{P}{\pi} \int_{-\infty}^{\infty} \frac{k(\omega')}{\omega' - \omega} d\omega' \tag{2.10}$$

$$k(\omega) = -\frac{P}{\pi} \int_{-\infty}^{\infty} \frac{n(\omega' - 1)}{\omega' - \omega} d\omega' \tag{2.11}$$

In this work Kramers- Kronig relations were used to calculate the phase angle θ(E) [15]:

$$\theta(E) = -\frac{E}{\pi} \int_{0}^{E_2} \frac{\ln R(E) - \ln R(E_0)}{E^2 - E_0^2} + \frac{1}{2\pi} \ln[\frac{R(E)}{R(E_2)}] \ln \frac{E_2 + E}{|E_2 - E|}$$

$$+ \frac{1}{\pi} \sum_{n=0}^{\infty} [4(\frac{E}{E_2})^{2n+1}](2n+1)$$

where E denotes the photon energy, E_2 the asymptotic limitation of the free-electron energy, and R(E) the reflectance. Hence, if E_2 is known, the $\theta(E)$ can be calculated. Then the real and imaginary parts of the refractive index were calculated, from which other parameters were obtained.

3 Results and discussion

Figure 1 shows the reflectance curves for the silicon layers deposited on the glass substrates at 300 K. Here different curves correspond to different thicknesses of layers. The results by Aspnes and $Thee'ten$ for silicon samples are included in Figure 1 and all the further figures for the sake

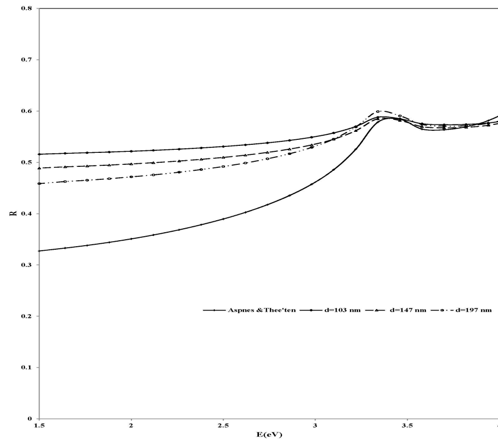

Figure 1

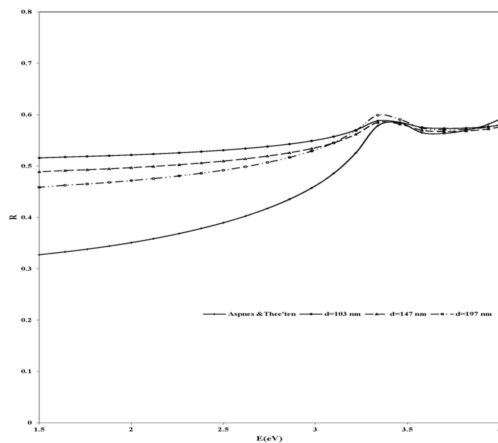

Figure 2

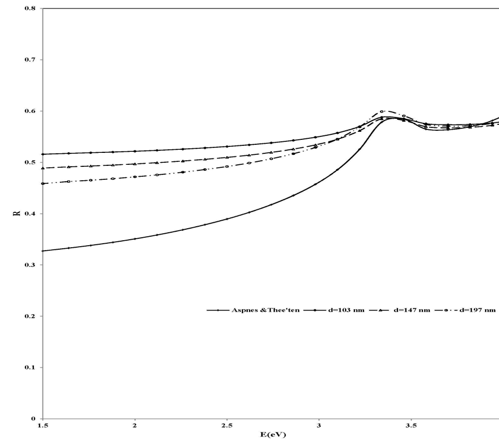

Figure 3

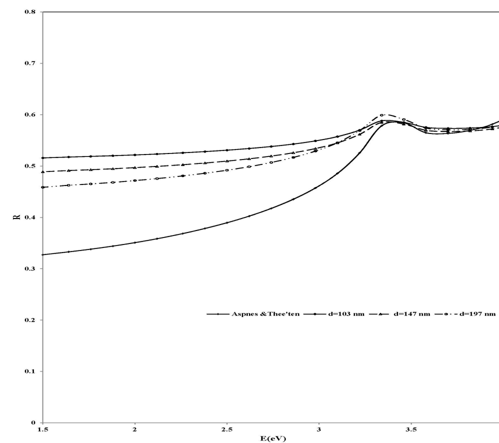

Figure 4

of comparison. By increasing thickness of layers, optical reflectance decreases. This is because layers become thicker in the shape of fractals so the voids formation between grains leads to increase in transmittance and as a result decrease in reflectance. In Figure 2 we depict the real part of the refractive index n. Here the main peculiarities also correlate with those seen in the data by Aspnes and $Thee'ten's$ [8]. There is a peak at 3.4 eV energy for all layers. This peak for Aspnes and $Thee'ten$ [8] result is sharper; which for our results is wide and short. It can be seen from Figure 2 that by increasing thickness real part of refractive index decreases which is because of configuration of homogeneous layers. Figure 3 shows the imaginary part of refractive index. It increases with increasing thickness. That is because of filling voids with silicon grains. Aspnes and $Thee'ten$ [8] data are also included for comparison. There is a peak at about 3.5 eV energy for all layers. Figure 4 displays the real part of the dielectric function for the layers produced in this work. The general trends of our results are same with Aspnes and $Thee'ten$ [8]. There is a peak at 3.4 eV energy for all layers that is sharp and tall for Aspnes and $Thee'ten$ [8], wide and short for our results. As it can be seen from Figure 4, by increasing thickness real part of dielectric function decreases. That is because of formation more metallic layers by increasing thickness. For thicker layers the effect of substrate is also observed. Figure 5, shows the imaginary parts of dielectric constant. The general trend of our results is the same as Aspnes and $Thee'ten$ [8]. There is a peak at 3.5 eV energy for all layers. As it can be seen from Figure 6, by increasing thickness, imaginary part of refractive index increases, that depends on more absorbance. Figure 6 shows, the real part of conductivity which in general agrees well with the results by Aspnes and $Thee'ten's$ [8] data. The general trend and the peak at 3.4 eV energy are the same for all layers. As it can be

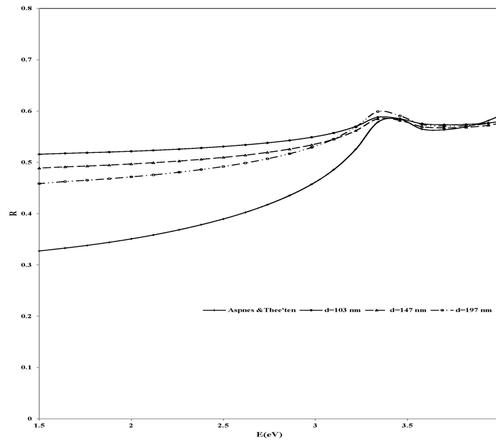

Figure 5

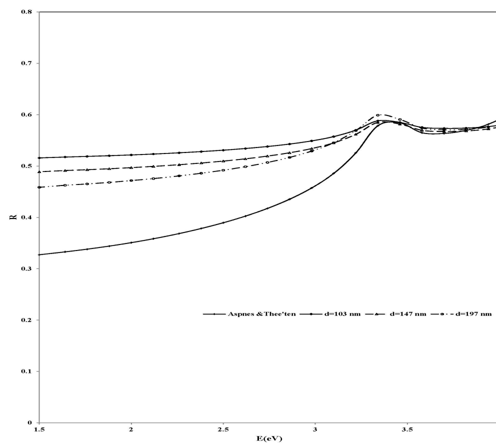

Figure 6

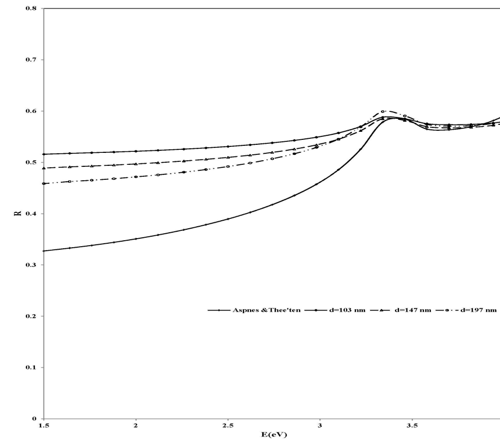

Figure 7

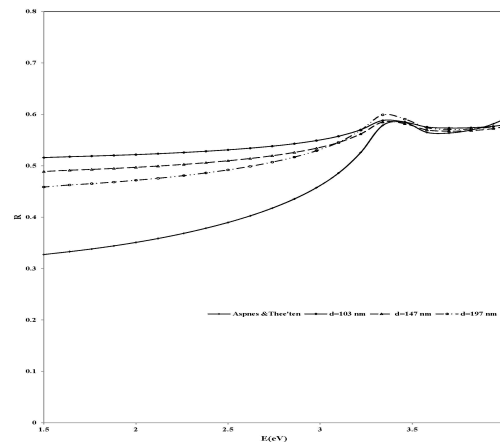

Figure 8

seen from Figure 6, by increasing thickness, real part of conductivity increases, that is because of formation of completed metallic silicon layers and that is in agreement with Figure 3 (real part of dielectric constant). The dependences of the imaginary part of the conductivity coefficient upon the photon energy is shown in Figure 7. The general trend of our results is the same with Aspnes and $Thee^{'}ten^{'}s$ [8], results. The peak is at 3.4 eV energy for all layers, sharp and tall for Aspnes and $Thee^{'}ten^{'}s$ [8], wide and sharp for our results. By increasing thickness, imaginary part of conductivity decreases that depends on absorbance as we discussed before. Figure 8 represents the dependence of the absorption coefficient on the photon energy. Our results are similar to those obtained in the earlier studies [8]. The general trend of all layers is the same. The peak at 3.4 eV is shown already. By increasing thickness absorption coefficient increases. That is because of formation of completed layers and filling up the voids with silicon metallic grains. Figure 9 illustrates calculations of the optical band gap energy for the layers under test and also for Aspnes and $Thee^{'}ten^{'}s$ [8] data. As it can be seen the band gap energies are close to each other at about 3 eV energy, but as it can be seen by increasing thickness band gap energy decreases which is in agreement with all optical parameter analyses. The void fractions of the silicon films calculated for the thicknesses of 103, 147, 197 nm using the known $Aspnes^{'}$ theorem [1]] are shown in Figure 10. By increasing thickness void fraction of layers decreases. It can be seen an anomaly behavior for the layer with the thickness of 103 nm, which is because of a competition between being a conductor or insulator.

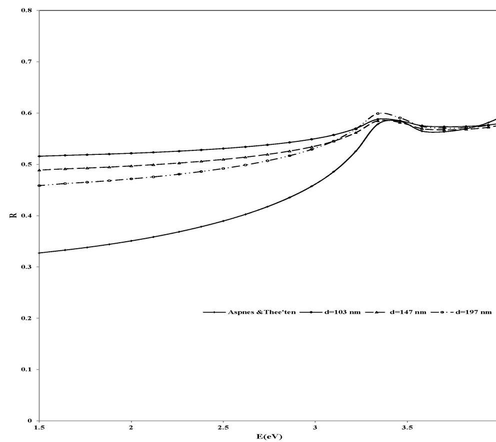

Figure 9

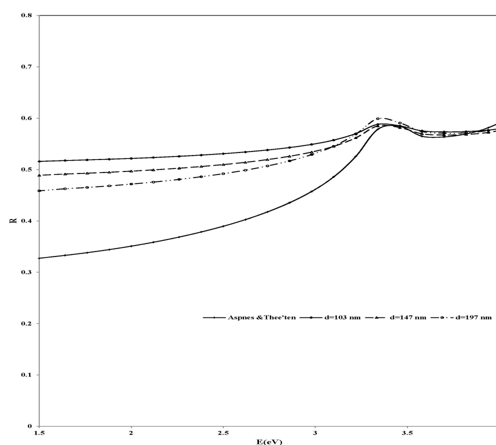

Figure 10

4 Conclusion

In this work we have deposited thin silicon layers on the glass substrates under the same deposition conditions with different thicknesses of 103, 147 and 197 nm. Optical reflectance and transmittance of the layers were measured. The optical constants of our samples have been calculated using the Kramers-Kronig method. We have compared all of our results with those obtained earlier by Aspnes and $Thee^{'}ten$ [8].The general features of our data are quite similar to those found in the works [8]. By increasing thickness real part of refractive index decreases and imaginary parts of refractive index increases, that was because of formation more completed layers and filling up the voids. By increasing thickness real part of dielectric constant shows a decreasing trend and imaginary part of dielectric constant increases. For the same reasons there is an increasing and decreasing trend for real part and imaginary parts of conductivity constant respectively. By increasing thickness, absorption coefficient increases and band gap energy decreases.

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