ORIGINAL PAPER

EXPERIMENTAL STUDY OF OPTICAL PROPERTIES AND INDEX OF CdS /CdTe /Si MULTILAYER

BAHOU YOUNOUSS[1], ABDESSITIR DERAOUI[1,2], ADIL BALHAMRI[1,3], MOURAD RATTAL[1], ABDELMOUMEN TABYAOUI[1], MOHAMED HARMOUCHI[1], AZEDDINE MOUHSEN[1], EL MOSTAFA OUALIM[1]

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Abstract. *The aim of the study on CdS/CdTe/Si multilayer is the determination of the optical properties: reflectance in visible [0.4 -0.8 µm] and infrared [0.8 -1.5 µm] ranges. The spectra obtained allowed us to plot the refractive index (n) and the extinction coefficient (k) of our multilayer, which was chosen due to the large use in solar cells applications.*

In this work, we use wafer silicon (Si) as a substrate with preferential orientation (111), the first layer of CdTe has been deposited in vacuum chamber by thermal evaporation, the second layer of CdS, is done by chemical reaction in the liquid phase. The layers of CdS and CdTe deposited on silicon have been characterized by Fourier Infrared Transformer (FTIR) to get optical properties. Finally, the Kramers-Kronig Transformer (KKT) applied to the reflectance allowed us to plot the refractive index and the extinction coefficient of the system for studied range.

Keywords: *CdS/CdTe/Si, optic properties, FTIR, Kramers-Kroning.*

1. INTRODUCTION

Deposit a simple thin film or multilayer thin film take an important place in applied optics; it's due to their large application in many experimental and industrial devices: Photovoltaic cells, polycrystalline thin films n-CdS/p-CdTe, fiber optics and semiconductors [1].

The cadmium telluride (CdTe) doped p constitute a transparent conductor layer deposited on silicon substrate (Si). At last cadmium sulfide (CdS) of type n has been added. CdTe is oriented for the terrestrial photovoltaic conversion of the solar energy. The width of the band gap of our system (1.45 eV), is conveniently adopted with solar spectrum and the very large absorption coefficient, and the CdS band gap, which is equal to 2.45 eV [2]. These materials belong to the group of semiconductor II-VI, having great potential for applications such as light emitting diodes [3, 4] and optoelectronics. The study put the light on the contribution of good performances demonstrated by interesting optical properties like coefficient of extinction and refractive index. Such properties of deposited layers are given

[1] Univ Hassan 1st, Faculté des Sciences et Techniques de Settat, Laboratoire Rayonnement & Matière: Equipe d'Optique Appliquée et Transfert d'Energie (LOPATE), B.P. 461 Settat, Maroc.
E-mail: ylouch2000@gmail.com.
[2] Université Catholique de Louvain, Institute of Condensed Matter and Nanosciences -Nanophysics (IMCN/NAPS), Louvain, Belgium.
[3] Univ Hassan 1st, Ecole Supérieure de Technologie Berrechid, Berrechid, Maroc.

thanks to FTIR spectrometer and the identification of the optical constants is done by mathematical operations.
The multilayer system deposited is characterized by a complex index:

$$N = n + ik \tag{1}$$

where n is the refractive index (real part), and k is the index of attenuation (imaginary part).

The Kramers-Kronig relations [5, 6] calculate the real part, which lead us to the imaginary part and vice-versa of a response function of passive linear system.
Response function is defined by oscillations of this kind:

$$\alpha(\omega) = \alpha_1(\omega) + i\alpha_2(\omega) \tag{2}$$

The $\alpha_1(\omega)$ is an even function and $\alpha_2(\omega)$ is an odd one, for the variable ω.
Considering following integral of Cauchy:

$$\alpha(\omega) = \frac{1}{\pi\, i} P \int_{-\infty}^{+\infty} \frac{\alpha(s)}{s-\omega} ds \tag{3}$$

where P is the principal part of the integral of superior semi-infinite circle, in the upper part of the complex plane. Let's start equaling real parts of above equation:

$$\alpha_1(\omega) = \frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{\alpha_2(s)}{s-\omega} ds \tag{4}$$

$$\alpha_1(\omega) = \frac{1}{\pi} P[\int_{0}^{+\infty} \frac{\alpha_2(s)}{s-\omega} ds + \int_{-\infty}^{0} \frac{\alpha_2(p)}{p-\omega} dp] \tag{5}$$

In the integral; we replace p by (-s) and use the fact that:

$$\alpha_2(-s) = -\alpha_2(s) \tag{6}$$

This integral becomes:

$$\int_{0}^{+\infty} \frac{\alpha_2(s)}{s+\omega} ds \tag{7}$$

Using the relation:

$$\frac{1}{s-\omega} + \frac{1}{s+\omega} = \frac{2s}{s^2-\omega^2} \tag{8}$$

We found:

$$\alpha_1(\omega) = \frac{2}{\pi} P \int_{0}^{+\infty} \frac{s\alpha_2(s)}{s^2-\omega^2} ds \tag{9}$$

It is the first relation of Kramers-Kronig. The other relationship is obtained by equaling the imaginary parts of the original equation:

$$\alpha_2(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{\alpha_1(s)}{s-\omega} ds = -\frac{1}{\pi} P[\int_0^{+\infty} \frac{\alpha_1(s)}{s-\omega} ds - \int_0^{+\infty} \frac{\alpha_1(s)}{s+\omega} ds] \quad (10)$$

Thus we have:

$$\alpha_2(\omega) = \frac{-2\omega}{\pi} P \int_0^{+\infty} \frac{\alpha_1(s)}{s^2-\omega^2} ds \quad (11)$$

The complex refractive index is also an analytic function, which can be written in the form of Kramers-Kronig relation:

$$n(\omega) = \frac{2}{\pi} P \int_0^{\infty} \frac{sk(s)}{s^2-\omega^2} ds \quad (12)$$

where P is the principal part of the integral, as we see in this equation. Kramers-Kronig relations, allow us to know the evolution of n (or k) in the whole range of wavelengths.

2. EXPERIMENTAL STUDY

2.1. PREPARATION OF SAMPLE

The process of substrate treatment was as follows: firstly, the substrate was dipped in acetone; secondly it was washed with water after dipping; finally the substrate was dried.

Deposition of CdTe onto Si substrate by CSD was carried out according to the literature methods [7]. In short, trisodium citrate (TSC) was used as complexing agent. An aqueous stock solution of 0.2 M CdSO4 and a 5 10^{-4} M of TeO_2 was used. The pH of the aqueous solution is adjusted to pH 2.2 and the temperature of the bath. Is maintained in the neighborhood of 0°C to produce a very low deposition. The Si substrate was placed in the CSD solutions for typically 24 h periods. The thin layer of CdTe has been put down to a cathodic potential equal to -0.7 V. The average thickness of thefilm CdTe is about 9.7 mm, based on deposition time.

A brown color layer is deposited on the substrate of silicon when this last be immersed in a solution containing $HTeO_2^+$ (none potential is applied). The formation of telluride produces via a mechanism of corrosion that can be explained by the following reactions:

Mechanism of oxidization:

$$Si + 2H_2O \rightarrow SiO_2 + 4H^+ + 4e^- \quad (13)$$

Mechanism of reduction:

$$HTeO_2^+ + 2e^- \rightarrow Te + 2H_2O \quad (14)$$

The processes of the deposition of CdS by CSD technique are widely described in the literature [8]. In short, trisoduim citrate (TSC) was used as complexing agent. Aqueous stock solution of 0.2 M $CdCl_2$ and a 0.01 M of Na_2S_2O3 was used. The pH of the aqueous solution is adjusted to pH = 2.2 and the temperature of the bath is maintained close to 90°C to have a very low deposition. The thin layer of CdS has been deposited for a cathodic potential equal to -0.6 V. In this manner, CdS is deposited in the form of transparent, uniform and adherent film. Based on deposition time, the average thickness of the film CdS is about 1 mm. The cathodic reactions that drive to the simultaneous deposition of the cadmium and sulphur are as follows:

$$Cd^{2+} + 2e^{-} \Leftrightarrow Cd \tag{15}$$

$$S_2O_3^{2-} + 6H^{+} + 4e^{-} \Leftrightarrow 2S + 3H_2O \tag{16}$$

2.2. MEASURING DEVICES

The infrared absorption spectroscopy is a physical-chemical characterization technique, often used for thin films. Materials absorb radiations, whose energy corresponds to one of vibration modes of a molecule. In this study we use the infrared spectrometer Fourier transform "FTIR" of "Bruker-Vertex70" type, This device is an entirely numeric spectrometer of resolution spectral standard 0.5 cm^{-1} and can cover the spectral range from 30 cm^{-1} in the far infrared to 25000 cm^{-1} in the visible, through the medium and the near infrared. This spectrometer is used to carry out experimental measurements of the reflection Rexp (λ) and transmission Texp (λ) in the spectral range of the visible and the infrared. The spectrometer presents various compartments, namely: He-Ne laser source with a wavelength of 633 nm and a power of 1mW, two beamsplitters : standard of layer KBr deposited on the medium infrared Ge covering a spectral band (7500-370 cm^{-1}) and the other for the visible along 25.000 to 1200 cm^{-1}. Two detectors of DLATGS types for the infrared mid (wavelength range of 12.000 to 250 cm^{-1}, sensitivity D *> 2.108 cm $Hz^{1/2}$ W^{-1}) and the other for the detection of the visible (wavelength range of from 25.000 to 9.000 cm^{-1}, NEP sensitivity: < 10^{-14} W $Hz^{-1/2}$). Its operation is based on the principle of the Interferometer of Michelson.

2.3. MEASUREMENT EQUIPMENT - INFRARED FOURIER TRANSFORMER SPECTROMETER (FTIR)

FTIR use the technology of the Michelson Interferometer. A monochromatic light beam impinges on a light-splitting plate, which divides the beam into two parts of nearly equal intensity. One part passes through the plate, while the other is deflected perpendicular to the incident beam direction. Then both beams fall normally onto two mirrors and return to the beam-splitting plate. Once again, the plate partially reflects and partially transmits the incident light, producing an output beam composed of two beams that have traversed different arms of the interferometer.

By moving one of the interferometer mirrors along the incident light beam, one can vary the optical path difference and observe a variation of the interference pattern.

The light-splitting plate is a plane-parallel glass plate the back surface of which is covered with a translucent silver film. The film is so thin that the plate partially reflects and partially transmits the light, thus serving as a semi-reflecting mirror.

FTIR’s output is an interferogram and consists of a plot of detector signal versus the mirror displacement in the interferometer.

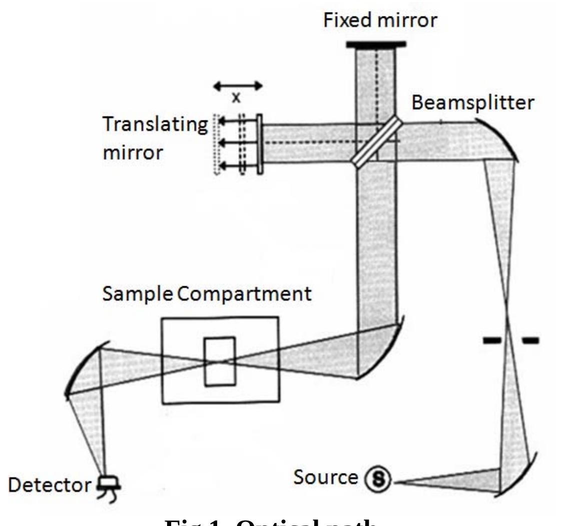

Fig.1. Optical path.

The interferogram must be mathematically transform to a more conventional "% transmission versus wavelength" spectrum by means of Fourier-Transform methods. This is done in a computer which is also used to control the spectrometer [9]. A complete FTIR assembly is shown in Fig1. Since collection of a usable spectrum takes only a few minutes the reference data may be collected immediately before or after the sample data without disturbances due to changing humidity, etc.

3. RESULTS AND DISCUSSION

We present bellow, reflectance measured by FTIR spectroscopy:

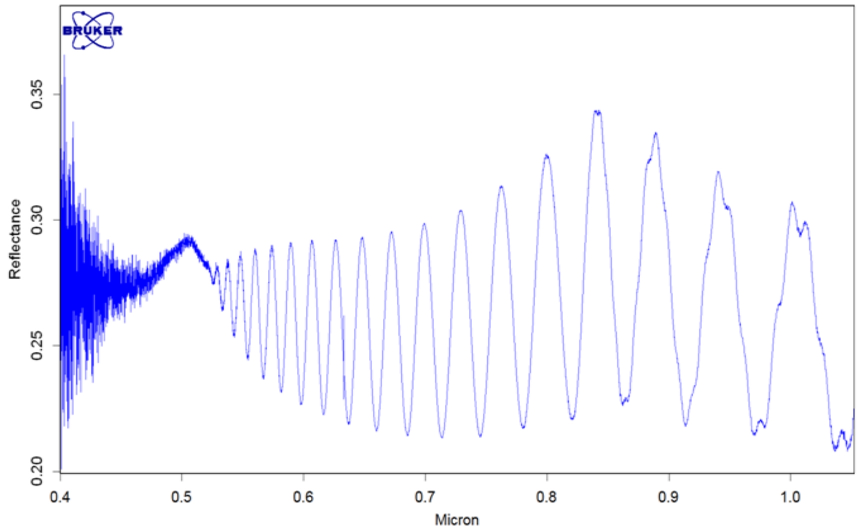

Fig. 2. Reflectance of CdS/CdTe/Si in the wavelength [0.4-1.5µm] range.

The oscillations in the spectrum (Fig. 3) are due to interference within the system. We observe redundancy fluctuations at 0.4µm to 0.5µm band. These oscillations are due to the resolution of the beamsplitter in visible.

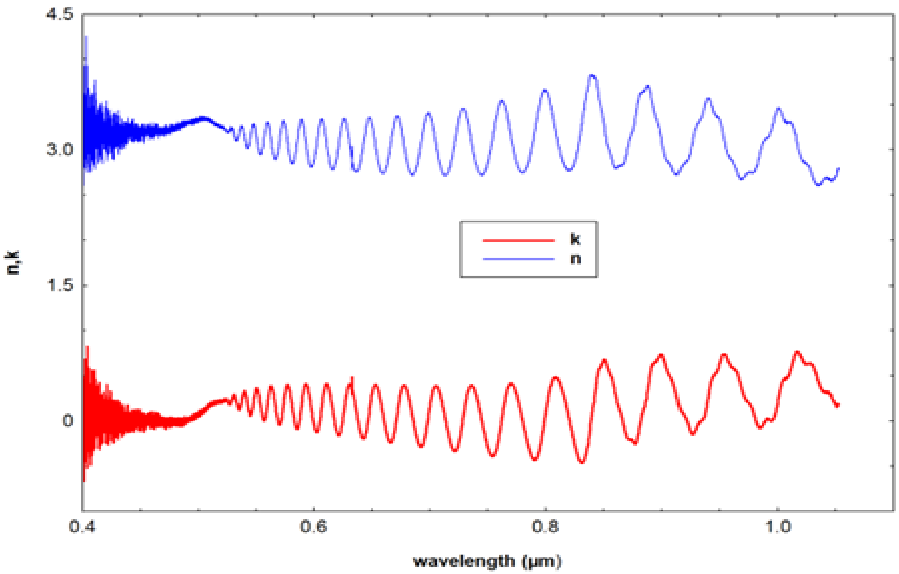

Fig. 3. Refraction index (n) and extinction coefficients (k) of the CdS/CdTe/Si in the range of [0.4-1.5µm].

We note that the numerical value Fig. 3 of extinction coefficient oscillates around an average value over a wide range of thicknesses. The oscillations are associated with interference within the system, and disappear when the thickness becomes large compared to the wavelength in the layer traversed [10]. At thermal equilibrium, the extinction coefficient k is positive because the lowest energy levels are more populated than the excited ones. Indeed, a count rate of transition absorption or emission leads to an expression of the absorption coefficient:

$$k = B_{12}\ f(N_1 - N_2) \tag{17}$$

K : Absorption coefficient

B_{12}: Einstein coefficient

If we consider that the balance is upset by optical pumping process, we can arrive at a situation which population inversion is to reverse the sign of the absorption coefficient.

4. CONCLUSIONS

The multilayer of CdS/CdTe/Si was chosen for its high reputation in the field of solar cells, indeed several research studies have reported that this system have significantly improved performance, compared to ordinary cells [11]. This study was aimed to determine optical constants, which are the refractive index (n) and extinction coefficient (k), for the spectral domain of the visible and infrared and their wavelength ranges are analyzed to complete the data reported in the literature [12]. The optical properties were analyzed by Fourier transform infrared, and by Kramers-Kronig transform applied to the reflectance of the system in the case of optical constants. The tables below presents refractives index and extinction coefficient for each wavelength.

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