Dielectric properties of flash – evaporated CuInSe₂ photovoltaic thin films

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Abstract - In this paper, we have analyzed the dielectric functions of CuInSe₂ photovoltaic thin films, \( \varepsilon = \varepsilon_1 + i\varepsilon_2 \). Thus we have obtained the dispersion spectra corresponding to \( \varepsilon_1(\lambda) \) and \( \varepsilon_2(\lambda) \) from spectrophotometry measurements for different thicknesses of thin films.

Résumé - Nous analysons dans cet article, les fonctions diélectriques des couches minces photovoltaïques CuInSe₂, \( \varepsilon = \varepsilon_1 + i\varepsilon_2 \). A cet effet, nous avons obtenu les spectres de dispersion correspondant à \( \varepsilon_1(\lambda) \) et \( \varepsilon_2(\lambda) \) à partir des mesures spectrophotométriques pour différentes épaisseurs de couches minces.

Keywords: CuInSe₂ films - Dielectric properties - Critical points - Band structure - Spectroscopic ellipsometry.

1. INTRODUCTION

CuInSe₂ is one of the ternary semi conducting compounds with good properties for solar cells applications [1]. It presents a direct band gap.

CuInSe₂ films are prepared by flash evaporation in vacuum from a single source [2]. We use films thicknesses: 100, 200, 300 and 400 nm. We have studied [3], the optical properties, i.e. index of refraction \( n(\lambda) \), extinction coefficient \( k(\lambda) \) and determined the absorption coefficient \( \alpha(\lambda) \) and optical energies gap of CuInSe₂ flash evaporation thin films, from the measured transmittance \( T \) and reflectance \( R \) at normal incidence in the range 300 to 2500 nm.

The interpretation of these results are based on the Mueller numerical method of resolution of nonlinear equation [4].

In this work, we report an analysis of dielectric properties of the thin films from the relations:

\[
\varepsilon_1 = n^2 - k^2 \quad \text{and} \quad \varepsilon_2 = 2\, n\, k
\]

From the \( \varepsilon_2 \) spectra, we have deduced the critical points related to its band structure correlation with optical parameters \( n \) and \( k \).

2. RESULTS AND DISCUSSION

The spectra of the real part \( \varepsilon_1(\lambda) \) and those of the imaginary part \( \varepsilon_2(\lambda) \) for different thicknesses are represented in figures 1, 2, 3 and 4 as function of wavelength.

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Reflectance $R(\lambda)$ and transmittance $T(\lambda)$ spectra of CuInSe$_2$ films at normal incidence of light in the visible and near infrared region exhibit a middle and strong absorption in the visible while a weak absorption in the near infrared range [3]. All these spectra of $\varepsilon_1$ present the same trend that the index of refraction $n$.

The imaginary part $\varepsilon_2$ of the dielectric constant of the film depends to the absorption coefficient $\alpha$: and to all the transitions (valence band to conduction band) and is closely related to its band structure.

The spectra of $\varepsilon_2$ present also the same behavior that the extinction coefficient $k$.

![Fig. 1: Dispersion spectra of the real part $\varepsilon_1(\lambda)$ and of the imaginary part $\varepsilon_2(\lambda)$ for different thicknesses (100 nm), as function of wavelength](a)

![Fig. 2: Dispersion spectra of the real part $\varepsilon_1(\lambda)$ and of the imaginary part $\varepsilon_2(\lambda)$ for different thicknesses (200 nm), as function of wavelength](b)
3. DETERMINATION OF CRITICAL POINTS

The spectra of $\varepsilon_1(\lambda)$ and $\varepsilon_2(\lambda)$ for different thicknesses are shown in figures 1, 2, 3 and 4 as function of wavelength. The real part $\varepsilon_1(\lambda)$ shows a maximum at 0.5 µm and then decreases for thickness 0.4 µm. For thickness 0.2 µm, it fluctuates around 3.6. For thickness 0.1 µm and thickness 0.3 µm, $\varepsilon_1(\lambda)$ presents the same trend that n.

The film absorption coefficient $\alpha$ was extracted from $R(\lambda)$ and $T(\lambda)$ measurements [6].

For direct transition materials, the absorption coefficient $\alpha$ is given by:

$$\alpha E = A \left( E - E_g \right)^{1/2}$$
where $E$ is the photon energy and $E_g$ is the band gap energy. The optical energy gap was calculated by extrapolating the linear portion of the absorption spectrum to $E = 0$.

Thus we obtain:

- $E_g = 0.98 \text{ eV}$ for $d = 0.1 \mu m$
- $E_g = 0.97 \text{ eV}$ for $d = 0.2 \mu m$
- $E_g = 1.02 \text{ eV}$ for $d = 0.3 \mu m$
- $E_g = 1.03 \text{ eV}$ for $d = 0.4 \mu m$

in good agreement with the published data [7].

However the spectra of $\varepsilon_2(\lambda)$ for thicknesses 0.2 and 0.4 µm show peaks energy of 2.9 eV and 2.61 eV respectively and decrease. While those for thickness 0.1 µm and 0.3 µm give singularities in the near infrared range and several peaks energy of 2.53 eV, 2.10 eV, 1.82 eV, 1.61 eV respectively.

This can primarily be associated to physical imperfections which were not taken into account in the calculations [8].

Different methods have been used to determine the band structure of CuInSe$_2$ [9, 10]. The values at 2.9, 2.61, 2.53, 2.10 eV can be attributed to transitions originating Cu 3d levels and the values at 1.82, 1.61 eV can probably be ascribed to transitions from the Se 4p levels [11].

Our results are compared with values measured by spectroscopic ellipsometry and with those reported in the literature. They are in good agreement [11].

REFERENCES