

Calculated and Measured Dark Conductivity in P-Type Polycrystalline CdTe Thin Films

H. Mohssine, H. Bouhouch, F. Debbagh

Abstract— In this study we describe a numerical procedure for modeling the dark conductivity in a p-type polycrystalline Cadmium Telluride (CdTe). We base our approach on the comparison between measured and computed conductivity. For this purpose, the Fermi-Dirac statistic combined with the numerical solution of the charge neutrality equation allows to calculate the exact dark conductivity as function of the temperature. The results are then used to fit the experimental conductivity. Measures have been undertaken on CdTe thin films produced by r-f sputtering on glass substrates at room temperatures. It is shown that the amount of the experimental conductivity can be modeled, quite precisely, by suitably choosing parameters of localized states, without needing complicated approaches like Mott and seto's models. However, from a point of view of experimental fitting, it is verified, in accordance with our previous general treatment that the model's parameters are not unique and cannot be derived from Arrhenius diagram analyses.

Keywords—Thins films, CdTe, Sputtering, Conductivity.

I. INTRODUCTION

A precise knowledge of the electric and photoelectric properties of semiconductors is of great importance in several technological fields such as conception and realization of modern optoelectronic devices (photovoltaic cells, Schottky diode, and sensor for page scanners or fax machines...) [1]. The efficiency of these materials depends strongly on densities N_i and energy levels E_i of localized states in the gap (donors and/or acceptors) The determination of these parameters plays therefore an essential role in the characterization of these materials. For this effects many experimental techniques have been implemented (Hall effect, thermally stimulated currents and conductivity, deep-level transient spectroscopy, conductivity at thermal equilibrium,). These techniques are based in their majority on simplified approaches of the Shockley-Read model (RS) [2] and on reducing Fermi-Dirac statistic to its boltzmannian form. They are often analyzed by means of Arrhenius diagrams (DA) that are deemed to give access to N_i and E_i whose graphic exploitation allows in principle to evaluate the N_i and the E_i Now, we have shown [3], that discarding these classical approximations allowed to put forward that (DA) was not a valid method of graphical determination of localized state parameters in dark conductivity experiments.

In this section we substitute the DA method to an exact computer simulation for modeling the dark conductivity in a polycrystalline Cadmium Telluride (CdTe). Computed

conductivity σ_c and measured conductivity σ_m is then compared.

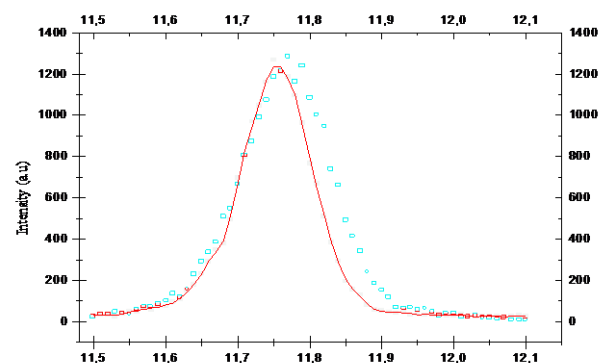
II. EXPERIMENTAL METHOD

The CdTe thin films are deposited from high purity (5N) target by r-f sputtering onto unheated glass substrates. Before deposition, a combination of mechanical and oil diffusion pumps pump the plasma chamber (down to around. 10^{-6} mbar). All the films reported here are produced in argon atmosphere. During the deposition, the argon pressure is maintained at 10^{-2} mbar The sputtering rate is approximately 0,5 nm/s. The film thicknesses' is determined using a Mickelson's interferometer associated with an optical microscope system.

Cu-Te/CdTe/Te-Cu sandwich structures are prepared in order to make ohmic contacts. The tellurium and copper electrodes are deposited at relatively low r-f power density ($1,5 \text{ W/Cm}^2$) In order to avoid interfacial contamination; the films are sequentially deposited without breaking the vacuum.

III. X RAY STUDIES

Conventional diffraction technique, using copper $\alpha(1.5418\text{\AA})$ radiation, is used to study the structural properties of CdTe thin layers. Rocking curve measurements around the (111) diffraction peak will be given.



X-Ray Rocking Curves for unheated (scatter) and heated 500K (line) films.

crystallite sizes were determined from XRay diffraction spectra using the Sherrer formula [1].

$$L = \lambda D \cos(\theta) \quad (1)$$

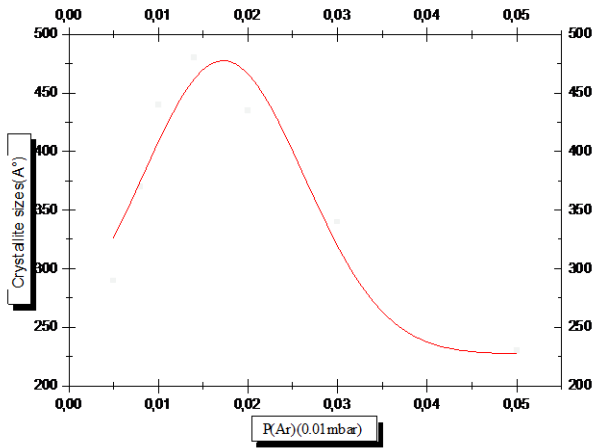
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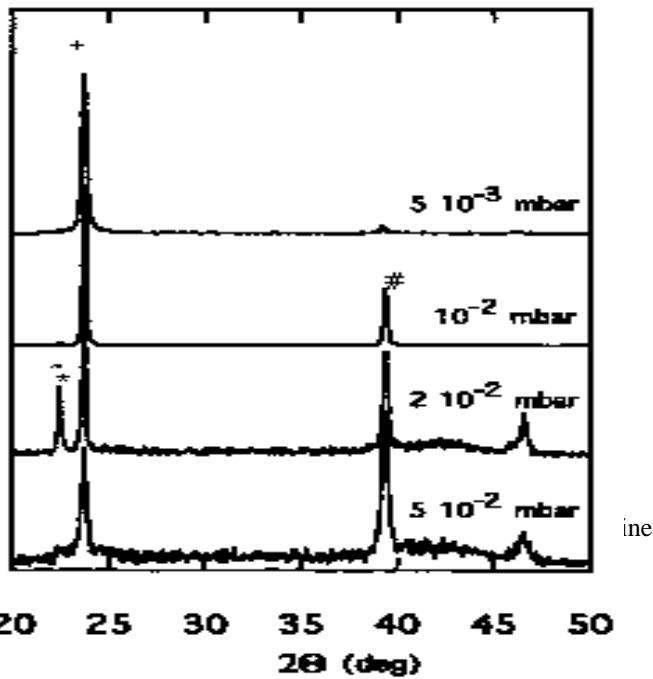
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Where l is the grain size, D the full width at half maximum of the peak and λ is the used wavelength. The results indicate that the preferential orientation of crystallites is along the (111) direction [3].



Sharp peaks of CdTe corresponding to the (111), (220) and (311) reflections of cubic phase are observed. The hexagonal phase is also present but in small proportion ((100) reflection). It should be noted that the hexagonal phase is only remarked at $P(\text{Ar})=2 \cdot 10^{-2}$ mbar. It is clear to show from these spectra that argon pressure has noticeable effect on crystallite orientation: When $P(\text{Ar})$ increased from $5 \cdot 10^{-3}$ to $5 \cdot 10^{-2}$ mbar, the intensity of (111) direction line is decreased while the corresponding (220) one is increased. This effect could be explained on the basis of change in the mean free path of sputtered atoms leading to an increase of defect density in the material. This explanation is very consistent with the conclusions given by other authors [4] which have interpreted this behavior in terms of deterioration in the films structure when the argon pressure changes. D.C. electrical conductivity is measured in the temperature range 140-500 K. All these measurements were performed in

a vacuum better than 10^{-6} mbar. The junction of thermocouple was bonded to the glass substrate close to the middle of the specimen for measuring the average sample temperature

IV. NUMERICAL CONSIDERATIONS

In thermal equilibrium the dark conductivity is given by

$$\sigma_c = n \cdot q \left(1 + \frac{\theta}{u} \frac{p}{n} \right) \quad (2)$$

Where, $\theta = N_v / N_a$, $u = \mu_n / \mu_p$. μ_n and μ_p are the mobility of free electrons and holes respectively. n and p are their densities. N_c and N_v are the effective densities of states in conduction and valence bands.

The precise calculation of n , p and σ_c , requires the determination of the Fermi level, which is obtained through the numerical solution of the charge neutrality equation. Fermi-Dirac statistics is required to describe the trapped and free carriers, because the Boltzmann approximation is not appropriate, especially at low temperatures or when the traps are located near the conduction or the valence band.

$$\frac{1}{C_b + e^{-\frac{(E_c - E_{F_0})}{KT}}} - \frac{\theta}{C_b + e^{-\frac{(E_{F_0} - E_v)}{KT}}} - \sum_{i=1}^M \frac{N_i}{N_c} \frac{1}{1 + e^{-\frac{(E - E_{F_0})}{KT}}} = 0 \quad (3)$$

Where the factor $C_b = 27/10$ is used in calculation as an approximation of the $F_{1/2}$ Fermi function [4], E_{F_0} is the Fermi level. We assume that the localized states are both acceptors like located in the lower half of the band gap.

The numerical solutions of equation (3) . give the E_{F_0} , then n and p , and σ_c . Nevertheless the numerical procedure is very difficult, especially at low temperatures when terms of equations (2) take very low or very high values. Another problem comes from the flatness shapes of these equations in the neighborhood of the roots. Consequently to get round these difficulties, a special program working with any arbitrary precision was developed from the BRENT algorithm [4]. Experimental and calculated conductivity for 500 nm thicknesses are plotting in fig.3 in order to show what

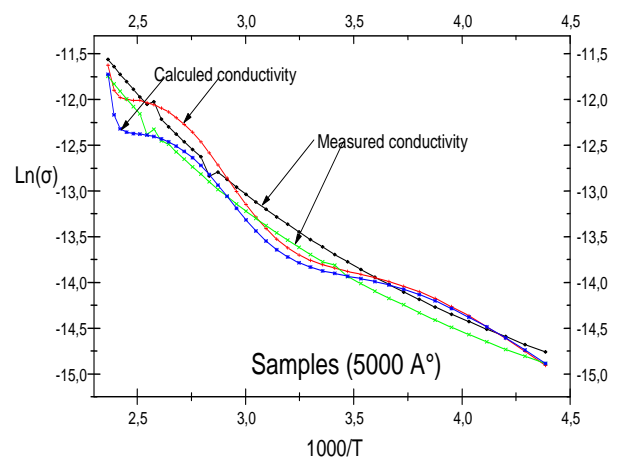


Fig.3. Variation of conductivity for 5000Å° thicknesses Unannealed films b) 500 K Heated Films



kind of behavior can result when 4 acceptors and 1 donor model is considered. This model is not otherwise different from the one of sub-section above. However it introduce two other parameters of characterization ($r = N_a/N_c$ and E_a).

We have processed thermally one sample during 2 hours in the elaborate vacuum in order to put in obviousness the influence of annealing on the electrical conductivity. The result, show a slow increase of the conductivity based on the increase of the concentration of acceptors in the band without all time to cause a variation notable of activation energy. Two observations can be made about these curves. First, it appears that the curves of calculated conductivity annealing and un-annealing films; enveloped the experimental ones. In each curves the relative ratio r , is varied by powers of 10. (From 10^{-10} to 10^{-11}). Secondly, the slope of curves depend upon

| E_1 (eV) | E_2 (eV) | E_3 (eV) |
|----------------------|-----------------------|--------------------|
| 0.95 | 1.1 | 1.3 |
| r_1 | r_2 | r_3 |
| $4.5 \cdot 10^{-11}$ | $0.95 \cdot 10^{-11}$ | $9 \cdot 10^{-12}$ |

the temperature range: at the low temperature (120 to 200 k), the curves seem to be confused leaving to claim a direct convergence between experimental and simulation.

The comparison between curves shows quantitatively good agreement. It is clear from figures that in contrast with an early work, the amount of the experimental conductivity can be approached quite precisely by adequately choosing values of localized states parameters without needing sophisticate approaches like Mott and Seto's models. But from a point of view of experimental fitting, it is verified, in accordance with our previous general treatment that the model's parameters are not unique and cannot be derived from Arrhenius diagram analysis. Another important result shows that for a given model (here three acceptors), one observes that the effect of the thermal annealing, is the change in densities of acceptors only. Activation energies are maintained constant because we have noticed that the conductivity is very sensitive to the lesser variation of these energies.

It should be noted that the hopping conduction in polycrystalline material is essentially remarked in the grain boundaries region. At low temperature, the carriers have insufficient energy to cross the potential barrier, and then the major contribution to the transport properties can be attributed to the transfer of the charge carriers from a charged trap state to a neutral one.

But this graphic analysis, based on the qualitative diagram behavior (D.A), does not allow determining, in a clear manner, the position of acceptor levels. Indeed, activation energy deduced of these diagrams cannot, in the most shares of cases, to be attributed to the real localized states [4]. It is elsewhere the good reason to find appropriated simulation models for be able to determine exactly the acceptor levels. Therefore, in our opinion, these diagrams do not offer, in the one hand, the opportunity to localize levels of acceptors in the gap, and on the other hand, the Mott's model, is not the unique tool of result interpretation in our case.

V. CONCLUSION

A numerical model has been developed to examine the exact dark conductivity in polycrystalline Cadmium Telluride in order to fit the experimental data. Three acceptors model was

used to carry out computations, but the same model, with different suitable values of parameters or another adequate model can be used. More essentially, it is shown that our simple model without needing complicated approaches can interpret the conductivity process.

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