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COMPOSITION MIXTURE PROBABILISTIC MODEL IN THE FORMATION OF SEMICONDUCTOR MATERIALS OBTAINED BY RANDOM GROWTH TECHNIQUES

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During the obtaining of semiconductor materials by some growth techniques the film structure forms randomly according to how the species arrive to the subtract. If the film is a material with three or more elements they can organize in several compounds, which have only local order and even become amorphous. As a consequence the physico-chemical parameters manifest non-typical behaviors other than in pure materials. In the present work we develop a dynamical-probabilistic model, which describes quantitatively such composition mixture and was applied on the behavior of the absorption profiles of CdTeO films grown by radio frequency (rf) sputtering with different oxygen concentrations. The model can be applied to films obtained by other growth techniques.

1 Introduction

The promissory possibilities of disordered semiconductors have led to deepen on its study. One of these materials is the CdTe oxide. In controlled atmosphere growth it was obtained with different oxygen contents in the film, and it was found to be amorphous since concentrations about 5 at.% oxygen.

From the measured characteristics the CdTeO films have been proposed to be associated with $CdTeO_3$ [2] and co-existing with $CdTe_2O_5$ [3], but a material with variable composition has also been suggested [5,6].

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The CdTeO growth by rf sputtering process takes place under the action of high energies, which induces the appearing of ionized species and multiple random bindings between them. In this case the formation of the amorphous material is ruled by the formation of TeO_2 primary chalcogen units which bound to Cd atoms and form, together CdTe molecules a compositional mixture [5]. In other words, such high-energy techniques lead frequently to the formation of compositionally and structurally mixed amorphous materials as has also been observed in CdNiTe [1], and in ternary oxides as CdPbO [4].

In this work we model the behavior of the optical absorption spectra of CdTeO films grown by rf sputtering as a function of the oxygen content from dynamical and probabilistic considerations of the composition of the amorphous CdTeO films. The model is, in principle, applicable to other amorphous compounds with similar behaviors.

2 Experiment

The CdTeO films, of 1 cm diameter, were deposited on Corning 7059 glass slides by rf reactive sputtering using a 2 in. diam CdTe target with 99.99 at. % purity in an argon-nitrous oxide atmosphere. The base pressure was $1.5\text{x}10^{-6}$ Torr and the gases used were Ar from Linde with 99.999 at. % purity and N_2O from MG Industries with 99.999 at. % purity. The total pressure in the chamber was $1\text{x}10^{-2}$ Torr. The N_2O partial pressure was varied between $8\text{x}10^{-6}$ and $9\text{x}10^{-4}$ Torr in order to vary the O concentration (r). The substrates were non-intentionally heated (50°C) and placed 8 cm from the target. The rf power was 30 W.

Oxygen concentration of each sample was determined by Auger Electron Spectroscopy in a Perkin-Elmer PHI 560/ESCA-SAM system. The absorption spectra were obtained by the transmission spectroscopy technique

3 Model

In a previous paper [5] we considered the existence of $Cd_xTe_yO_z$-$(CdTe)_n$ clusters mixture with localized band-gap energy in the films. The O concentration of each compound is given by $r_{j,n} = z/(x+y+z+2n)$. By employing the combinatorial analysis we found that the probability of formation of the $Cd_xTe_yO_z$ is given by [5]:

$$p_j(r,j) = \frac{C_x^X C_y^Y C_z^Z}{C_{x+y+z}^N} = \frac{(x+y+z)!}{x!y!z!} r^z \left(\frac{1-r}{2}\right)^{x+y}.$$

However, those subunits can bound to CdTe subunit through Cd bridge with Te^{-2}. The number of possible Cd bridge in a $Cd_xTe_yO_z$ subunit is $2x$. From these bounds would follow tying other Cd and Te successively until any Cd ties to an O.

The probability of such *2x* Cd-Te bridges obviously depends upon *r* and is given by:

$$p_n(r,j,n) = \left(\frac{C_{2x}^{Y}}{C_{2x}^{N}} \cdot \frac{C_{2x}^{X}}{C_{2x}^{N}}\right)^{n} = \left(\frac{1-r}{2}\right)^{2xn}.$$

Therefore the total probability of $Cd_xTe_yO_z$-$(CdTe)_n$ unit formation is $p(r,j,n)=p_j(r,j)p_n(r,j,n)$.

On the other hand, the absorption coefficient of each $Cd_xTe_yO_z$-$(CdTe)_n$ molecular unit is given by $\alpha(j,n) = A_{j,n}\,[h\nu - E_g(j,n)]^{1/2}$, where E_g is the band-gap energy, $h\nu$ the photon energy and $A_{j,n}$ is a constant proper of each material. E_g can be estimated from the Vegard's law taking into account that E_g=1.5 eV for CdTe and E_g=3.8 eV for $CdTeO_3$ [6]. As the formation dynamics of CdTe is different of $Cd_xTe_yO_z$, separated formation terms must be considered. Hence, the general absorption coefficient expression must be set as:

$$\alpha(r) = \alpha_{CdTe}F(r) + \sum_j \sum_n \alpha_{CdTeO}(r,j,n)\, p(r,j,n)\, G(r,j,n),$$

where α_{CdTe} and $\alpha_{CdTeO}(r,j,n)$ are the absorption coefficients of CdTe and of each $Cd_xTe_yO_z$-$(CdTe)_n$ cluster respectively.

4 Results

F(r) and *G(r,j,n)* are the CdTe and $Cd_xTe_yO_z$-$(CdTe)_n$ dynamic factors. They, in fact, are related with the volume fraction of the compounds in the sample and include the factor $A_{j,n}$ which depends on the characteristics of each compound [5]. In order to simplify the calculus, *G(r,j,n)* was considered dependent only on *r*, and thus it becomes in a factor *G(r)* out the sums over *j* and *n*

F(r) and *G(r)* were determined from experimental absorption spectra. Employing numerical methods and fitting the obtained values we found that:

$$F(r) \approx 2.2\times10^{4} \exp\left(-\frac{r}{0.18}\right) cm^{-1}eV^{1/2},$$

and

$$G(r) \approx \left[(2.5\times10^{6})^{-1} + \left(1.2\times10^{5} + 7\times10^{6}\, e^{-\frac{r-0.346}{0.028}}\right)^{-1}\right]^{-1} cm^{-1}eV^{1/2},$$

This function indicates the prevalence of a constant value $G(r) \cong 2.5\times10^{6}$ $cm^{-1}eV^{1/2}$ for low *r*, which agrees with the assumption that the $Cd_xTe_yO_z$-$(CdTe)_n$ cluster formation is mainly influenced by the CdTe subunits. For high *r* the $Cd_xTe_yO_z$ subunit formation dynamics dominates.

Figure 1(a) shows the simulated absorption profiles for the same O concentrations as the experiment. Observe the similarity of the profile shape

behavior according our model as compared with experimental absorption profiles in Figure 1(b).

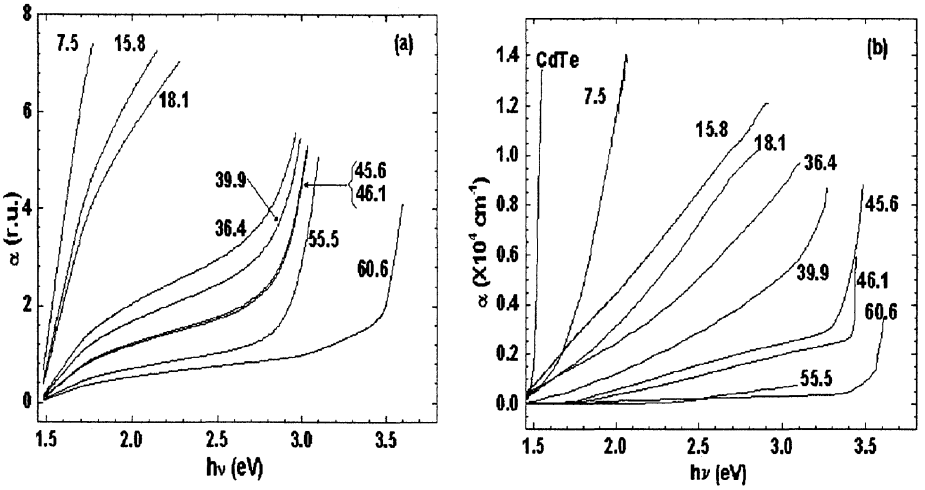

Figure 1. (a) Simulation of the absorption profile with the model. (b) Experimental absorption profiles of CdTeO films. The numbers near the curves correspond to the O concentration.

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References

1. Alvarez-Fregoso O., Mendoza-Alvarez J. G., and Zelaya-Angel O., J. Appl. Phys. **82**, 708 (1997).
2. El Azhari M. Y., Azizan M., Bennouna A., Outzourhit A., Ameziane E. L., and Brunel M., Thin Solid Films **295**, 131 (1997).
3. Espinoza-Beltrán F.J., Ramírez-Bon R., Sánchez-Sinecio F., Zelaya-Angel O., Torres-Delgado G., Mendoza-Alvarez J. G., González-Hernández J., Faras M. H., and Baños L., Braz. J. Phys. **24**, 425 (1994).
4. Hosono H., Yamashita Y., Ueda N., and Kawazoe H., Appl. Phys. Lett. 68, 661 (1996).
5. Iribarren A., Menéndez-Proupin E., Castro-Rodríguez R., Sosa V., Peña J. L., Caballero-Briones F., J. Appl. Phys. **86**, 4688 (1999).
6. Zapata-Navarro A., Bartolo-Pérez P., Zapata-Torres M., Castro-Rodríguez R., and Peña J. L., J. Vac. Sci. Technol. A **15**, 2537 (1997).