Urbach Energy and Dispersion Parameters of $(Cr_2O_3)_{1-x}(I)_x$ thin films

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Abstract

The effect of Iodine (I) doped on some optical properties and Urbach energy of chromium oxide (Cr_2O_3) films is studied . The optical transmission (T %) in the wavelength range (350-850) nm was measured, The oscillator energy E_0 and dispersion energy E_d have been determined by Wemple DiDomenico single oscillator model. Parameters like absorption coefficient, and skin depth are investigated. The results shown that all these parameters were affected by doping .

طاقة اورباخ ومعلمـــات التفريق لأغشية أوكسيد الكروم المشــوب باليـــود

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الخلاصة

في هذا البحث تم دراسة تأثير الأشابة باليود على بعض الخصائص البصرية وطاقة اورباخ لأغشية أوكسيد الكروم. اذ قيست النفاذية البصرية (T%) ضمن مدى الأطوال الموجية (350-850) nm كدالة للطول الموجي. حددت قيم طاقة الاهتزاز E_0 و طاقة التفريق لـ E_d باستخدام نموذج المهتز الأحادي Wemple DiDomenico. وعلى ضوء ذلك تم حساب بعض المعلمات كمعامل الامتصاص، وعمق الاختراق. أظهرت النتائج أن جميع العوامل البصرية التي تمت دراستها تتأثر نتيجة التشويب.

Keywords: Urbach Energy, Dispersion Parameters, Wemple DiDomenico, E_d, Cr_2O_3

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Introduction

Chromium oxide (Cr_2O_3) thin films are of great interest due to their wide variety of technological applications. This oxide exhibit high hardness and high wear with corrosion resistance which are important properties for protective coating applications[1], it has already found several applications as protective coatings on read–write heads in digital magnetic recording units and in gas-bearing applications ,It has been studied for optical and electronic uses such as selectively absorbing films for solar energy conversion , solar energy shielding films for windows , and electrode material for electrochromic windows[2]. The most stable phase is the corundum structured (Cr_2O_3). This form of oxide has important industrial applications, for instance in catalysis and solar thermal energy collectors. chromium oxide is an insulating antiferromagnetic material it is also suitable as a tunnel junction barrier[3]. On the other hand, despite its intrinsic insulator nature, (Cr_2O_3) films can either p-type or n-type semiconductor behaviors, depending on the growth conditions. the confluence of all these properties in a single material makes (Cr_2O_3) a key material for the development of a broad range of industrial applications[4].

We present in this work the effect of Iodine (I) doped on some optical properties and Urbach energy of chrome oxide (Cr_2O_3) films prepared by the chemical spray pyrolysis.

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Experimental part

$(Cr_2O_3)_{1-x}(I)_x$ thin films were deposited using spray pyrolysis technique. The spray pyrolysis was done with a laboratory designed glass atomizer, which has an output nozzle about 1 mm. An homogeneous was prepared by adding (0.888816 g) from ($CrCl_3.6H_2O$) on (1.4495 g) from (NH_4I) with (91 % purity) in distilled water and stirred by magnetic stirrer . The films were deposited on preheated glass substrates at temperature of (390 °C), The optimized conditions were determined by the following parameters, spray time (10 sec) , average deposition (10 cm^3/min) , distance between nozzle and substrate (30 cm) and the carrier gas (filtered compressed air) was maintained at a pressure of (10^5 Nm^{-2}). The thickness of the sprayed samples were in the range of (200±2 nm) by using the weighting method.

Absorbance and transmittance measurements were carried out using double bean UV/VIS spectrometer (shimadzu Japan) in the wavelength range (380-900) nm

Results and discussions

Fig.(1) shows the transmission spectra of as-deposited $(Cr_2O_3)_{1-x}(I)_x$ film. It was found that the absorption edge shifts towards high wavelength due to doping (red shift). Furthermore, the transmission was found to decrease with doping.

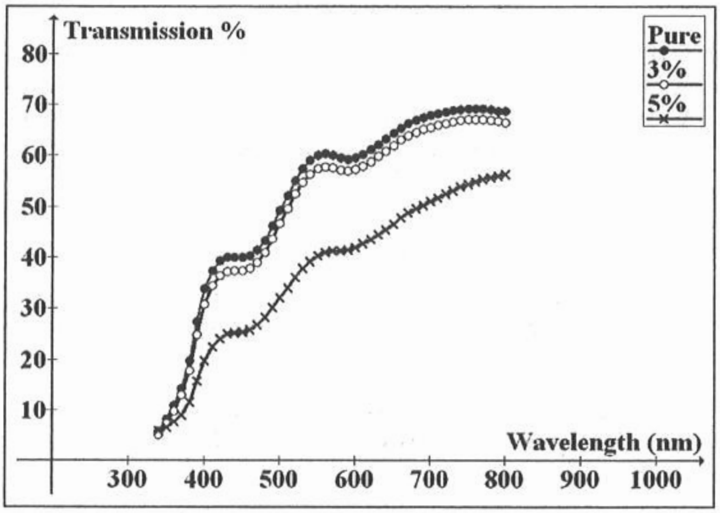

Fig. (1) Transmission % of $(Cr_2O_3)_{1-x}(I)_x$ films

The variation of absorption coefficient (α) with photon energy is shown in Fig. (2).

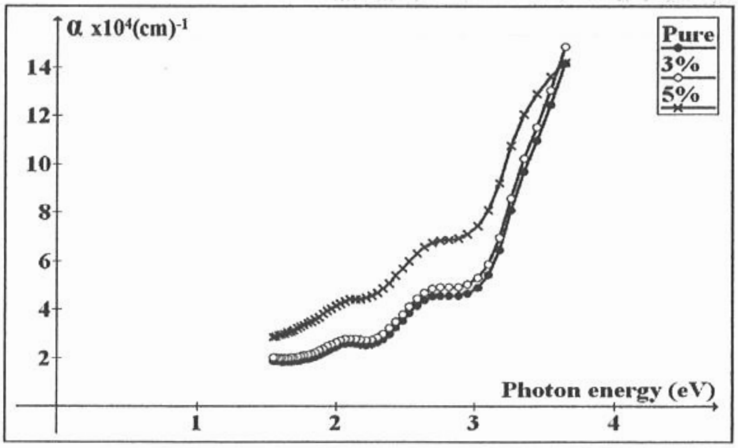

Fig. (2) Absorption Coefficient as a function of Photon energy (eV).

All films show higher absorption on the shorter wavelength, but `5wt % (I)doped (Cr_2O_3)sample has highest value. The marked increase of the absorption coefficient at higher energies may be attributed to extra transition from the bonding molecular orbit to nonbonding molecular orbit [4].

Plotting the relation between ln(α) and photon energy produced straight lines as shown in Fig. (3). The reciprocal of the slope was taken as the band tail of the $(Cr_2O_3)_{1-x}(I)_x$ films . Localized states increases with increasing the percent of (I) as illustrated in Fig. (4) which shows the relationship between doping percentage and the band tail. The presence of dopant and its interaction results in the creation of new molecular dipoles could be a result of point defects created within the band gap [5].

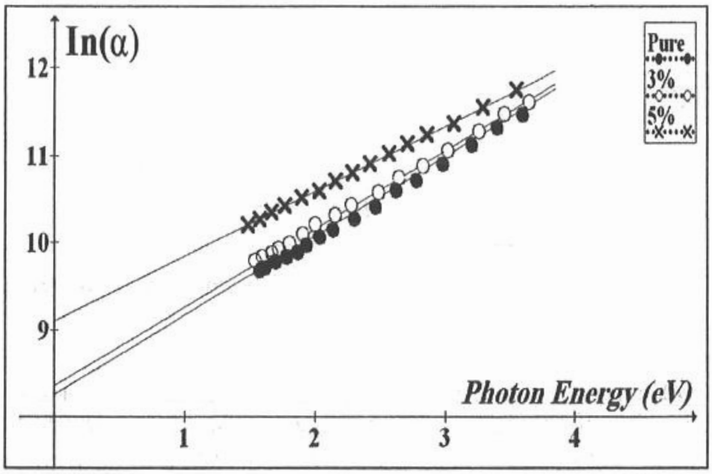

Fig. (3) Relation between lnα and photon energy of $(Cr_2O_3)_{1-x}(I)_x$ films.

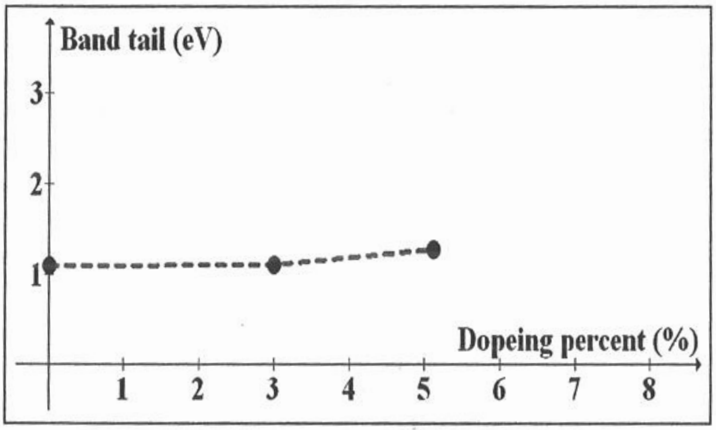

Fig. (4) The dependence of band tail on doping percent of $(Cr_2O_3)_{1-x}(I)_x$ films.

Wemple and DiDomenico have developed a model where the refractive index dispersion is studied in the region of transparency below the gap, using the single-effective oscillator approximation [7]. According to the this model the optical data could be described to a very good approximately by the following formula [7]:

$$n^2 = 1 + \frac{E_d E_0}{E_0^2 - (h\nu)^2} \quad \text{.............(1)}$$

Where, n is the refractive index, E_o is the average excitation energy for electronic transitions, $h\nu$ is the photon energy and E_d is the so–called dispersion energy. The dispersion energy E_d is a measure of the strength of interband optical transitions and can be considered as a parameter having very close relation with the charge distribution within unit cell and therefore with the chemical bonding [8].

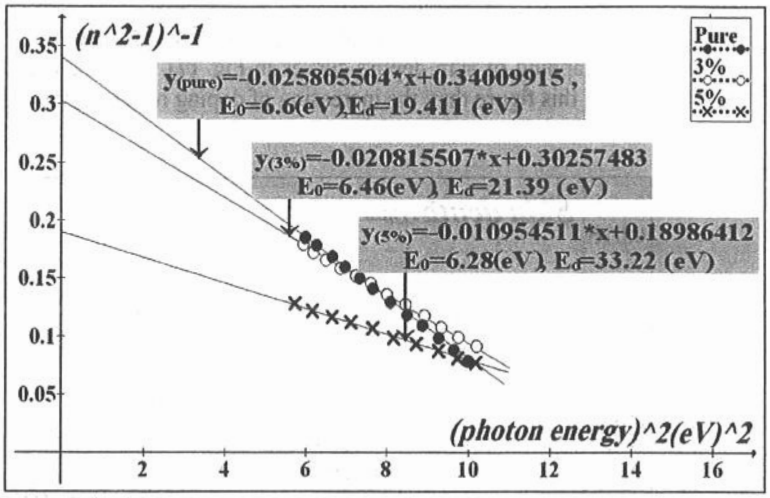

Fig. (5) The plots of the variations of $(n^2-1)^{-1}$ vs. $(h\nu)^2$ for the $(Cr_2O_3)_{1-x}(I)_x$ films.

Plotting $(n^2-1)^{-1}$ against $(h\nu)^2$ allows the determination of the oscillator parameters by fitting a straight line to the points Fig. (5) . The value of E_o and E_d can be directly determined from the slope $(E_oE_d)^{-1}$ and the intercept on the vertical axis, (E_d/E_o). The oscillator energy, E_o is an average energy gap as pointed out in many references [9]. The values of E_o and E_d are listed in Table (1). The oscillator energy E_o is related by an empirical formula to the optical gap value: $E_o \approx 2Eg$.

Table(1): The values of E_o and E_d

Type of Samples	$E_o(eV)$	$E_d(eV)$	$E_g\ (eV)$
Pure	6.6	19.41	3.3
3%	6.46	21.39	3.23
5%	6.28	33.22	3.14

The electromagnetic will have its amplitude reduced by a factor 'e' after traversing a thickness (called the skin depth) such that : $\chi = \lambda / 2\pi k$

Which may be the order of 100 to several thousand angstroms, depending on the material [10]. In spite of the overlapping of skin depth's curves in Fig. (7), but it can recognized from the amplification part in this figure that; the increasing of doping results decreasing skin depth.

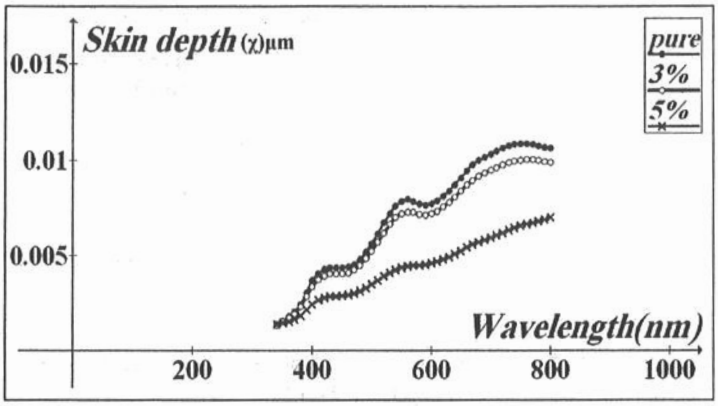

Fig. (6) Skin depth (χ) as a function of wavelength.

Conclusions

$(Cr_2O_3)_{1-x}(I)_x$ thin films were successively prepared by chemical spray pyrolysis. The doping affect of Indium on the optical properties of (Cr_2O_3) were investigated. Optical measurements show that the film possesses transmittance over 60% in the visible region. and absorption coefficient, band tail and dispersion energy increases with doping. and The oscillator energy and Skin depth decreases with doping.

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