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Substrate Temperature Effect on the Optical Properties of ZrO_2 Films Prepared by Thermal Evaporation

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ABSTRACT

The pure substance of Zirconium oxide (ZrO_2) was deposited on substrate of glass with various substrate temperatures using thermal evaporation under pressure of (2×10^{-5} mbar) and with a deposition rate of (0.5 nm/S) with an average thickness of (300 nm). The optical properties of these prepared films were concentrated as a function of the substrate temperature. It was found that the values of each of the refractive index, packing density, together with the extinction coefficient increased with the increase in the substrate temperature of the prepared films.

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تأثير درجة حرارة تأثير درجة الحرارة ارضية الترسيب على الخصائص البصرية لأغشية ZrO_2 المحضرة بواسطة التبخر الحراري

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الكلمات المفتاحية:

الخواص البصرية
كثافة التعبئة
معامل الانكسار
ZrO_2

الــخُـلاصــة

تم ترسيب مادة اوكسيد الزركونيوم (ZrO_2) النقية على ارضية من الزجاج ولمختلف درجات الحرارة باستخدام تقنية التبخير الحراري تحت ضغط مقداره (2×10^{-5} mbar) وبمعدل ترسيب مقداره (0.5 nm/S) لمعدل سمك (300 nm). ان الخصائص البصرية للأغشية المحضرة تكون كدالة لدرجة حرارة الارضية الزجاجية .لقد وجد أن قيم كل من معامل الانكسار وكثافة التعبئة ومعامل الخمود تزداد مع زيادة درجة حرارة ارضية الترسيب للأغشية المحضرة.

1. Introduction

Zirconium dioxide (ZrO_2) has three phases, monoclinic, tetragonal and cubic phases [1]. It is important in many applications due to its specification in terms of the mechanical and optical properties such as high hardness and high refractive index[2,3].ZrO_2 is used in the systems of diodes ,sensors (light and gas sensors) and solar cells. It is also used in coatings processes due to its high melting point and resistance to corrosion and in medical applications such as dentistry and other medical applications [3,4]. The ZrO_2 encounter from a state of change in the value of the optical refractive index when the thickness of the thin films changes. To illustrate, phenomenon known as negative inhomogeneity, meaning that the optical refractive index decreases with an increase in the thickness of the film, and it is one of the problems that is facing the use of this oxide in multi-layer anti-reflective films[5]. Kirvosheev and his group have studied this effect as a function of substrate temperature and thin film thickness[6]. The effect of substrate temperature plays an important role in forming the thin film during evaporation [6], as it affects the coefficient of adhesion with the ground and the structural properties of the thin films and packing density. Packing density can be calculated by using Kinosita and Nishibori equation's [7].

$$n_f = (1-p)n_v + pn_s \qquad (1)$$

Where (n_f) represents the refractive index of thin film,(p p) packing density, (n_v) represents the refractive index of an unoccupied spaces in the film, and (n_s) the refractive index of the solid parts of the film and it is equal to (2.1) for Zirconium dioxide (ZrO_2) at the wavelength 550 nm [8]. The Zirconium dioxide (ZrO_2) is a very important material due to its multiple applications and due to its possession of a group of unique qualities represented by its excellent mechanical properties and resistance to the weather conditions [9]. In this study we report the deposition and structural, optical properties of ZrO_2 thin films by thermal evaporation method.

2. Experimental details

Thermal vacuum evaporation technique was used to prepare pure the (ZrO_2) thin film by using system of A700Q type supplied by LEYBOLD-HERAEUS. The vacuum unit system with a minimum vacuum pressure of ($1x10^{-6}$ mbar). The pumping system , which consists of two evacuation pumps (stages); the first stage is the rotary pump (roughing stage), while the second stage is the turbo pump with a pumping rate of 1500 lit/S. The chamber of the system supplied with a crystal monitor unit of type (IC-5) equipped with INFCON company to control the deposition rate as well as the thickness of the films. The Zirconium dioxide was evaporated using an E-beam unit ESV-6 with electric power equal to 6 kW, this unit equipped with an electronic scanner unit towards the X and Y coordinates. The substrates used to make the required films were chemically cleaned, followed by a topical and physical cleaning procedure using the flash glow unit. To obtain uniformity in the thickness of the films, the substrates were suspended on a rotating stand with a rotation speed of 20 rpm. For the purpose of studying the crystal structure of the prepared films, the X-ray diffraction pattern was performed using (XRD- 6000 SHIMADZU) and within the range of examination from (20^o-80^o). Regarding the optical properties of the prepared films, they were diagnosed using an optical spectrometer of the type (Spectrophotometer model 190-SHIMADZU) with a double beam and within the range of wavelengths (200 to 1100 nm) and using the swanepoel equation [10] . The optical constants of these films were calculated

3. Results and discussion

Fig. 1 represents the X-ray diffraction spectrum of the ZrO_2 thin film . This figure shows four peaks (011), (110), (112) and (121)) planes corresponding to the angles 30.37^o, 35.22^o, 50.65^o and 60.22^o respectively which indicate for a perfect agreement with the JCPDS data card (ASTM data file No. 50-1089). The results show the dominance of the (011) plane over the rest of the levels, which made it the level with a preferential orientation for crystal growth, where the intensity of diffraction is the highest possible. When comparing the results this work found, one can observe that there is a good matching with the researchers findings[11,12].

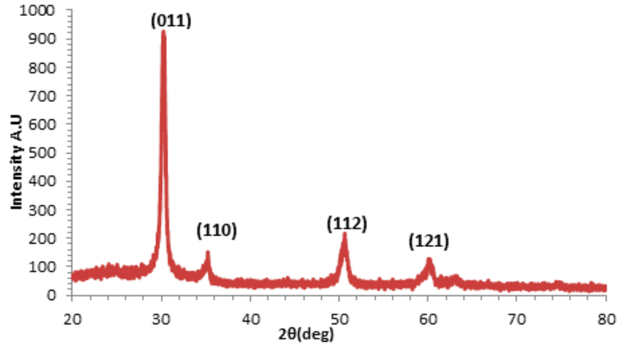


Fig. 1: XRD spectra of ZrO_2 thin films

Fig.2 shows the transmittance spectrum of the ZrO_2 films prepared at a temperature of 30,100,200 and 300°C. The relationship between the refractive index and the coefficient of extinction as a function of the substrate temperature at a wavelength of 550 nm can be illustrated in Fig. (3) and (4), respectively. It is clear that the refractive index increased from 1.82 for the films deposition at a temperature of 30 °C to 1.95 when the films is deposited at 300°C , and this could be attributed to an increase in the density of the packing density with an increase in the substrate temperature, in addition to the crystallization of the film at a temperature of 150°C [6,13].

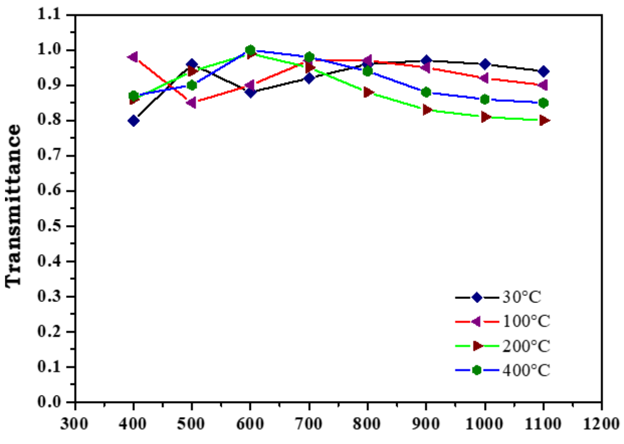
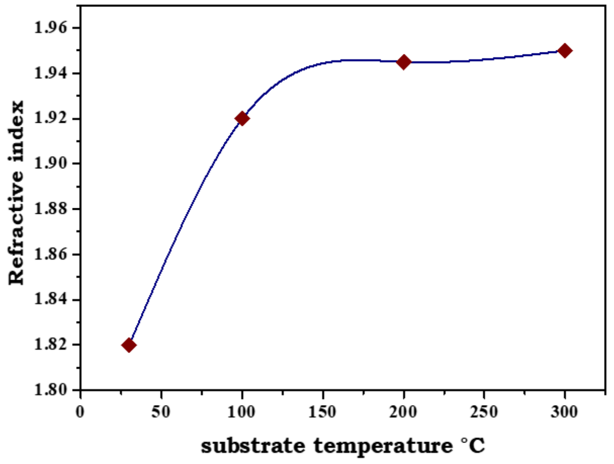
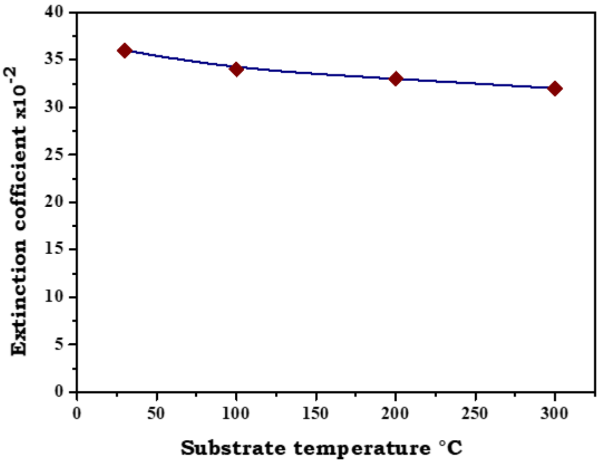


Fig. 2: The Transmittance Spectrum of ZrO2 film



Fig(3): Refractive Index as a function of the substrate temperature.



Fig(4): Extinction coefficient as a function of the substrate temperature.

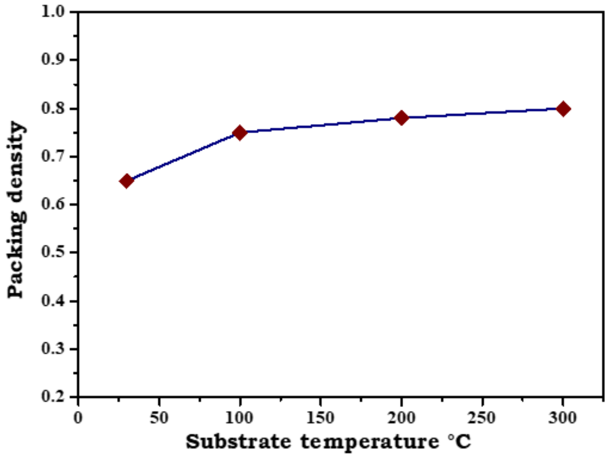


Fig. 5. Relationship of the packing density to the substrate temperature

4. Conclusions

The current research have shown that the substrate temperature had an obvious effect on the optical constants for thin films prepared from ZrO_2. It was found that both the refractive index and the packing density increased with the increase in the substrate temperature , and it was also observed that the extinction coefficient values were approximately constant with an increase in the substrate temperature.

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