Energy band diagram of In_2O_3/ Si heterojunction

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Abstract:

Crystalline In_2O_3 Thin films have been prepared by flash evaporation. We have studied the crystal structure of as deposited at 303K and annealed at 523K using X-ray diffraction. The Hall Effect measurements confirmed that electrons were predominant charges in the conduction process (i.e n-type).It is found that the absorption coefficient of the prepared films decreases with increasing T_a. The d.c conductivity study showed that the conductivity increase with increasing T_a , whereas the activation energy decreases with increasing T_a. Also we study the barrier tunneling diode for In_2O_3/Si heterostructure grown by Flash evaporation technique. (capacitance-voltage C-V) spectroscopy measurements were performed at 303 K and at the annealing temperature 523K. The built in voltage has been determined and it depends strongly on the annealing process of the heterojunction.

From all above measurements we assumed an energy band diagram for In_2O_3 /Si(P-type) heterojunction.

Key words: Thin films grown; Band diagram ;InO

Introduction:

Important new applications are possible today in the field of energy conversion and storage by the application of thin and nanostructure solid films on surfaces. These special films, or multiple films, will be integral parts of the energy systems in the near future for the production of useful thermal and electrical energy and for energy saving application [1]. Indium oxide is one of the most promising polycrystalline materials for thin film solar cells due to its physical properties : It has high absorption coefficient (larger than 10^5 cm^{-1} at wavelength 600nm) so that only thin layers (a few microns) are needed for the absorption of the most solar spectra photons with energy higher than band gap [2]. In_2O_3 thin films are suitable for technological application where high transparency in the visible region and high conductivity are required .Indium oxide is a wide band gap semiconductor (~3.7eV), which obtained by means of reactive sputtering deposition onto soda lime substrates. Nevertheless, when it is prepared in an oxygen-deficiency way. it can reach a high n-type doping level due to the intrinsic defects such as oxygen vacancies[3]. Tthis unique combination of electrical and optical properties has led numerous researchers to a thorough investigation of the growth and characterization of thin semiconducting indium oxide films because of their obvious application in optosensistive over layer in telecom and sensor wave guide applications.[3,4]

Growth of III-V semiconductors on Si substrates has been investigated more than three decades. These investigations have aimed at several goals .the monolithic integration of devices consisting of III- oxide semiconductors and Si, and tandem

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type solar cells. Replacement of GaAs or InP substrate by Si substrates has been attracted for fabrication of discrete devices intern of either the high thermal conductivity or the low cost of Si[5,6].

The aim of the present work is to pay more attention to study of the junction of In_2O_3 /p-Si heterojunction and effect of annealing temperature on the structural, optical and electrical behaviors on indium oxide thin films prepared by flash evaporation technique.

Materails and Methods:

Thin In_2O_3 films were deposited on corning glass substrate and Silicon (P-type (111 orientation),using flash evaporation method under vacuum treatment 10^{-5} mbar. The evaporation powder was continuously dropped into the molybdenum boat heated at a temperature of about 1600K through an Edward(216E). The film thickness was (100±15 nm).Aannealing treatment of thin In_2O_3 films was carried out in air for duration 1 hr at temperature of 523K .the structure of the films was examined via X-ray diffraction (XRD-6000-shemadzu with CuK_{α}, wavelength=1.54A^0). Al metal contact electrodes were thermally deposited in vacuum 10^{-5} mbar, coated electrode was 300nm thick. The glasses were immersed in a distill water for 30 minutes and afterward they ultrasonically cleaned in acetone for 10 min. finally they were rinsed with water. The substrate temperature during the deposition process was kept at 303K.

The UV-Visible optical transmission spectra of the thin films were recorded by (Shemadzu UV-160/UV-Visible recorder spectrophotometer) where the films investigated by means of experimental measurements of transmittance (400-900 nm).Dc electrical conductivity, Hall effect were measured to determine the electrical transport properties and the type of Indium Oxide film(Digital electrometer type Ketheley 616 was used for these purpose), also the C-V characteristic were carried out (using LCR meter model HP-R2CC4274) .

Results and Discussion:

The X-ray diffraction of In_2O_3 films at 303K and 523K were carried out in order to get an information about the structural changes produced by prepared samples .Obviously, the structure of the as deposited In_2O_3 films and annealed at 523K are polycrystalline structure as shown in Fig.(1),However, the intensity of annealed sample is increases with increasing annealing temperature this is may be due to the increasing in grain size or the arrangement in the structure. It can inferred from Table(1) that the comparison between the values of diffracted angle(2θ),inter-planner distance(d) of the peaks of as deposited and annealing samples.

Table(1) The value of 2θ and inter-planner distance (d) of Indium oxide thin films at 303K and annealed at 523K

Experimental		**Standered (ASTM)**		
2θ	**d**	**2θ**	**d**	**hkl**
17.1	5.179	17.512	5.09	200
20.71	4.283	21.49	4.13	211
35.50	2.525	35.466	2.527	400

The electrical properties of the films were found to be related to the microstructure and crystallographic structure which is in turn strongly depend on the annealing temperature,

The variation of $Ln\sigma$ as a function of reciprocal temperature for the as deposited and annealed films at 523K is shown in Fig.(2) The plots suggest that there are two distinct regions corresponding to low and high temperatures(303-473K).For the as deposited and annealed at 523K.The d.c conductivity exhibits an activated temperature dependence, in accordance with the stuckes equation[7] $\{\sigma = \sigma_0 Exp.(-E_c-E_f/k_BT)\}$, where σ_0 is minimum metallic conductivity (E_c-E_f) is activation energy for electrons conduction, k_B is Boltezmann constant and T is absolute temperature. At higher temperature ranges the conduction mechanism of this stage is due to carriers excited into extended states beyond the mobility edge and for the other temperature range the conduction mechanism is due to carriers excited into localized states at the edge of band edges and hopping at energy close to the tail, while for annealing samples there one mechanism of conductivity, so the mechanism of this stage is due to carriers excited into extended states. (see Table 2)

The transparency of thin films for as deposited and annealing samples exhibits a sharp decrease in about the UV region as shown in figure(3).The transmission percent of In_2O_3 films were also changed from 8 to 6% for as deposited and annealed at 523K , respectively. All the samples show optical transparency in the spectral region (500-900nm).The transmittance decreases in the band gap region for annealing treatment films. From the transmittance spectra the absorption coefficient (α) can be calculated from the relation [8] $\{\alpha=2.303\, A_0/t\}$

Where A_0 is absorption t is thickness of the film. The optical band gap values of the In_2O_3 films were obtained from transmission measurements and by plotting $(\alpha h\upsilon)^2$ against ($h\upsilon$) the absorption spectra of In_2O_3 films are shown in Fig.(4)the linear nature of the plot after the absorption edge indicates the presence of direct transition. The extrapolated of the linear portion to the x-axis gives the values of optical band gap,E_g, are 2 eV and 1.65 eV for as deposited and annealed at 523K for 1hr respectively. The value of energy gap is less than that obtained by Luis et.al.[3],because of the difference of preparation conditions. The data of Fig.(4) clearly shows the progressive sharpening of the absorption edge upon heat treatment, the reason for the sharpening might be due to a change in the stoichiometry or intrinsic (defect population of the heat treatment samples [9-11].

The variation of capacitance as a function of forward and reverse bias voltage in the range of (0-1) Volt at frequency equal to 2 MHz has been studied, for In_2O_3/p-Si heterojunction for as deposited and annealing samples. The inverse capacitance square is plotted against applied voltage as shown in Fig.(5).the plots revealed straight line relationship which means that the junction was of an abrupt type. This is in agreement with the result of Ryu and Takashi[12],Jain and Melehy[13].The interception of the straight line with the voltage axis at $(1/C^2)$=0 represents the built-in voltage[14].we observed from Table(2) that the built-in voltage increases with increasing of T_a as a result of the decreases in the capacitance value and the increase of the depletion width.

The energy band diagram of In_2O_3 /p-Si heterojunction was determined by analysis on a very thin In_2O_3 grown of a p-type Si (111) substrate (0.01 ohm.cm).

In the formation of heterojunction with narrow-band gap material and wide –band gap material, the alignment of the band gab energies is important in determining the characteristics of the junction [15,16].

In the case of heterojunction, the properties of the interface vary greatly from material to material and largely depend on the method of formation.

An equilibrium energy band diagram of an abrupt P-n heterojunction formed as shown in Fig.(6) with the aid of dc-conductivity, optical energy gap and C-V measurements. The main parameters in order to plot the energy band diagram are ΔE_v and ΔE_c which can be calculated from equation (1 to 3)[17] :

$\Delta E_c = \chi_n - \chi_p$ ...1

$\Delta E_v = (E_{gp} - E_{gn}) - (\chi_n - \chi_p)$ 2

$\Delta E_v = V_{bi} + E_{an} + E_{ap} - E_{g1}$ 3

Where V_{bi}=Built in potential, E_{an},E_{ap}=activation energy for n and p-type semiconductor,E_{g1},E_{g2}=optical energy gap for n and p-type semiconductors. This energy band profile in which a "spike" and "notch" occur in the conduction band edges at the interface is the case in which $\chi_n > \chi_p$. Experimentally it is found the two semiconductors have different energy gaps (E_g), different dielectric constants (ε), different work function (ϕ) and different electron affinity (χ).

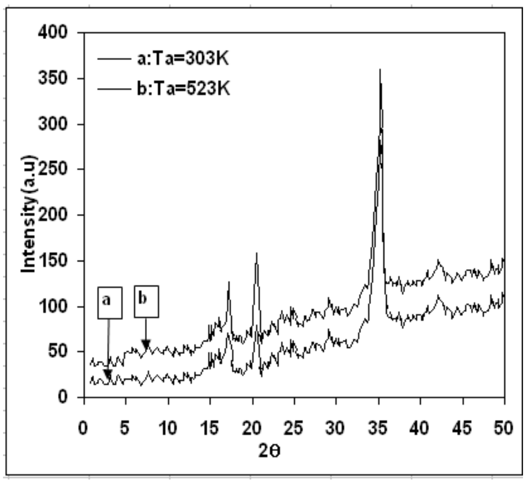

Fig. (1) XRD spectrum of the as-deposited In_2O_3 thin films, and annealed at 523K

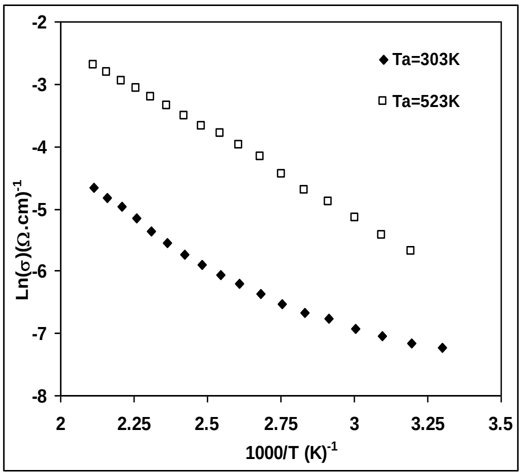

Fig. (2) Temperature dependence of D.C. conductivity σ of the as-deposited In_2O_3 thin films, and annealed at 523K

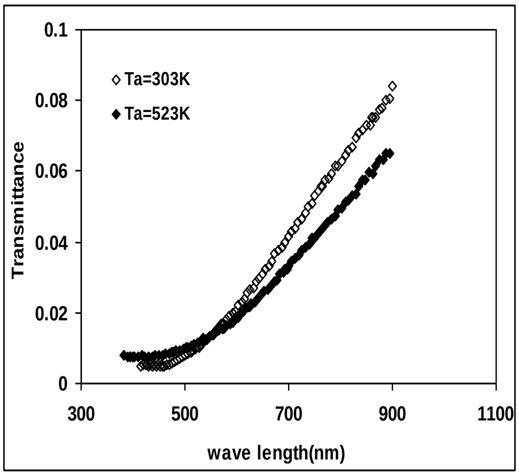

Fig. (3) Transmittance spectrum of the as-deposited In_2O_3 thin films, and annealed at 523K

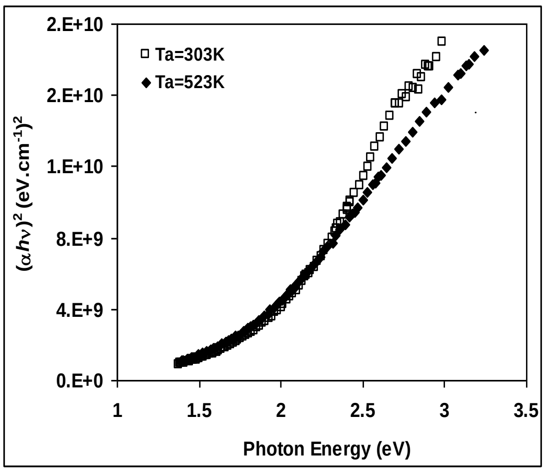

Fig. (4) $\alpha h\upsilon$ vs. $h\upsilon$ for samples as prepared and annealed at 523K

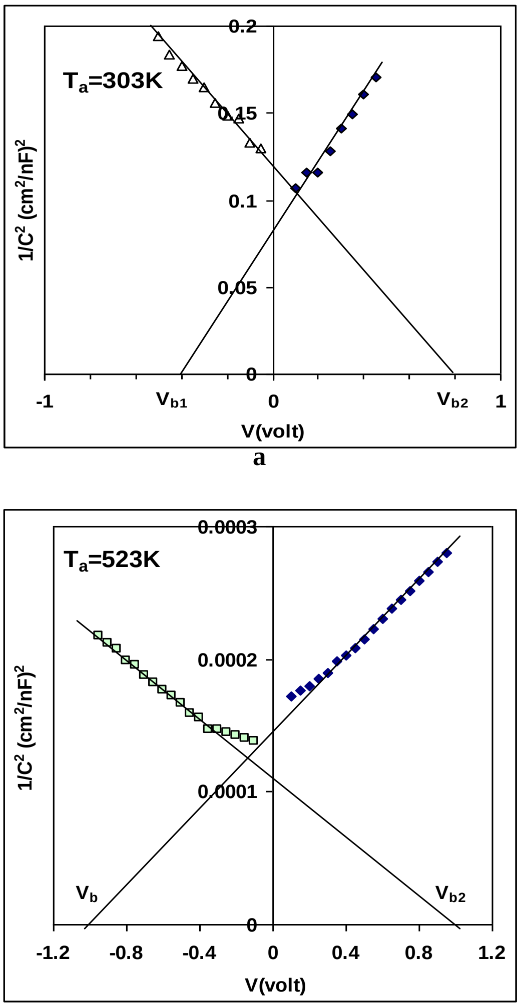

Fig. (5) Built-in voltage of the as-deposited In_2O_3 –Si heterojunction, and annealed at 523K

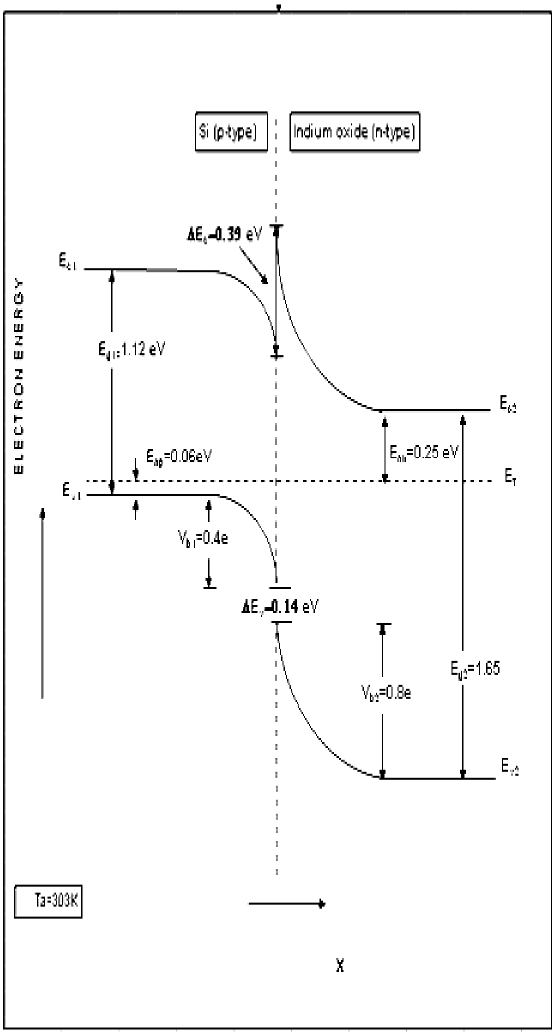

Fig. (6) Energy Band diagram of the as-deposited n-In_2O_3/p-Si Heterojunction.

Table(2) The activation energy, optical energy gap, difference in valence and conduction band.

T_a (K)	E_{a1}(eV)	E_{a2}(eV)	E_g(eV)	ΔE_v(eV)	ΔE_c(eV)	V_{bi}(eV)
303	0.11	0.26	2.0	0.37	1.05	1.2
523	0.25	--------	1.65	0.14	0.39	2

Conclusion:

The crystal structure of In_2O_3 thin films prepared by flash evaporation reveal suitable electrical and optical characteristics when grown at a pressure $2x10^{-5}$ mbar. With substrate temperatures equal to T_s=303K, which appeared n-type charge carriers. The optical energy gap decreases with increasing annealing temperature. From 2 eV to 1.65 eV which made this material is suitable for cell devices.

Refference:

[1] Yianoulis P. and Giannouli M. .2008.,Thin Solid Films Conversion and Energy Saving

Applications, J.Nano search 2:49-60.
[2] Al-Zubaidi M.F.and Ibrahim W.N. .2009.Increasing the conductivity of cadimium telluride Films,J.Eng.&Tech. 27(14):2682-2691.
[3] Luis C.,Jimcnez B.,Henery A.,Mendez P., and Peynor A.2006.Production and Characterization of Indium Oxide and Indium Nitride, Brazilian J.of Physics 36(3B):1017-1020.
[4] Al-Ajili A.N. and Bayliss S.C.1997.Astudy of the optical,Electrical and Structural Properties of Reactivity Sputtered InOx and ITOxThin Films,Thin Solid films306:116-123.
[5] Dekkers J.M.,Rijnders G.,and Btank H.A.2006.Role of Sn doping in In_2O_3 thin films on Polymer substrates by Palsed laser Deposition at room temperature,Appl.physics letters88.
[6] Hossein M.and Telebain N. 2005.The effect of Annealing on Structural,optical,and Electrical Properties of Nanostructural Tin Oxide Thin Films, J.Acta chim.slov.52:53-59.
[7] Zhen G.M. and Shey X.D.2008.Thickness Dependence of Resistivity and optical Reflectence of ITO films,Chinese Phys.Lett.25:1380-1385.
[8] Khairnar U.P., Bhavsar D.S., Vaidya R.U., Bhavsar G.P.2003.Optical Properties of thermally evaporated Cadimuim telluride thin films,J. Materials Chemistry and Physics80:,421-437.
[9] Chein-Jung,Huang,Kuo-Chien L.and Yan-Kuins S.2008.Structure Properties of Titanium Dioxide Thin Films in sintered temperature by the Sol-Gel Method,Engineering Materials 368:1465-1467.
[10] Latitha S., Sathyamoorthy R.,Subbarayan A.2006.Modelling and Simulation Single Layer Anti-Reflective Coating,J.Solar energy materials and Solar cells90:694-703.
[11] Vorontsov A.V.,Savinov E.N.,Zhengsheng J. 1999. Fabrication of Porous TiO_2 thin films prepared with low temperature for Photocatalytic degradation of Methylene Blue Solution,J.Photochem.Photobiol.A: Chem.125:113-117.
[12] Ryu I.S.,and Takashi K.1965.Preparation of Ge-GaAs Heterojunctions by vacuum Evaporation, Japanies J. of Applied Physics 4(11):850-853.
[13] Jain F.C. and Melehy M.A.1975.Grating add-drop filter Application resonator coupling, Applied Physics letter 27(1):36-38.
[14] Streetman B.G.1980. Solid State Electronic Devices, prentice-Hall,Inc,printed Englewood,USA 126:12-24.
[15] Neaman D.A.2003. Semiconductor Physics and Devices, 3rd edition,University of New Maxico,THE MCGRAW-HILL COMANIES.
[16] Sharma B.L. and Purohit R.K.1974. Semiconductor heterojunction, Pergamen Press, Oxford.
[17] Yoshimoto M., Nnakano T.,Yamashita T., Suzuki K. .2000.MBE growth of InN on Si toward hot Barrier Structure in Si Devices, IPAP conf. Series 1:186-189.

مخطط حزمة الطاقة للمفرق الهجينIn_2O_3 /Si

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الخلاصة:

تم تحضير أغشيةIn_2O_3 بطريقة التبخير الوميضي في الفراغ.ثم دراسةالتركيب البلوري للعينات كما تم ترسيبها (as-deposited) عند درجة حرارة 303K وتلك الملدنة عند درجة 523K . أظهرت فحوصات هول ان حاملات الشحنة السائدة هي الألكترونات وهذا يعني ان الأغشية كانت من النوع السالب. وجد ان معامل الامتصاص للاغشية المحضرة تقل بزيادة درجة حرارة التلدين من خلال دراسة التوصيليةالمستمرة وجد ان التوصيلية تزداد بزيادة درجة حرارة التلدين بينما طاقة التنشيط تقل بزيادة درجة حرارة التلدين .

تم دراسة خواص (السعة-الفولتية)وخساب جهد البناء الداخلي لهذا المفرق حيث اظهرت النتائج ان جهد البناء الداخلي يعتمد بشكل كبير على المعالجةالحرارية للمفرق.ومن خلال جميع الحسابات المذكورة اعلاه تم افتراض موديل لمخطط طاقة التنشيط للمفرق الهجين المحضرIn_2O_3/p-Si.