Effect of substrate temperature on some structural and optical properties of ZnTe films

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Abstract
Zinc telluride thin films of various thickness are deposited onto clean corning glass substrates kept on different tempretures(T_s=323,393 and 473 k),by vacuum evaporation method under the pressure of 10^{-5} Torr. The thickness of the films were measured by optical interference method(Tolansky).All the films prepared at different substrate temperatures were studied by X-ray diffraction method and shown that ZnTe films with (100nm) thickness have single crystal structur at substrate temperatures(323,393k) and polycrystalline structure at substrate temperature(473k),while we show that the films with (160 nm) thickness have single crystal at substrate temperature(323k) and polycrystalline structure at substrate temperatures(393,473k).Optical behaviour of the films were analyzed from transmittance spectra in the visible region(400-800 nm).The optical transition in ZnTe films is direct and allowed type.The optical band gap energy shows an inverse .dependence on substrate tempreture and thickness .

تاثير درجة حرارة الاساس على بعض الخصائص التركيبيه والبصريه لاغشية ZnTe

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الخلاصه:
تم ترسيب اغشيه رقيقه باسماك مختلفه على قواعد من الزجاج النظيف نوع (Corning) بدرجات حرارة اساس مختلفه (T_s=323,393 and 473 k) بطريقة التبخير الحراري في الفراغ تحت ضغط (10^{-5} Torr). تم قياس سمك الاغشيه المحضره بطريقة التداخل الضوئي(تولانسكي). تم دراسة الخصائص التركيبيه للاغشيه المحضره باستخدام تقنية حيود الاشعه السينيه ووجد ان الاغشيه ذات السمك ((100 nm احادية التبلور عند درجة حرارة اساس(323,393k) ومتعددة التبلور عند درجة حرارة الاساس(473k) ، بينما وجد ان الاغشيه ذات السمك (160nm) احادية التبلور عند درجة حرارة اساس (323k) ومتعددة التبلور عند درجة حرارة اساس(393,473k)). الخصائص البصريه للاغشيه تم دراستها من خلال طيف النفاذيه ضمن المنطقه المرئيه (400-800nm) اظهرت القياسات البصريه بان اغشية ZnTe تمتلك فجوة طاقه مباشره ذات انتقال مسموح. كما لوحظ ان فجوة الطاقه تتناسب عكسيا مع درجة الحراره والسمك.\

Introduction .1

Zinc telluride(ZnTe)is an important semiconductor material for the development of various modern technologies of solid state devices(blue light emitting diodes,laser diodes,solar cells,microwave devices,etc)[1-4]. The 11-V1 compound semiconductors have considerable potential for Integrated-optics applications due to their high electro-optics coefficients,wide transparency range from the visible beyond to 10 μm [5].Zinc Telluride (ZnTe) is a 11-V1 compound semiconductor with Zinc-blend structure with lattice constant of 6.1037 Å ,direct band gap of 2.26 Ev at room temperature[6],and melting point of 1295ċ.ZnTe and its alloys may effectively be used as window materials in CdTe heterojunction solar cells.These thin films were also used in tandem solar cell structure,which utilizes CdZnTe as the absorber material,and for the fabrication of a CdZnTe/ZnTe quantum well structure[7].Since optical response is of great importance for many device applications,much work has been done to determine the reflectivity,band gaps,and refrective index of ZnTe.Because of its importance several works [8] have made a detailed study on structure of ZnTe thin films.They have observed that these films deposited on glass substrates kept at room temperature have cubic Zinc-blende type structure.Saleem[9] has carried out studies on the optical properties on ZnTe thin films and calculated the optical constants..Raheem G.K[10] has measured structurel properties of ZnTe which used as heterojunction as $CdTe_{1-x}Se_x$/ZnTe.A theoretical model has been proposed by Pawlikowski[11]for ZnTe films and he determined the absorption coefficient near the fundamental absorption edge at normal incidence.Mondal et al.[12] have reported the dependence of refractive index,absorption and extinction coefficients on incident photon energy (hυ)for ZnTe films deposited on glass substrates by hot wall evaporation technique.Akkad and Thomas[13]have prepared ZnTe-cu thin films and measured the room temperature transmission and reflectivity in the wavelength range 300 nm.Rusu et.al [14] have deposited ZnTe thin films(d=0.12-180 μm) onto glass substrates by the quasi-closed volume technique under vacuum of 10^{-5} Torr.Optical gap was calculated from the absorption spectra situated in the range of (1.70-2.40)Ev .However not much work has been carried out on substrate temperature and optical properties of ZnTe films and their dependence on substrate temperature(T_s).Hence,this paper reports about the temperature dependence of structural,and optical properties of .vacuum evaporated ZnTe thin films

Experimental details

The bulk ZnTe alloy was prepared from its own constitutional elements.Appropriate weights of Zn and Te were mixed together,charged in a quartz tube and sealed under a vacuum of 10-5 Torr.The sealed quartz ampoule with the charge was placed in a rotating furnace.The temperature of the furnace was raised gradually to 1523 k and left at this temperature for about three hours with a rate of 5^o/min using a programmable furnace type carbolite.After that the ampoule was cooled down in . furnace and then broken to bring out the alloy

Thin films of ZnTe were prepared by thermal evapopation using an Edward E306A coating unit onto cleaned glass substrates maintained at various temperatures (T_s= 323,373and 473k)during evaporation.A Molybdenum boat was used as the source holder and the pressure in the chamber was of order($2x10^6$)mbar.The ZnTe films were evaporated thermally with a deposition rate of 0.5 nm/s with (100 and 160)nm thicknesses.The thicknesses of the films were evaluated using a Fizeau interferometric method. The structural aspects of the films were analyzed,using X-ray diffractometer with filtered CuKα radiation(λ=1.5418Å).The optical transmittance spectra of these . films were recorded using UV-VIS-NIR spectrometer

Results and discussion .3

structural characteristics 3-1

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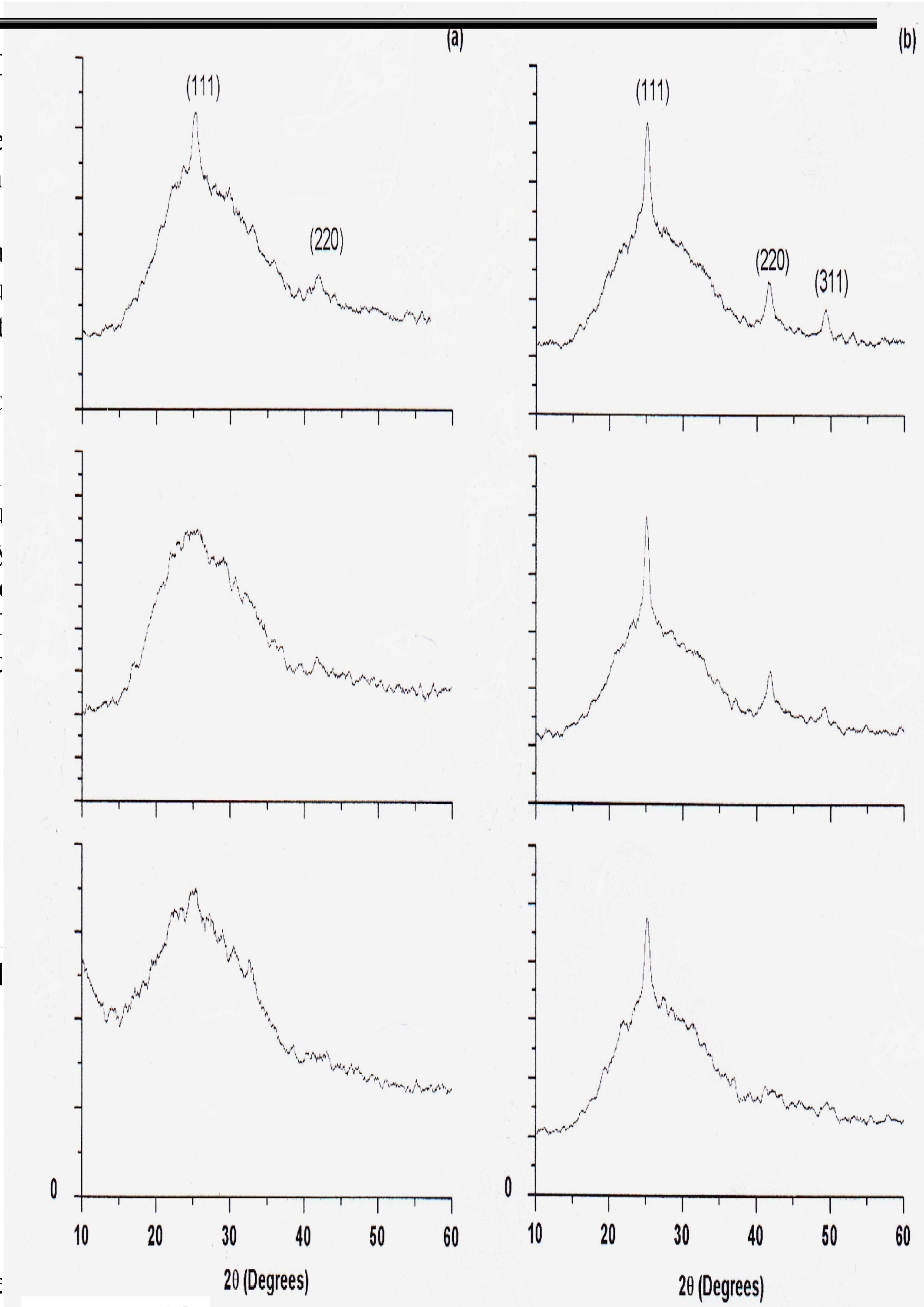

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Fig.1 XRD spectra of ZnTe thin films of thickness (a)100 nm and (b) 160 nm deposited at different substrate temperature

substrate temperature is a consequence of the larg ... y of the atoms at high temperature;thus,there is a decrease in the density ... ation centers,and under these circumatances a smaller number of centers start to grow.Adecrease in grain size at higher substrate temperature may be due to the some Zn reevaporation,which changes the stoichiometric,leaving an excess of Te on the film,which forms crystalline .grains

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Table 1 structural parameters of ZnTe films

(Thickness(Å	(T_s(k	Lattice constant a(Å	Grain size D(Å	hkl
1000	443	6.230	92	111
1600	323	552 .6	158	111
	393	6.560	175	111
	443	6.572	146	111

Optical properties 3-2

The transmittance spectra for ZnTe thin film of thickness 1000Å and 1600Å deposited at various substrate temperatures(T_s=323,373 and 443 k) are shown in figure 2.It is clearly observed that the film has very low transmittance in the visible region and further increases to higher values at higher wavelength region.The transmittance falls steeply with decreasing wavelength.It can be positively concluded that the material is of highly absorbing nature in the visible region (4000-8000Å).This is in good agreement with the earlier investigation[ ].For the semiconducting films with with the thickness below 1000Å important role in the optical absorptrion(transmission)also begin to play non-confined effects on the borders film-substrate and amorphous-like background-microcrystallites,how it was shown during investigations of the optical and non-linear optical properties of the ZnS doped films[15].These nano-confined levels also may cause observed short wavelength .shift of spectra

The total absorption coefficient was calculated from transmittance measurements :[with the aid of the expression[16

$$\alpha = \left(\frac{4\pi k_f}{\lambda} \right) \quad (1)$$

:The extinction coefficient (k_f) can be calculated from the relation

$$k_f = \frac{2.303\lambda \left(\frac{1}{T_0} \right)}{4\pi t} \quad (2)$$

.Where T_0 is the transmittance and t is the thickness of the film

The refractive indices were calculated using Manifacier's formula[23] by the iterative :method

$$T_0 = \frac{16n\ n_g n^2 \exp(-\alpha t)}{R^{\ 2} + R_2^{\ 2}\exp(-2\alpha t) + 2R_1R_2\exp(-\alpha t)\cos\left(\frac{4\pi nt}{\lambda}\right)} \qquad (3)\ldots\ldots\ldots$$

Where $R_1=(n+n_a)(n_g+1)$, $R_2=(n-n_a)(n_g-1)$ are the absorption coefficient n ,n_a and n_g : .are the refractive indices of the film , air and substrate respectively

Figures 3,4,5 and 6 show the variation of k and n with wavelength for ZnTe films of thickness 100 nm and 160 nm for different substrate temperatures.These optical constants(k and n)are found to be very sensitive to the substrate temperature of the film.The refractive index n decreases monotonically with increasing substrate temperature.This was found to be most noticeable near the absorption edge.An unexpected decrease of n was observed at shorter wavelengths,which have also been .reported for ZnTe[by various investigators

Figure 6 and 7 depict the variation of square of (αhυ) versus photon energy(hυ) for ZnTe films of the thickness 100 and 160 nm for different substrate temperatures T_s =323,393 and 443 K respectively.The optical band gap energy has been evaluated by extrapolating the linear portion of the curve to the energy axis and the corresponding .values with respect to the substrate temperature were given in table 2

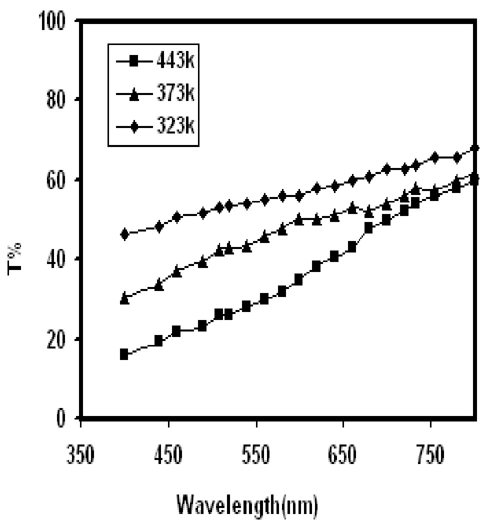

Fig.2 Transmittance spectra of ZnTe film of thickness (100 nm) deposited at differnnt substrate temperatures.

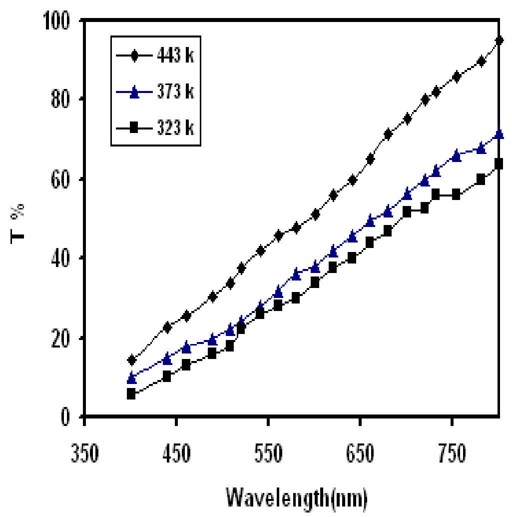

Fig.3 Transmittance spectra of ZnTe film of thickness(160 nm)deposited at different substrate temperatures

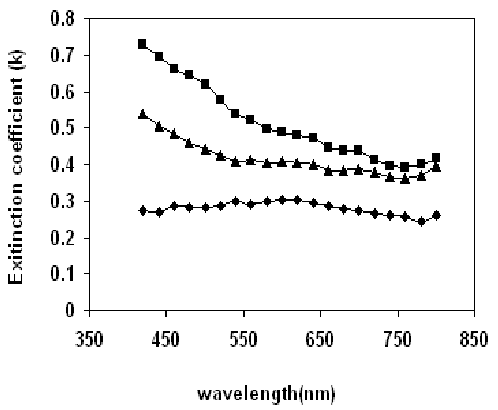

Fig.4 Extinction coefficient of ZnTe films of thickness 100 nm deposited at different substrate temperatures.

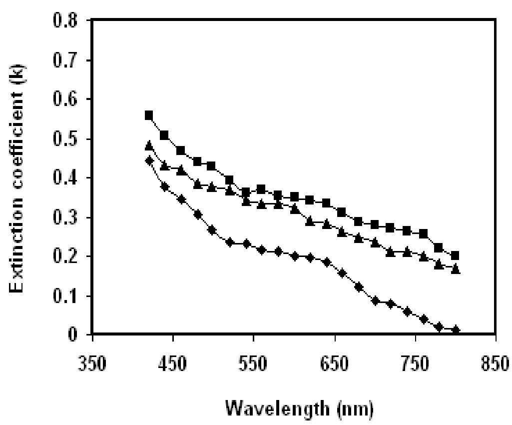

Fig. 5 Extinction coefficient of ZnTe films of thickness 160 nm deposited at different substrate temperatures.

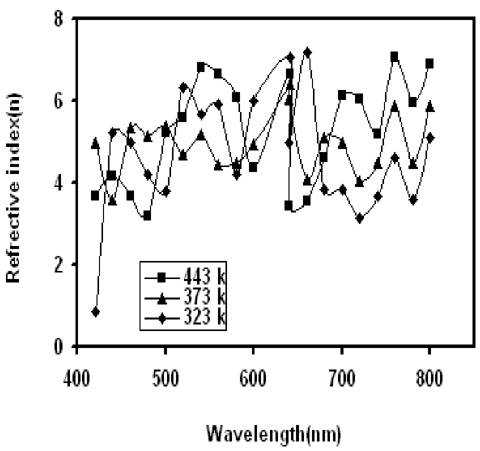

Fig.6 Refractive of ZnTe films of thickness 100 nm deposited at different substrate temperatures.

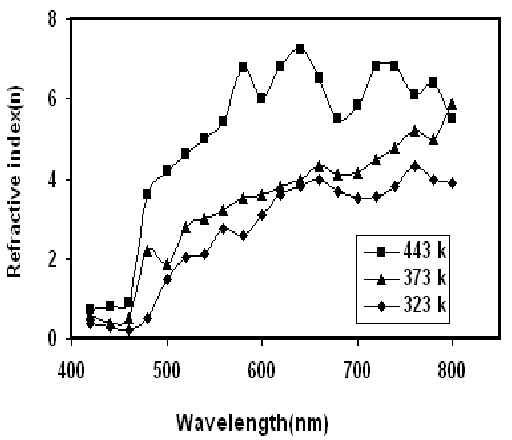

Fig.7 Refractive index of ZnTe films of thickness 160 nm deposited at different substrate temperatures

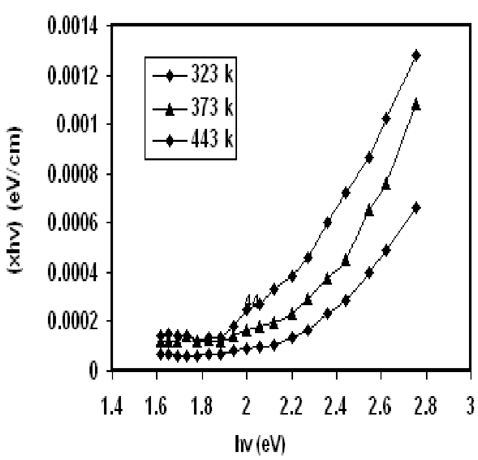

Fig.8 The dependence of ( ) on hv for ZnTe films of thickness 100 nm deposited at differnt substrate temperatures

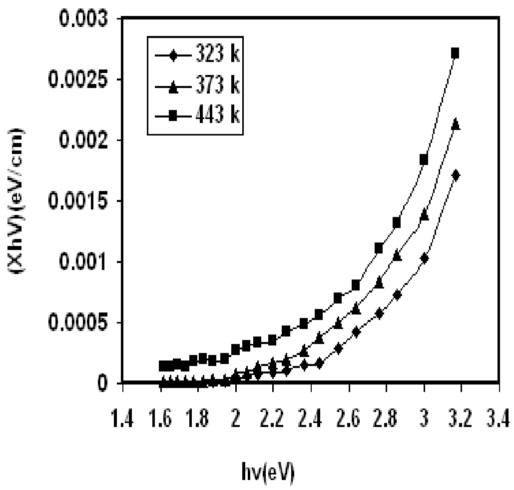

Fig.9 The dependence of ( ) on hv for ZnTe films of thickness 160 nm deposited at difference substrate

Table 2 The band gap for ZnTe films of thicknes 100 and 160 nm deposited at .different substrate temperatures

Substrate (Temperature(K	Band gap energy of 100 (nm(eV	Band gap energy of (160 nm(eV
323	2.25	2.15

393	2.10	2.06
443	2.05	2

The direct band gap decreases with increase of ubstrate temperature and thickness of the films.The decrease of direct band gap with increase of substrate temperature and thickness is attributed to an increase of particle size and increase of lattice constant[11].From the microstructural analysis it is observed that the particle size increases with the increases of substrate temperature.The decrease in optical band gap with increase in film thickness is due to the increased grain size of the higher .thickness films

.Conclusion 4

ZnTe thin films were deposited onto well-cleaned glass substrates by vacuum evaporation.The X-ray diffraction analysis indicates that the crystalline nature of the film increases with increase in the substrate temperature.From the transmission spectra,the transmission is found to decrease with increase of substrate temperature and thickness.The optical transitrion in ZnTe films is direct and allowed type.The optical band gap energy shows an inverse dependence on substrate temperature and .thickness

Refrences

.M.Jain(ed),1993,11-V1 Semiconductor Compounds,World Scientific,Singapore. 1

.V1 Semiconductors,Inspec.London. R.Bhargava (ed),1997,Properties of Wide 2-11

.M.Schall,M.Walther,P.Uhd Jepsen,2001,Phys.Rev.B64,94301 . 3

G.I.Rusu,P.Prepelita,N.Apetroaei,G.Popa,2005,The Electronic Transport and Optical .4 Properties of ZnTe thin films,Jornal of Optoelectronics and Advanced .Materials,Vol.7,No.2,P.829-835

R.Amutha,A.Subbarayan, and R.Sathyamoorthy,2006,Influnce of substrate temperature on .5 microcrystalline structure and optical properties of ZnTe thin .films,Cryst.Res.Technol.Vol.41,No.12,p.1174-1179

.M.Nishio,K.Hayashida,Q.Guo,and H.Ogawa ,2001,Appl.Surf.Sci,Vol.129,No.223 .6

.B.Maiti,P.Gupta,S.Chaudhuri,and A.K.Pal,1994,Thin Solid Films,V0lume,239,No.239 .7

U.Pal,S.Saha,A.K Chaudhuri,V.V.Rao,and H.D.Banerjee,1989,Optical properties .8

S.Ezara ,2006,Study of Al-CdTepAl and Al-ZnTe-Al for switching applications, PhD .9 .Thesis,Baghdad university

R.G.K Almorshdy,2007,Study of structural,electrical and optical Characterization of the .10 .Heterojunction $Cd(Te_{1-x}Se)/ZnS(Te)$,PhD Thesis,Baghdad university

J.M.Pawlikowski,1985,The effect of thickness on some optical properties of ZnTe films,Thin .11 .Solid Films,Vol.39,No.127

A.Mondal,S.Chaudhuri,and A.K.Pal,1987,Study of some optical properties of ZnTe films by hot .12 .wall evaporation technique,Appl.Phys.A,Vol.43,N0.81

F.El.Akkad and M.Thomas, 2005,Optical properties of ZnTe-Cu films .13 .,Phys.Stat.Sol(c),Vol.2,No.3,pp 1172-1174

G.I.Rusu,P.Prepelita,N.Apetroaci,G.Popa,2005,Journal of Optoelectronic and advanced .14 .Materials,Vol.7,N0.2,pp 829-835

.A.Lopz-Otero,1977,J.Cryst.Growth,Vol.42,N0.157 .15

O.Zelaya,F.Sanchez-Sinencio,J.G.Mendoza-Alvarez,M.H.Faarias,L.Cota-Araiza,and .16 .G.Hirata-Flores,1998,J.Appl.Phys.,Vol.63,N0.49