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Effect of Molar concentration on Structural and Optical properties of MgO thin films prepared by SILAR method.

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ABSTRACT:

Different molarities of MgO thin films were grown on the glass substrate by successive ionic layer adsorption and reaction (SILAR) method. The effect of molar concentration on the structural and optical properties was studied by using X-ray diffraction (XRD), UV-Vis spectrometer, Raman spectroscopy and FTIR spectroscopy.XRD measurements demonstrate the cubic MgO structures and samples have (200), and (220) peaks with (200) preferred orientation. The crystalline size was found to be increased with increase of molar concentration.UV-Vis spectrometer showed that the absorption edge of prepared samples in UV region, and the band gap values of MgO thin films decrease with increasing of molar concentration.

Keywords: MgO, Molar concentration, Thin film, SILAR

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1. Introduction:

Recent researches have shown a special interest in nanomaterials due to their unique properties. Among the nanomaterials, metal oxides nanostructure have gained great attention due to their applications in various electronic fields such as sensors, solar cells and so on[1, 2].
Among these metal oxide nanostructure materials magnesium oxide gained much interest from the researchersdue to its special functional, optical and electrical properties which are made it suitable candidate to use in different technology applications such as sensors, solar cells, capacitors[3] and antibicterial agents[4].MgO thin films have high durability, high transparency, wide band gap, low optical loss and low refractive index which allowed to use it as protective layers against ion bombardment, buffer layers and ferroelectric materials[5].
Different physical and chemical methods can be used to producemagnesium compounds MgO or Mg(OH)2 in a variety of shapes, including needle, rod, coverslip, flake, and wire architectures, thin films on different substrates[6], such as SILAR method [7, 8], sol-gel spin coating [9], pulsed laser deposition [10].
Although there are several different techniques for growing MgO nanostructures, SILAR is favoured because to its superior qualities, including its straightforward, affordable, and quick development rate [8].
In this report we synthesized of MgO thin films at different molar concentration by using SILAR method, and study the effect of molar concentration on structural and optical properties of prepared films.

2. Experimental:

To prepare of magnesium oxide thin films by SILAR method, magnesium nitrate hexahydrate was used as cationic source and distilled water as anionic source. Different molarities of magnesium nitrate (0.2, 0.4, 0.6) M, were dissolved in 100 ml distilled water and equivalent quantity of distilled water was adjusted its PH up to 12 by adding ammonia solution. The pre- cleaned glass substrate was immersing for 30 sec in cationic and anionic solutions at 60 ^{0}C, this repeat for 90 cycle. Finally the deposited films were annealing at 200^{0}C, for 2h.

3. Results and discussion:

3.1. XRD analysis:

The X-ray diffraction spectra of different molarity MgO thin films are shown in Figure1(a-c). All peaks of MgO thin films corresponded (200), and (220) peaks and the cubic structure according to card number 00-45-0946 and that reported by [8].The figure showed there are no new peaks when cationic molarity are 0.2 and 0.4 M. when the molarity increased upto 0.6 M there is a peak at$2\theta(36.75^0)$. The $d_{(200)}$ and $d_{(220)}$ were calculated by using Bragg's law

$n\lambda = 2d\sin\theta$

where n= 1, λ= 1.5406 A^0 (wavelength of incident x-ray), d inter- planer distance and θ is the diffraction angle, the values where 2.11 and 1.49 A^0 respectively which were conform with standard values according to card number (00-45-0946). The dominant peak was at 2θ(42.76) degree, which reveals that the prefer orientation along (200). The crystalline size was calculated from the dominant peak show that the size increasedF with increased in molarity. For calculated the crystalline size Debye-Scherrer formula,was used

$$D = \frac{0.9\,\lambda}{\beta COS\Theta}$$

Where D is crystalline size of MgO thin films, λ is the incident X-ray wavelength, β is the full width at half maximum of the diffraction peak, and θ is the half of the observed peak angle. The result showed in table 1.

Table 1 Crystalline size of MgO thin films prepared at different molarities

Sample	Molarity(mol/liter)	Crystalline size (nm)
MgO (0.2 M)	0.2	11.4
MgO (0.4 M)	0.4	12.1
MgO (0.6 M)	0.6	15.6

The lattice constant can be calculated by using the formula

$d = \frac{a}{\sqrt{(h^2+k^2+l^2)}}$,

Where a is the lattice constant and h,k and l are miller's indices.

The value was a = 4.22 A^0.

The volume (V) of unit cell of cubic MgO thin films was calculated by using the relation

$$V = a^3$$

The calculated volume (V) of unit cell of cubic MgOwas $75.15A^{o\,3}$.

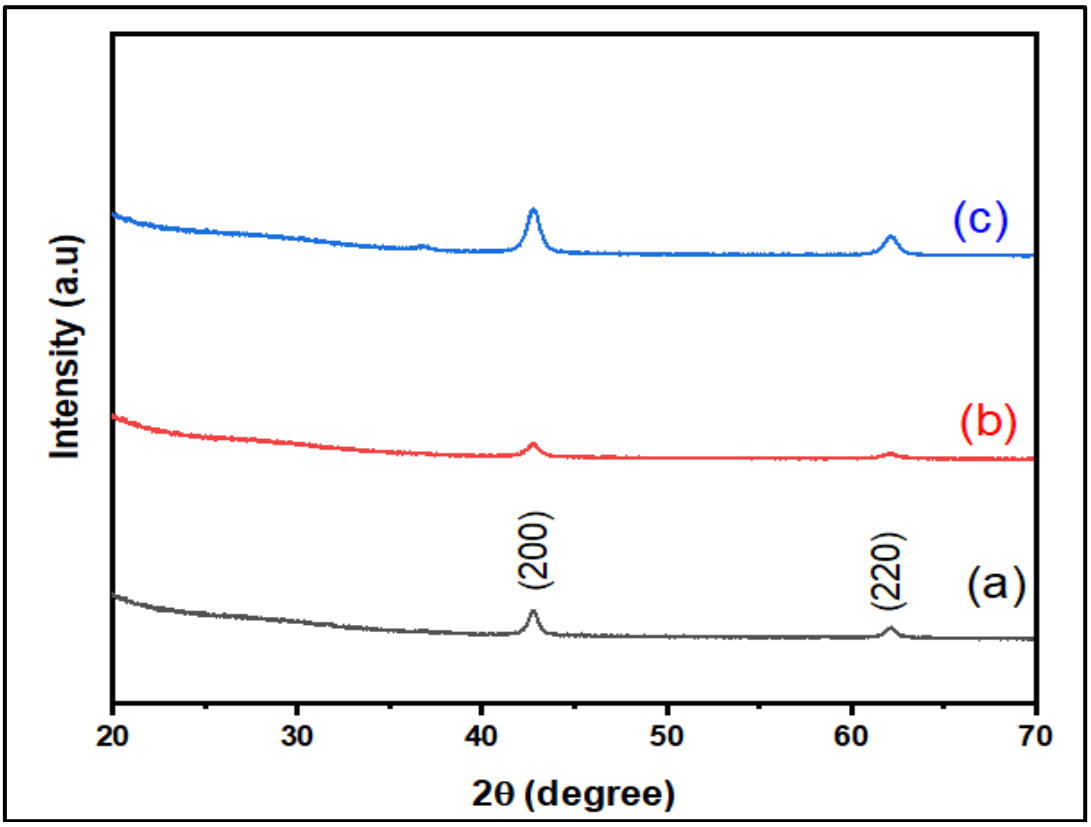

Figure 1. XRD pattern of MgO films (a) 0.2 M (b) 0.4 M (c) 0.6 M.

3.2. UV-VIS analysis :

The optical characterization of prepared MgO thin films were done by using UV–Vis spectrophotometer. Figure 2 shows the plot of absorption spectra of MgO thin films in 300–800 nm wavelength range. In absorption spectra, the peaks were observed in UV region at 309 nm, 311 nm and 311.5 nm for films prepared at 0.2 M, 0.4 M and 0.6 M respectively.

The values of direct band gap energy of MgO thin films were obtained from the absorption spectra by using Tauc plot versus $(\alpha h\nu)^2$ and $(h\nu)$ as shown in the inset Figure 2. The optical band gap was calculated by using Tauc equation, as given blow

$$\alpha h\nu = B\left(h\nu - E_g\right)^n$$

Where α is the "absorption coefficient," Eg is the material's "optical band gap," B is a "constant," h is the "Planck's constant," ν is the "frequency," and n is an exponent that depends on the type of transition and can have values of 1/2, 2, 3/2, or 3 that correspond to allowed direct, allowed indirect, forbidden direct, and forbidden indirect transitions, respectively [11]. The calculated values of energy band gap are listed in table 2.

Table 2.Optical energy band gap of MgO films.

Sample	Energy band gap (eV)
MgO (0.2 M)	3.35
MgO (0.4 M)	3.30
MgO (0.6 M)	3.29

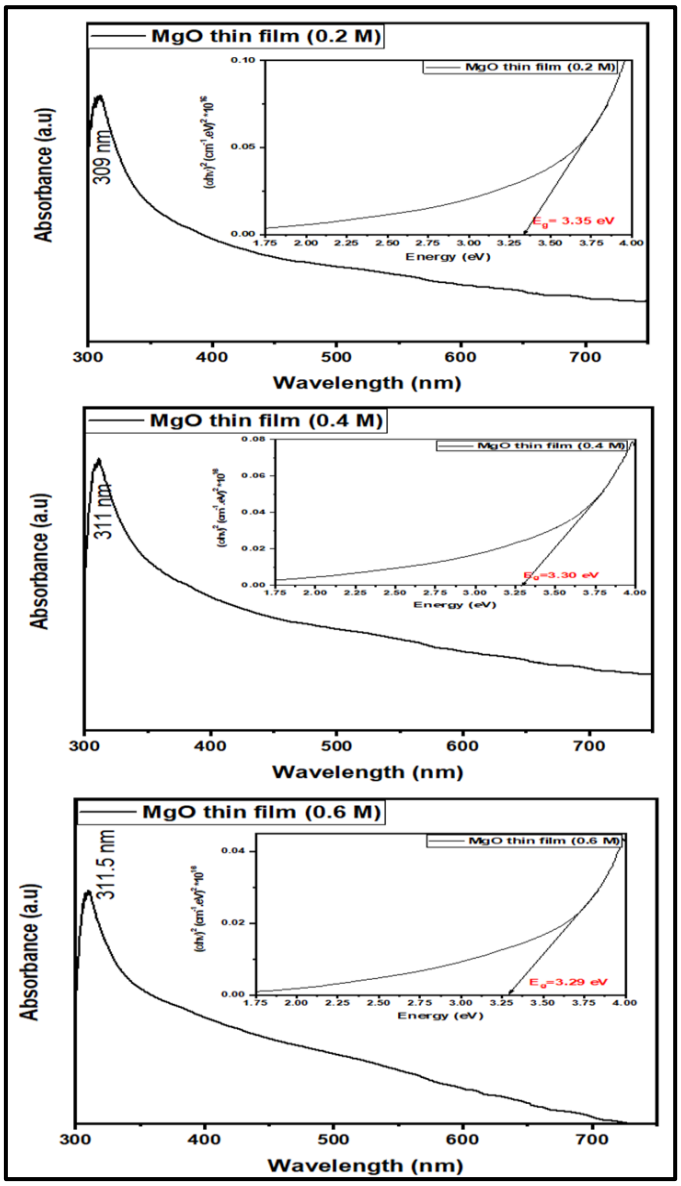

Figure 2 Absorption spectra and energy band gap of different molarities MgO thin films.

3.3. Raman analysis:

A flexible nondestructive method to examine the vibrational and structural characteristics of thin films is Raman spectroscopy. Room-temperature Figure 3 displays the Raman spectra of produced MgO films. Peaks located at 478 cm^{-1} and 1098 cm^{-1} are attributed to *E*2 (high) first-order Raman modes and TO–LO surface phonon mode in MgO lattice respectively[12]. The peak at 1460 cm−1 is associated to D-band also known as breathing mode [12, 13]. The peak at 1520 cm−1 represent as a G-band [13].

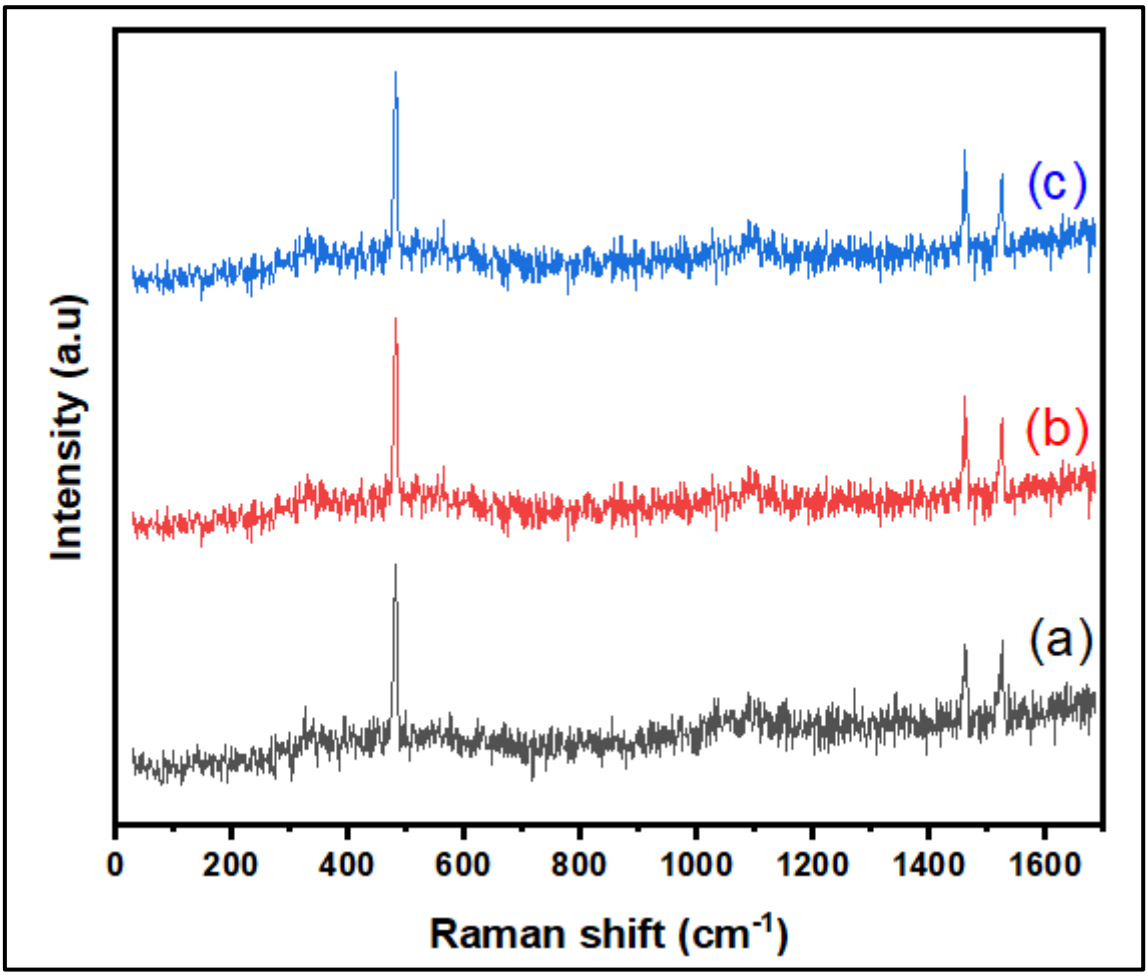

Figure 3 Raman spectra of different molarities MgO thin films (a) 0.2 M (b) 0.4 M (c) 0.6 M

3.4. FTIR analysis:

The FTIR spectrum of the MgO thin films in the wavenumbers range 4000 - 650 cm^{-1} depicted in Figure 3 shows broad absorption band at 3697cm^{-1} due to the stretching vibration of O–H. This absorption peak attributes to adsorbed water on the surface of MgO crystallites [14]. The peak at 2355 cm^{-1} is assigned to the bending vibrations of CO_2, which coming due to atmosphere. Absorption band in a range of 1300 -1500 cm^{-1} is assigned to symmetrical and asymmetrical carbonyl group vibrations. The peak observed at 793 cm^{-1} is indicates the Mg-O stretching vibration.

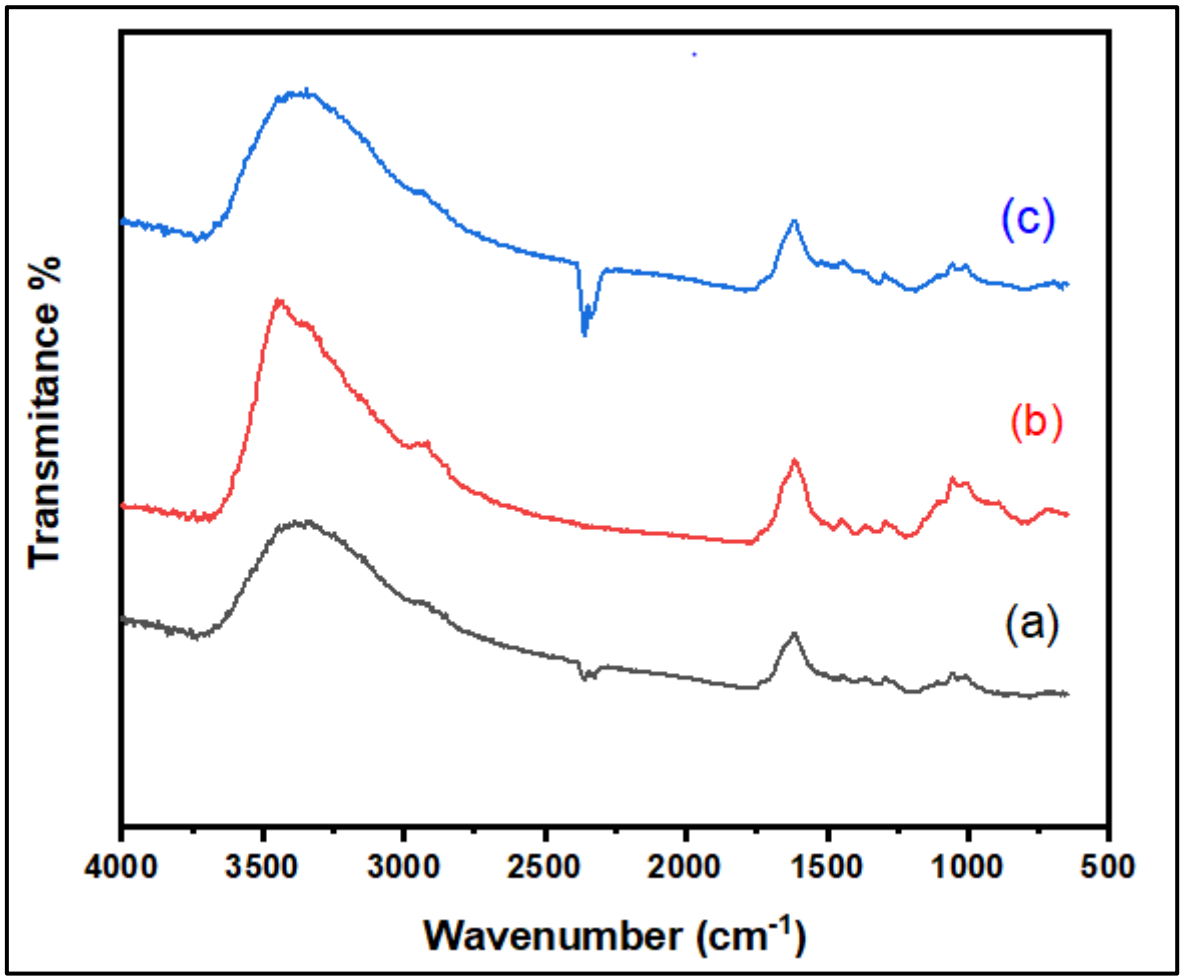

Figure 4 FTIR spectra of different molarities MgO thin films (a) 0.2 M (b) 0.4 M (c) 0.6 M.

4. Conclusion:

Magnesium oxide, MgO films with different molarities (0.2, 0.4 and 0.6M) has been successfully deposited on glass substrates by using SILAR technique. The structural of prepared samples was studied by using X-ray diffraction (XRD). XRD result showed that the obtained films have cubic structure with two peaks corresponded (200), and (220) planes. The dominant peak was at 2θ (42.76) degree, which reveals that the prefer orientation along (200). when the molarity increased upto 0.6 M there is a peak observed at 36.75^0. The crystalline size was calculated from the dominant peak show that the size increased with increased in molarity. UV-Vis spectra showed , the absorption edge of samples in UV region at 309 nm, 311 nm and 311.5 nm for films prepared at 0.2 M, 0.4 M and 0.6 M respectively. The calculated energy band gap was found to be decreased with increase in molarity.

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References:

[1]. Balakrishnan, G., et al., Microstructure, optical and photocatalytic properties of MgO nanoparticles. Results in Physics, 2020. **16**: p. 103013.

[2]. Verma, R., et al., Morphology, mechanism and optical properties of nanometer-sized MgO synthesized via facile wet chemical method. Materials Chemistry and Physics, 2014. **148**(3): p. 1064-1070.

[3]. Thirupathi, R., et al., A comparative study of chemically and biologically synthesized MgO nanomaterial for liquefied petroleum gas detection. Journal of Electronic Materials, 2018. **47**(7): p. 3468-3473.
[4]. Sundrarajan, M., J. Suresh, and R.R. Gandhi, A comparative study on antibacterial properties of MgO nanoparticles prepared under different calcination temperature. Digest journal of nanomaterials and biostructures, 2012. **7**(3): p. 983-989.
[5]. Bazhan, Z., F. Ghodsi, and J. Mazloom, Effect of stabilizer on optical and structural properties of MgO thin films prepared by sol–gel method. Bulletin of Materials Science, 2013. **36**(5): p. 899-905.
[6]. Habibah, Z., et al., Chemical solution deposited magnesium oxide films: influence of deposition time on electrical and structural properties. Procedia Engineering, 2013. **56**: p. 737-742.
[7]. Güney, H. and D. İskenderoğlu, Characterization of MgO: Cd thin films grown by SILAR method. Canadian Journal of Physics, 2018. **96**(7): p. 804-809.
[8]. Güney, H. and D. İskenderoğlu, Synthesis of MgO thin films grown by SILAR technique. Ceramics International, 2018. **44(**7): p. 7788-7793.
[9]. Zulkefle, H., et al. Molar concentration effect on MgO thin films properties. in 2011 IEEE Symposium on Industrial Electronics and Applications. 2011. IEEE.
[10]. Zhu, T.-J. and L. Lu, Orientation of MgO thin films on Si (001) prepared by pulsed laser deposition. 2003.
[11]. Singh, N., et al., Synthesis and characterization of nanostructured magnesium oxide: insight from solid-state density functional theory calculations. Journal of Inorganic and Organometallic Polymers and Materials, 2016. **26**(6): p. 1413-1420.
[12]. Visweswaran, S., et al., Characterization of MgO thin film prepared by spray pyrolysis technique using perfume atomizer. Journal of Materials Science: Materials in Electronics, 2020. **31**(17): p. 14838-14850.
[13]. Athar, T., A. Hakeem, and W. Ahmed, Synthesis of MgO nanopowder via non aqueous sol–gel method. Advanced Science Letters, 2012. **7**(1): p. 27-29.
[14]. Halder, R. and S. Bandyopadhyay, Synthesis and optical properties of anion deficient nano MgO. Journal of Alloys and Compounds, 2017. **693**: p. 534-542.