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Studying the Effect of Annealing Temperature on Some Optical Properties of Lithium Fluoride Thin Films

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Abstract:

Lithium Fluoride (LiF) thin films were prepared by thermal evaporation under vacuum (TEV), on glass substrate at room temperature of (303K). After that the films were treated thermally at temperature of (473,573 K) for one hour, with thickness of (400±10 nm). The optical properties of (LiF) thin films were studied within the wavelength range of (200-1100) nm. It was found that it has a high transmittance between (80 – 95 %) percentage, and low absorption and reflectivity in the (visible, near infrared) region. The value of energy gap was calculated and it was found that it is value is (5.1 eV) and the energy gab decreased to (5eV) with increasing annealing temperature. The value of some optical constants such as Absorption (α), Extinction coefficient (K_o) and Reflective index (n) were also calculated.

Keywords: Lithium Fluoride (LiF), Optical properties (OP), Thermal Evaporation Vacuum (TEV), Annealing Temperature (AT).

Introduction:

Optical properties of LiF thin films include high spectral transparency for visible light over a wide spectral range (300-6000 nm) (Rodrigues, Fleming, & Hennessy, 2022). LiF thin films have a low refractive index of (1.39) at a wavelength of (550 nm), these properties are very important and are considered in various optical applications such as lenses, filters (Scaglion & Montereali, 2005).

Lithium fluoride (LiF) is a highly ionic crystalline solid with a melting point of 480°C, a density of 2.639 g/cm^3, and a molecular weight of 25.94g/mol (Quijada, Hoyo, & Rice, 2014). LiF crystallizes in the form of a sodium chloride (NaCl) (salt) structure. It has an FCC lattice consisting of a Li^+ ion and a F^- ion, with a lattice constant of 4.03 Å (Motecchi & Baccaro, 2001).

Lithium fluoride (LiF) is widely used for microelectronics (electro-optics) applications, as a passivation layer for organic light-emitting diodes (OLEDs), and as a detector for contact-mode imaging. It is also widely used as a substrate and dielectric material for the growth of thin films in materials science and engineering (Rodríguez-de Marcos, Larruquert, & Méndez, Optimization of MgF2-deposition temperature forfar UV Al mirrors, 2018). Thin films of LiF were prepared using many depositions technique pulsed laser deposition (PLD), sol-gel, chemical spray (Glavic & Björck, 2022). Among these, thermal evaporation vacuum deposition is often preferred because it provides the best environment for deposition of thin films and enables the production of thin films with high purity and at varying substrate temperatures (Forasiere & Montereali, 2003).

Materials and Method:

Lithium fluoride thin films were obtained by (LiF) powder [a white powder which is a typical alkaline substance with a purity of (99.99)]. The deposition of (LiF) thin films by the of heated thermal evaporation by electrical resistance, where electrical energy passes through the source to form a vapor of lithium fluoride material that moves in straight paths and then condenses to form (LiF) thin films deposited on the substrate.

In this work the evaporation processes have been performed at room temperature (303K). The pressure during the evaporation was approximated to 10^{-6} torr, and the distance between the source and substrate was kept at (10) cm. on the other hand, these films have been annealed at different annealing temperatures (473, 573K), the thickness was measured using the optical interference method (laser method) by using a helium-neon laser light (He-Ne) where the thickness was calculated through the interference resulting from the difference in phase difference between the rays reflected from the back surface and the front surface of the thin film. The thickness (t) was calculated using the following relation (Weijtens & Van loon, 2015):

$$t = \frac{\Delta L}{L} \times \frac{\lambda}{2} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

Whereas:

λ: Wavelength of the laser light used and its value (632.8nm).

L: Width of the bright fringe (nm).

ΔL: Width of the dark fringe (nm).

Results and Discussion:

1. Transmittance (T):

The figure (1) shows transmittance value the films have high value (more than 90%) at wavelengths (λ) greater than (400 nm) (the visible and near infrared regions), but at wavelengths less than (290 nm) there is a sharp decrease in the transmittance of the films due to the increase in absorbance in this region. Figure (1) also shows the transmittance value decreases slightly with increase annealing temperature, and this behavior is annealing leads to an increase in the material's density, which represents an increase in the number of atoms per unit volume, leads to an increase in collisions between the incident photons and the atoms, thus increasing the absorbance and decreasing the transmittance, these results are consistent with what was stated by (Ibrahim & Murali, 2009).

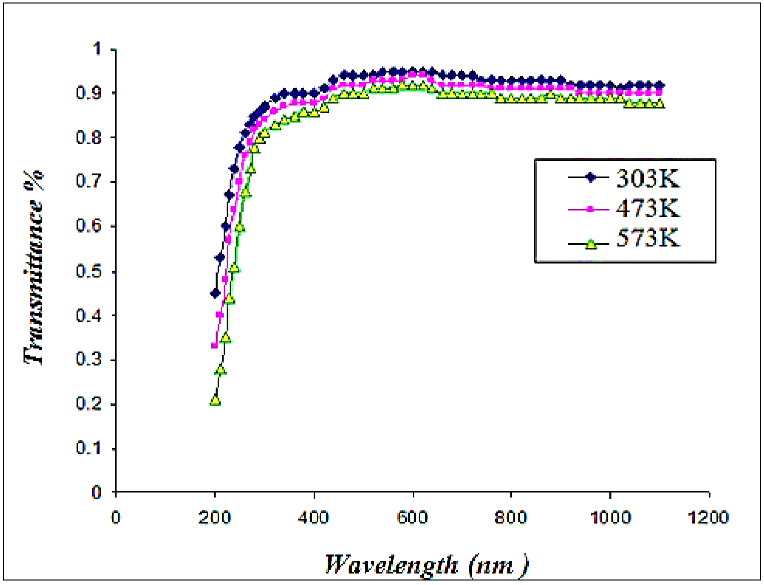

Figure (1): Relationship between transmittance with wavelength for different annealing temperatures.

2. Absorption (A):

The figure (2) absorbance of thin films has high value at wavelength (230nm), then its value decreases with increasing wavelength. The absorbance values are low in the (visible and near infrared regions) .

This behavior can be explained by the fact that at higher wavelengths the incident photons do not have enough energy to interact with the atoms and thus the photons will be transmitted from the films surface. But when the wavelength decreases and the energy of the photons increase, and thus absorbs between the incident photon and the material will occur, and thus the absorbance will increase (Şenay & Pat, 2014). Figure (2) also shows the absorption spectra increase with increasing annealing temperature. This behavior can be attributed to the increasing in the grain size with annealing temperatures; our results are consistent with those of
(Saadatyi, Grayeli, & savalon, 2010).

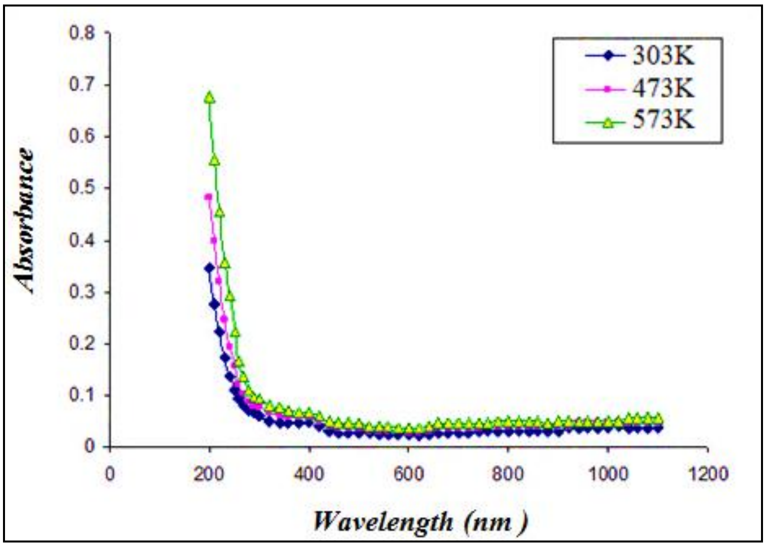

Figure (2): Relationship of absorbance with wavelength for different annealing temperatures.

3. Reflectivity (R):

The reflectivity was calculated from the following equation (Chiad & Mubarak , 2020):

$$R + T + A = 1 \ldots\ldots\ldots\ldots\ldots\ldots\ldots..(2)$$

The Figure (3) shows that the reflectivity value for films is very small in the visible region, and its value increases slightly with a decrease in the wavelength value. Figure (3) also shows that the reflectivity value increases slightly an increase the annealing temperature. This behavior is consistent with the transmittance results and absorbance according to equation (2).

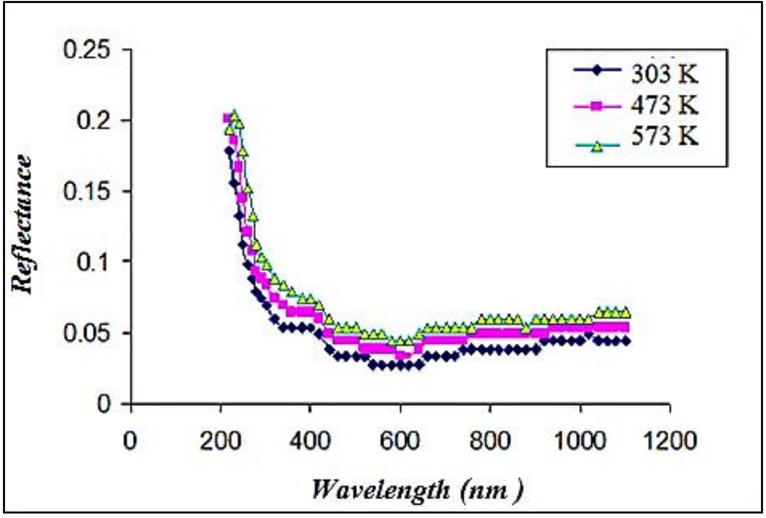

Figure (3): Relationship between reflectance with wavelength for different annealing temperatures.

4. Absorption coefficient (α):

It was calculated from the following equation (3) (Priyadarshini, Sahoo, & Naik, 2022):

$$\alpha = \frac{2.303(A - A`)}{t} \ldots\ldots\ldots\ldots\ldots\ldots (3)$$

Whereas:

A: The amount of absorbance at specific wavelength.

A `: The amount of correction factor.

Figure (4) shows the absorption coefficient increases with increasing incident photon energy. It was showing the absorption coefficient increases with the annealing temperature. Annealing leads to an increase in the material's density, which leads to an increase in absorption value, we note that found all films have a high absorption coefficient $(\alpha > 10^4\ cm^{-1})$. this is suggests the occurrence of direct electronic. The behavior is consistent with that of (Dines, Kmar, & Mehra, 2006).

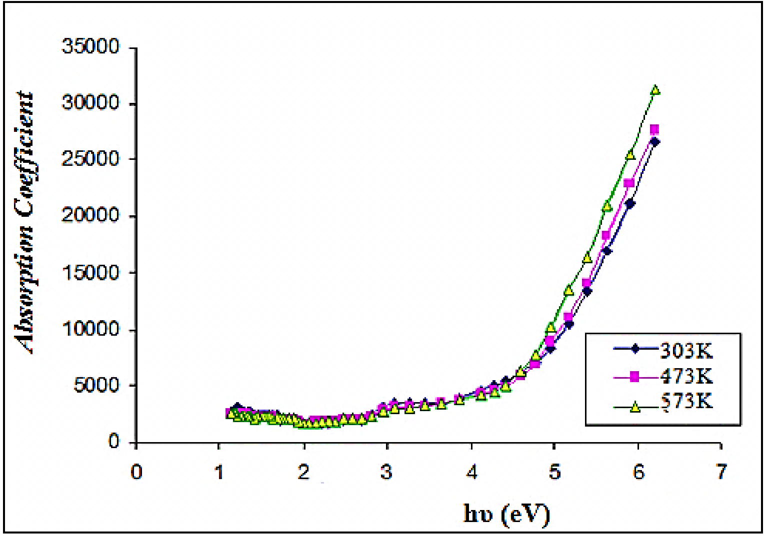

Figure (4): Relationship between absorption coefficient with photon energy for different annealing temperatures.

5. Optical energy gap (Eg):

Direct optical energy gap was determined the relationship between $(\alpha h v)^2$ and photon energy as shows in figure (5). It was observed the value of energy gap decrease with increasing annealing temperature. Annealing leads to an increase in the material's density. As the material's density increases, the interactions between atoms increase, leading to a broadening of energy levels and a reduction in the energy gap. This behavior consistent result of researchers (Rodríguez-de Marcos, J. Méndez, & Larruquert, 2016) . The energy gap values can be tabulated in Table (1).

Table (1): Direct energy gap for thin films (LiF) with different annealing temperatures.

Annealing Temperatures(K)	Energy Gap(eV)
303	5.1
473	5.05
573	5.0

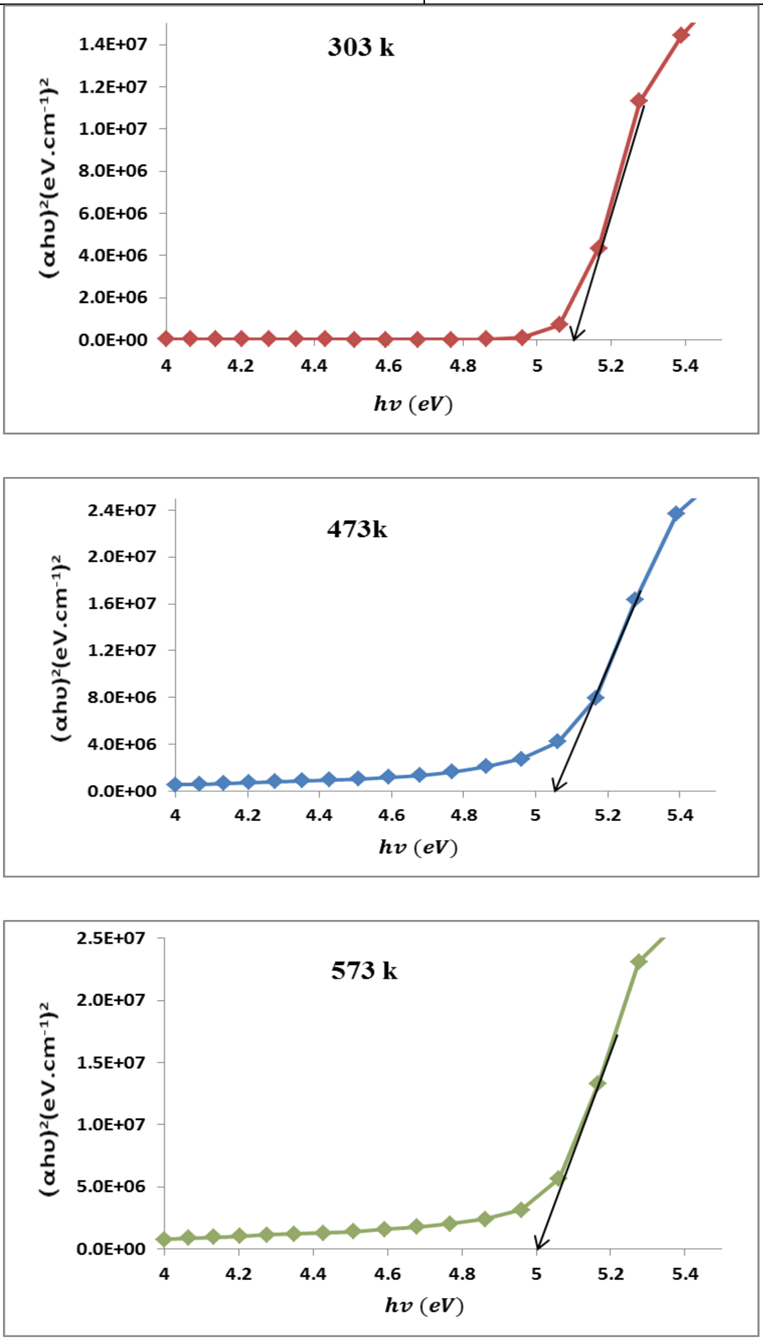

Figure (5): Relationship between $(\alpha h\upsilon)^2$ with photon energy for different annealing temperatures.

6. Extinction coefficient (K_o):

The extinction coefficient was found using the following relationship (Almaviva, Bonfigli, & Franzini, 2006)

$$K_o = \frac{\alpha\lambda}{4\pi} \dots\dots\dots\dots\dots\dots\dots.(4)$$

Whereas:

λ: Wavelength of beam.

The figure (6) shows the value of extinction coefficient increases with increase of the photon energy within the range ($hv > 2eV$). This behavior is consistent of the behavior of the absorption coefficient which has a direct relationship with (K_o) as shown in equation (4).

Also, figure (6) shows that the value of the extinction coefficient increases annealing temperature. This behavior attributed to the increase in the density of carries, which confirms increase in the value of absorption coefficient with annealing temperature, which in turn leads to an increase in the value of the extinction coefficient with an increase in the annealing temperature. (Mäntymäki, Hämäläinen, & Puukilainen, 2013).

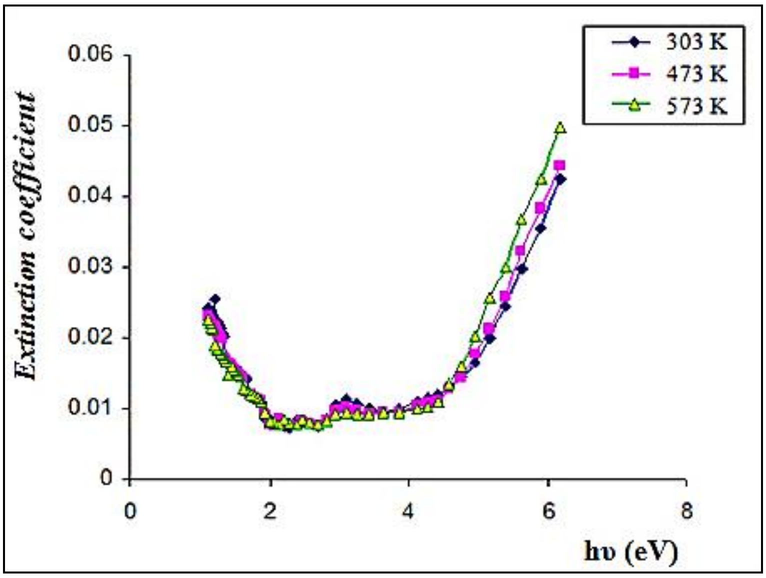

Figure (6): Relationship between extinction coefficient with photon energy for different annealing temperatures

7. Reflective index (n):

The reflective index was found using the following relationship (Sagadevan & Podder, 2023).

$$n = \frac{1+\sqrt{R}}{1-\sqrt{R}} \dots\dots\dots\dots\dots.(5)$$

Figure (7) shows the value of refractive index increases with increase photon energy. We can also notice from figure (7) that the value of refractive index increases with increase the annealing. Increased annealing of the material leads to an increase in the material's density, and thus an increase in the refractive index. The refractive index values of the deposited films vary in the range (1.35 – 1.52) at photon energy $(h\nu = 2.5)$(λ= 530nm). These values agree well with the value (1.36) reported by (Cremona, Pelli, & Pereira, 2003) for the same wavelength.

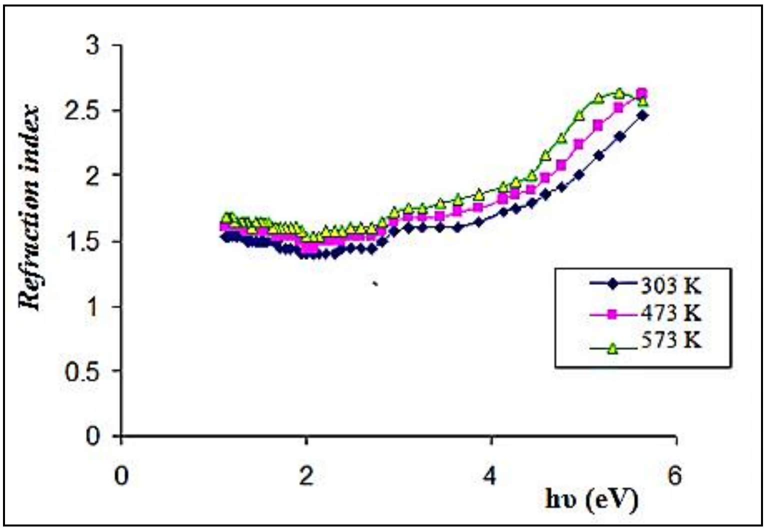

Figure (7): Relationship between refractive index with photon energy for different annealing temperatures

Conclusion:

1. All the deposited (LiF) thin films have high transmittance values (80% to 95%) in the (visible and near infrared region), which provides the possibility of using these films as optical window.
2. All (LiF) thin films have a high absorption coefficient ($\alpha > 10^4\ cm$). This suggests that they have direct electronic transitions at wavelengths of (200 – 1100) nm, and thus have energy gap for direct transition.
3. The energy gap decreasing with increasing annealing temperature.
4. The values of (extinction coefficient and absorption coefficient) increases with increasing annealing temperature.

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دراسة تأثير درجة حرارة التلدين على بعض الخصائص البصرية للأغشية الرقيقة من فلوريد الليثيوم

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مستخلص البحث :

تم تحضير أغشية رقيقة من فلوريد الليثيوم (LiF) بالتبخير الحراري تحت الفراغ (TEV) على ركيزة زجاجية عند درجة حرارة الغرفة (303 كلفن). بعد ذلك، عولجت الأغشية حراريًا عند درجة حرارة (473، 573 كلفن) لمدة ساعة واحدة، بسماكة (400 ± 10 نانومتر). دُرست الخصائص البصرية لأغشية فلوريد الليثيوم الرقيقة ضمن نطاق الأطوال الموجية (200-1100 نانومتر). وُجد أن لها نفاذية عالية تتراوح بين (80-95%)، وامتصاصًا وانعكاسًا منخفضين في منطقة الضوء المرئي والأشعة تحت الحمراء القريبة. حُسبت قيمة فجوة الطاقة، ووُجد أنها تساوي (5.1 إلكترون فولت)، وأن فجوة الطاقة تنخفض إلى (5 إلكترون فولت) مع ارتفاع درجة حرارة التلدين. كما حُسبت قيم بعض الثوابت البصرية مثل معامل الامتصاص (α)، ومعامل الانقراض (K_o)، ومعامل الانعكاس (n).

الكلمات المفتاحية :فلوريد الليثيوم (LiF)، الخصائص البصرية (OP)، التبخير الحراري في الفراغ (TEV)، درجة حرارة التلدين (AT).

ملاحظة : هل البحث مستل من رسالة ماجستير او اطروحة دكتوراه ؟ نعم : كلا : كلا