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Substrate Temperature Influence on Optical Properties of C_{60} Thin Films Within the Visible Range

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Abstract
Fullerene thin films of about 200 nm thicknesses have been deposited by thermal evaporation method on soda lime glass at substrate temperature 303 and 403K under pressure about 10^{-5} mbar. This study concentrated on the influence of substrate temperature on the optical properties of C_{60} thin films within the visible range. Optical characterization has been carried out at room temperature using the absorption spectra, at normal incidence, in range (200-900) nm.

The absorption and extinction coefficients of the samples have been evaluated according to the variation in the UV- Visible spectrum. Increasing substrate temperature causes decreasing in optical band gap energy, for direct allowed transitions, and slightly changing in refractive index. This incident was due to the reducing of interatomic intervals, which may be correlating a decrease in the amplitude of atomic vibrations around their equilibrium sites.

Keywords: Absorption, Extinction Coefficient, Refractive Index, Energy Band gap.

تأثير درجة حرارة الركيزة على الخصائص البصرية لأغشية C_{60} الرقيقة ضمن المدى المرئي

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الخلاصة
تم ترسيب الأغشية الرقيقة من الفوليرين بسمك حوالي 200 نانومتر بواسطة طريقة التبخير الحراري على زجاج الجير الصودا عند درجة حرارة الركيزة 303 و 403 كلفن تحت ضغط حوالي 5^{-10} ملي بار. ركزت هذه الدراسة على تأثير درجة حرارة الركيزة على الخواص البصرية للأغشية الرقيقة C_{60} ضمن المدى المرئي. تم إجراء التوصيف البصري عند درجة حرارة الغرفة باستخدام أطياف الامتصاص، لسقوط الاشعة العمودي ، في نطاق (200–900) نانومتر.

تم قياس معاملات الامتصاص والخمود من العينات وفقا لتغييرات الطيف المرئي– الفوق البنفسجي للأشعة. تؤدي زيادة درجة حرارة الركيزة إلى تقليل فجوة الطاقة البصرية، للانتقال المباشر المسموح، وتغيرًا طفيفًا في معامل الانكسار. قد يكون هذا التصرف بسبب تقلص المسافات بين الذرات، والتي قد تكون مرتبطة بانخفاض في سعة الاهتزازات الذرية حول مواقع الاستقرار الخاصة بها.

Introduction
There is flexibility in synthesizing new molecules of organic semiconductors through inducing a change in the electronic properties of them by changing either the functional groups or atomic arrangement, and hence makes these organic semiconductors good candidates for optoelectronic applications [1].

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Fullerenes molecules arrange at high symmetric sites. They can be collected in a solid structure like a spherical cage to form a new class of molecular combination semi to a football. They have wide applications in the field of superconductors, electronics, magnetics, medicine, biochemistry and physics of optoelectronics [2, 3]. C_{60} thin films which show a significant optical performance is mostly used in electronic devices such as light emitting diodes [4] and solar cells [5]. That's why there is an increasing interest in these materials over the last decades. Fullerene is an n-type, air stable, an organic semiconductor with applications in field effect devices and photovoltaics. Optical absorption properties in thin film form are important parameters for the suitability of a material for opto-electronic device applications. There are a lot of studies consider solids based on fullerenes as semiconductor materials and collect all physical properties of them [6, 7].

Morphology and structural properties had been studied in other paper of this author [8]. In this study, the influence of substrate temperature on Fullerene optical properties has been studied. In the visible region, the absorption band for the thin film is known as the Q-band, and also in the near UV region the B-band.

Experiment

Powder of C_{60} 99% (Sigma Aldrich), with melting point 800 K, is put in a molybdenum boat heated with DC current governed by a variac transformer. The transformer is capable to supply the necessary current for heating the molybdenum boat which it was used for the evaporation operation. Before starting evaporation operation and to get rid of unuseful gases the evaporated material was guardedly degassed for 0.5 hour while the shutter was closed. Thin films of C_{60} were deposited at temperatures 303 and 403 ºK on a cleaned soda lime glass substrates through pressure about 10^{-5} mbar using a (15 F6 Hind Hivac) evaporation system. The thin film was deposited at a rate of 3-5 Aº/s while it has been sublimating from a molybdenum boat. The evaporation rate was maintained constant through every evaporations process. The films thicknesses were 200 nm which was measured by a device named Quartz crystal monitor. This manner is used for synthesis C_{60} thin film on a cleaned soda lime glass substrate. The film seems to have a good adhesion with substrate. The absorption spectra of the C_{60} films were measured at room temperature using a double-beam spectrometer (RAY LIGH, UV – 2100).

Results and discussion: Optical behavior of material was used to determine its optical constants. The Coefficient of absorption α was calculated from the formula [9];

$\alpha = 2.303A / \boldsymbol{\tau}$

Where $\boldsymbol{\tau}$ is the film thickness and A is the absorbance, the absorption coefficient spectra of thin films deposited at both temperatures have been shown in Figure-1.

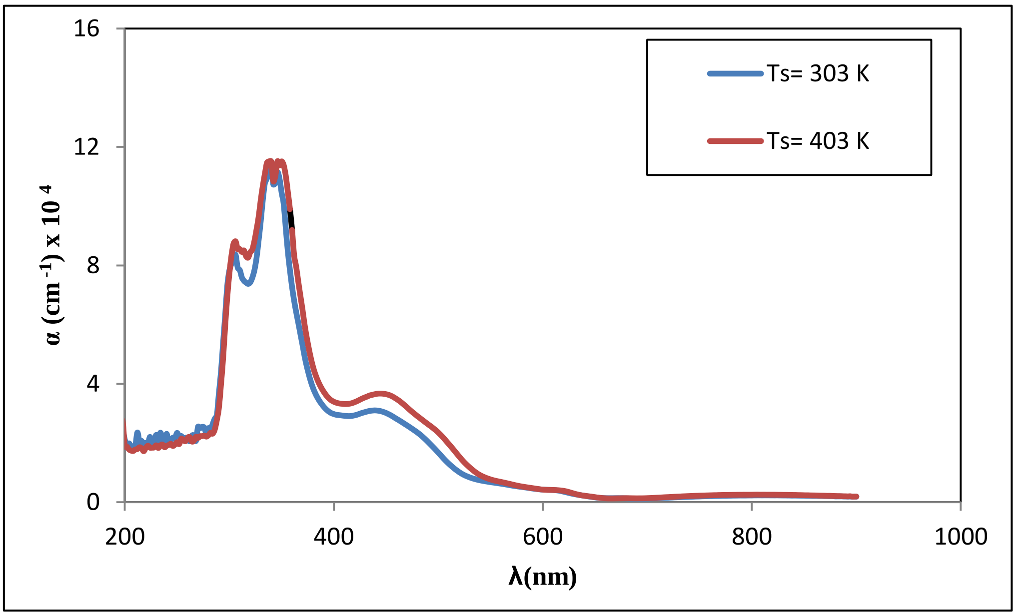

Figure 1-The absorption coefficient as a function of wavelength for C_{60} films deposited at 303K and 403 K.

The optical transmittance spectra of thin C_{60} films deposited at both substrate temperatures have been shown in Figure-2.

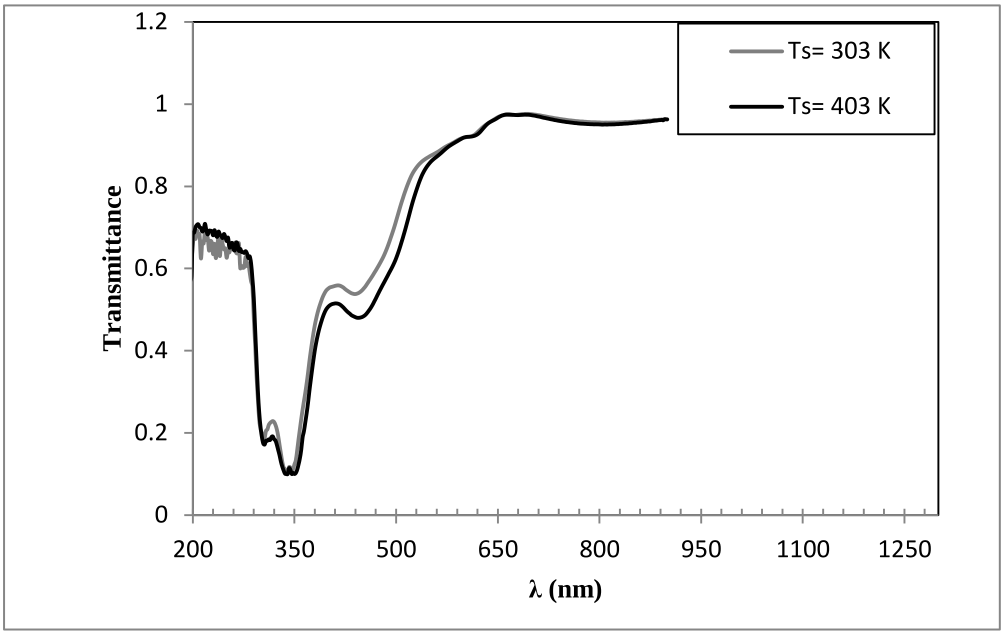

Figure 2-Transmittance vs wavelength for C_{60} films deposited at 303K and 403K.

Annealing process often increases the crystallinity of the film, so the absorbance will be increased too as seen in two figures above. Since C60 is organic material, so it cannot stand for high temperatures, and if it reaches decomposition temperature it will lose its characteristics.
Band gap was calculated using Tauc relation [10];

$$\alpha h \nu = \boldsymbol{\beta} (h \nu - E_g)^n$$

Where **β** is the energy band edge parameter and the value of n defines the nature of optical transition (n = 0.5 refers to direct transition and n = 2 refers to indirect transition). Variation between $(\alpha h\nu)^2$ and hν has been recorded in Figure-3 and Figure-4.

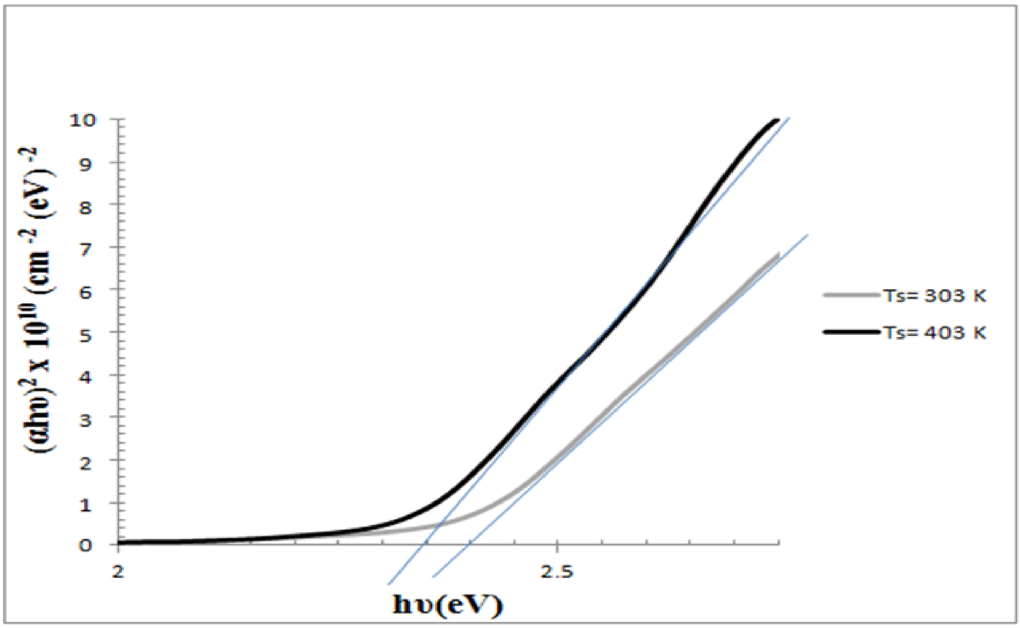

Figure 3-Variation of $(\alpha h\nu)^2$ with hν for films deposited at 303K and 403K.(Onset energy gap).

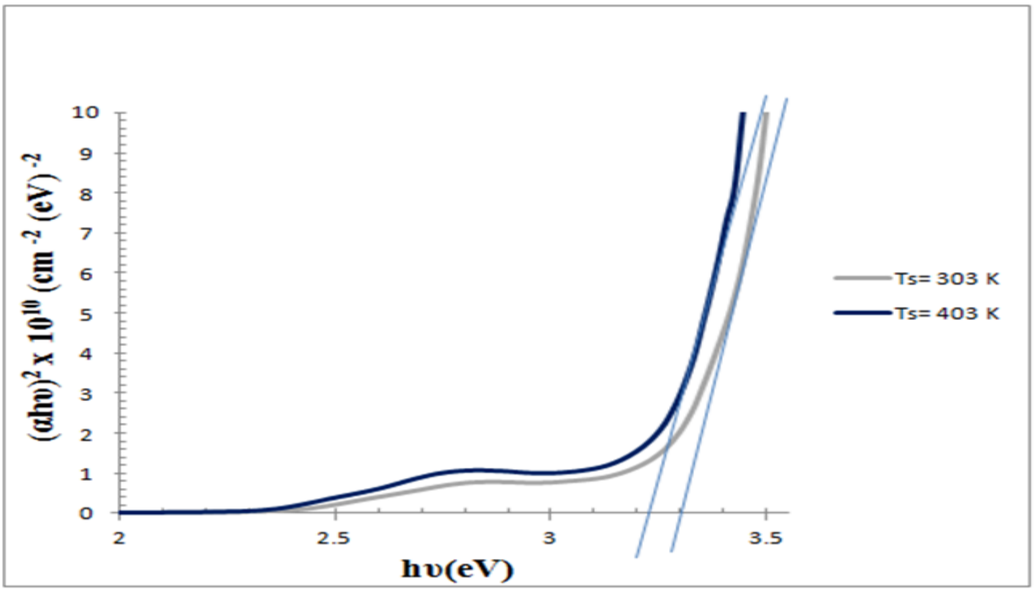

Figure 4-Variation of $(\alpha h\nu)^2$ with hν for films deposited at 303K and 403K. (Fundamental energy gap)

The linearity of the dependence indicates direct transitions. The extension of the linear regions to α h ν = 0 gives the value of the energy band gap. These values calculated for films deposited at different substrate temperatures are listed in Table-1.

Table 1-he variations in optical energy gap with substrate temperature for C_{60} thin films

Substrate Temperature K	E_g (eV)	
	onset (Q-band)	**fundamental (B-band)**
303	**2.4**	**3.3**
403	**2.35**	**3.2**

The results show that both onset and fundamental energy gaps are decreased from 2.40 eV for the film deposited at 303K to 2.35 eV for film deposited at 403K corresponds to the so-called onset energy gap (Q-band) while the absorption energy gap decreased from 3.30 eV for film deposited at 303K to 3.20 eV for film deposited at 403K corresponds to the fundamental energy gap (B-band).

This can be referred to the lowering of the interatomic spacing which may be correlating with a decrease in the amplitude of atomic vibrations around their equilibrium sites [11]. According to this observation, we conclude that C_{60} film becomes more conducting when it deposited at a high temperature substrate. It can be attributed also to the upward shift in Fermi level toward the conduction band whose position is determined by the distribution of electrons through the localized states [12].

Optical properties of a material depend upon the interaction of the material with the electric field of the electromagnetic wave. The extinction coefficient is a measure of damping of incident wave in the material [13].

The extinction coefficient has been calculated by using the relation:

$K = \alpha \lambda / 4\pi$

Both the absorption and extinction coefficients are found to vary with incident photon energy. The extinction coefficient depends directly on absorption coefficient. Variation of extinction coefficient with wave length for the samples at different substrate temperatures is shown in Figure-5.

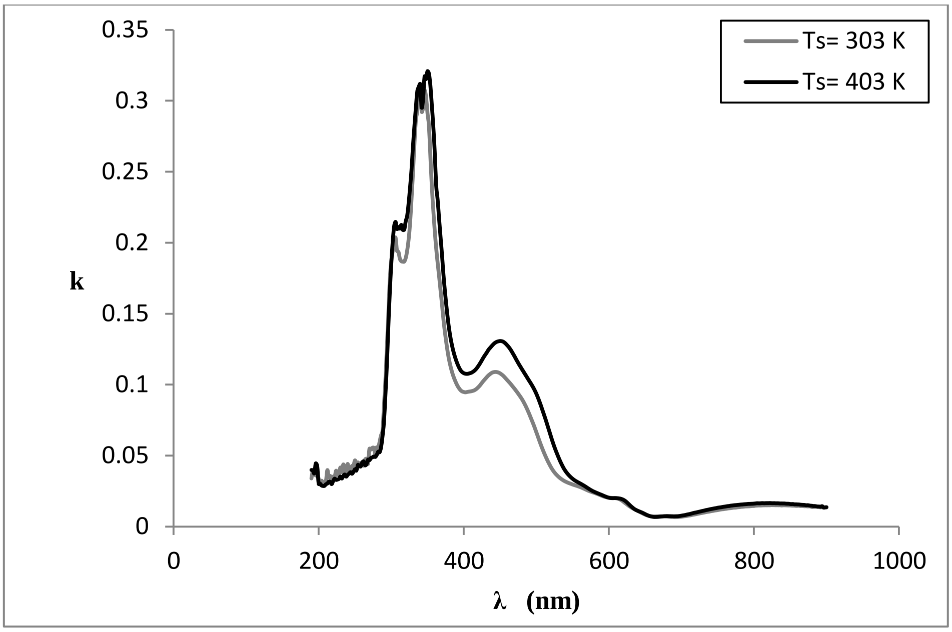

Figure 5-Extinction coefficient as a function of wavelength for C_{60} films deposited at 303K and 403K.

From the reflectance R data refractive index of C_{60} was estimated using the following formula [14]:

$$n = \sqrt{\frac{4R}{(R-1)^2} - k^2} - \frac{R+1}{R-1}$$

Variations of the refractive index with the wave length in the range 400–500 nm have been shown in fig.6.

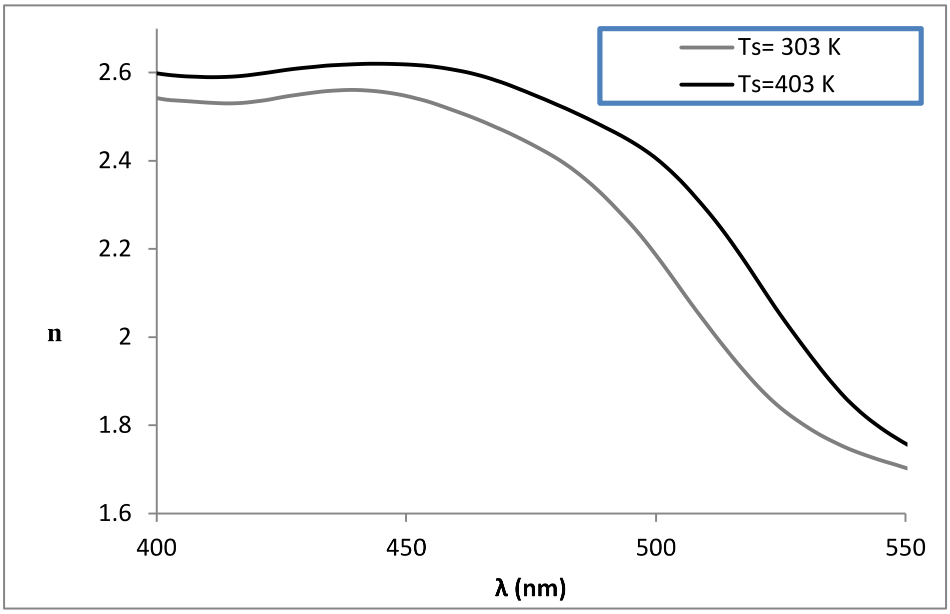

Figure 6-Dependence of refractive index with wave length for C60 films deposited at 303K and 403K.

The refractive index in general increases with increasing of substrate temperature as shown in Figure-6. It was attributed to the increase of absorbance of C_{60} thin films i.e. increasing of interactions between incident photons and C_{60} molecules.

By using the relations: $\varepsilon_1 = n^2 - k^2$ and $\varepsilon_2 = 2nk$ the real and imaginary part of dielectric constant were evaluated [14] which show that the dielectric constants depend on the value of the refractive index and also the dielectric loss depends mainly on the values of extinction coefficient. The variation of the real and imaginary parts of dielectric constants values with the variation of wave length have been shown in Figures-7 and 8.

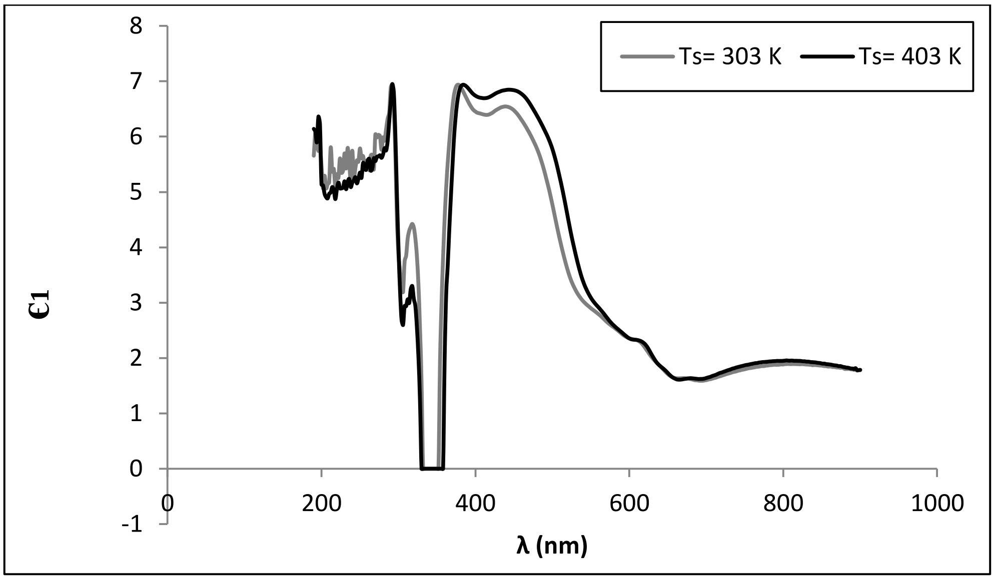

Figure 7-Dependence of the real part of dielectric constant with wave length for C_{60} thin films deposited at 303K and 403K.

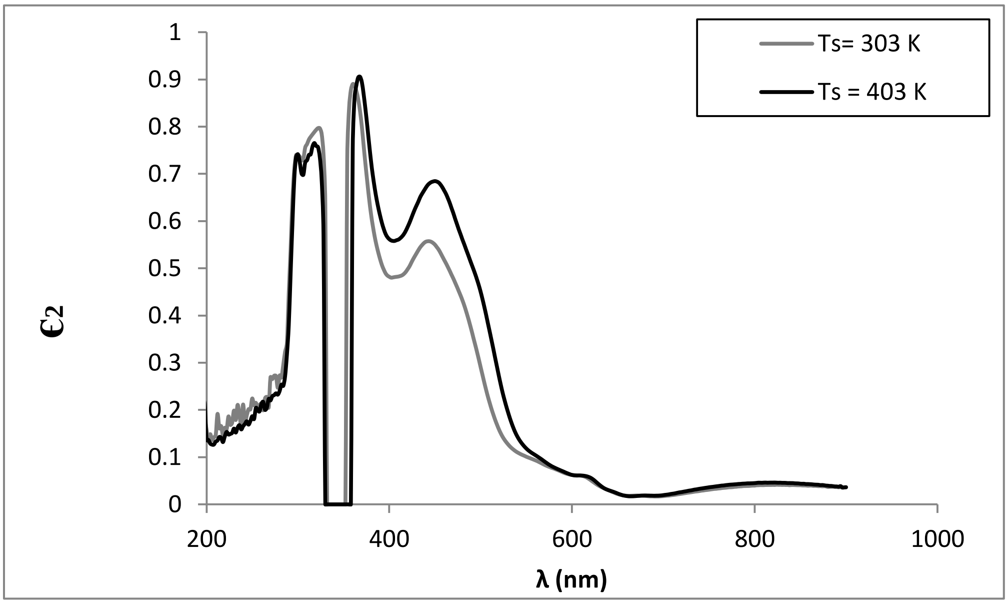

Figure 8-Dependence of the imaginary part of dielectric constant with wave length for C_{60} thin films deposited at 303K and 403K.

Conclusion

Absorption and extinction coefficients of C_{60} thin films vary with wavelength and they increase with the increasing of substrate temperature. Refractive index through the range (400–550) nm was increased with the increasing of substrate temperature. The optical energy gap decreases with the increasing of substrate temperature, this incident was referred to the reducing of interatomic spacing of C_{60} structure, which may be correlated to a decrease in the amplitude of atomic vibrations around their equilibrium sites. It is possible to consider C_{60} as a good candidate for optoelectronic applications.

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