

**THERMAL ANALYSIS OF GOLD NANOPARTICLES IN
POLYMER SOLUBLE WHICH ARE IN VACUUM CONDITION
AND EXPOSED TO LASER BEAM GAUSSIAN PULSE WITH A
WAVELENGTH OF 532 NM FOR CONSTRUCTION OF
ELECTRO-OPTICAL DEVICES OLED AND OFET**

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ABSTRACT. Today, gold nanoparticles due to their special properties have many applications in different fields of electronic industry and in particular in electro-optics. One of these applications is the layer deposition of organic materials in the process of constructing electro-optical device OLED, using gold nanoparticles. To achieve this, the characteristics of melting and desorption temperatures for gold nanoparticles in polymer soluble, which are exposed to a pulse laser with a wavelength of 532 nm is used and finally, the process of layer deposition is achieved. In this paper the thermal behavior of gold nanoparticles in polymer soluble, which are in the vacuum conditions and interactions with pulsed laser light, is studied and the results thus obtained explained and compared with experimental result.

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1. INTRODUCTION

Today's organic semiconductor materials have found many applications in the electronics industry [5, 9]. Examples of this application are flexible displays, flexible solar cells and organic field effect transistor (OFET)[1, 10]. There are various methods for making this electro-optical devices based on organic materials. Semiconductor material of the small molecules are first evaporation and then with using the deposition methods such as vapor phase deposition and organic vapor phase deposition (OVPD) the deposition will occur[2]. But the semiconductor material of the polymer with its solvent and by methods such as inkjet printing and spin coating, the process of deposition occur[3, 11]. In recently presented method for deposition of semiconductor polymer and sintering of gold nanoparticles for construction of electro-optical devices OLED and OFET, used the some of properties like the melting temperature, desorption temperature and plasmonic resonance of gold nanoparticles which are in a polymer soluble (hexanethiol). In this method by applying a pulse laser with 532 nm wavelength on the soluble of gold nanoparticles and polymer (donor multilayer), nanoparticles melt and cause melting and deposition the polymer under the nanoparticles soluble (for example Alq3) on the sub layer (Figure1). Using this method can be performed with nanometer deposition [8]. In this method, laser beam with a wavelength of 532 nm by using a lens focus on the solution of gold nanoparticles and polymers. Gold nanoparticles absorb the laser beam with this wavelength and its temperature increases[6]. Laser used as a local heat source to further minimize the thermal damage and also to enhance the resolution of the process. Local laser heating is advantageous due to the reduced heat affected zone and more efficient energy deposition induced by the strong absorption peak generated by surface plasmon oscillation modes around the 532 nm wavelength. This is in turn important for application on polymer substrates with low transition/melting temperature that is sensitive to blanket heating in a furnace or on a heater. Gaussian beam Nd: YAG Laser with a wavelength of 532 nm and

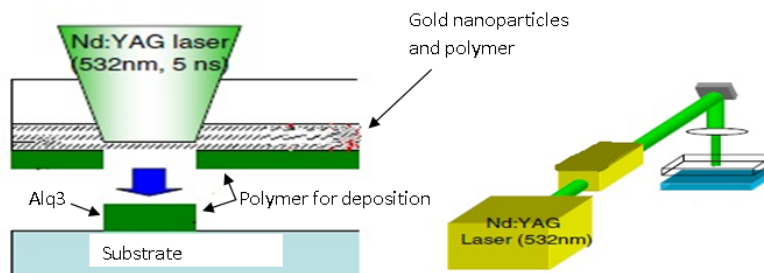


FIGURE 1. setup of method that use for deposition of polymer material by gold nanoparticles [8].

pulse width of 5 ns FWHM is applied on the substrate donor which composed of three layers :

- 1- Transparent layer (borosilicate glass slide)
- 2- Laser to heat conversion layer
- 3- Polymer layer of OLED for example Alq3 In this experiment two types of monolayer of gold were used as a laser to heat conversion layer : type I : Au nanoparticles and type II : Au thin film (Figure 2)[8] . Optical property measurements by spec-

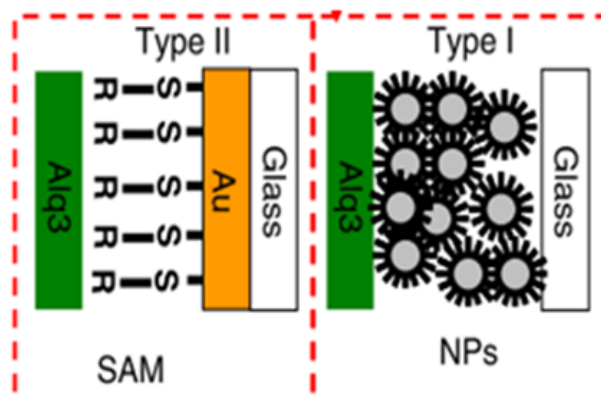


FIGURE 2. Magnified schematic illustration of the two types of donor multilayer [8].

troscopic ellipsometry show that the gold nanoparticles at 532 nm Nd YAG laser

have strong absorption while the polymer material has little absorption [8]. (Figure 4).

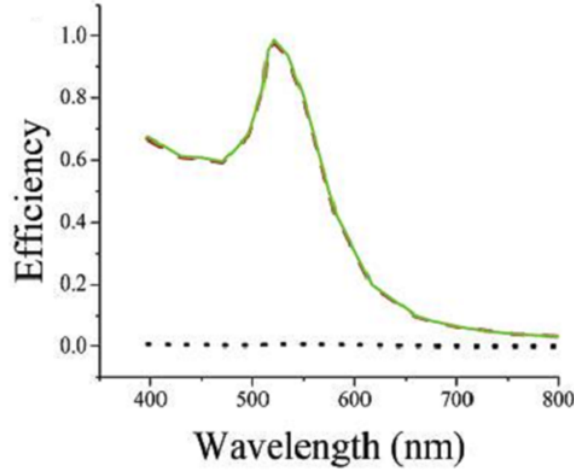


FIGURE 3. Calculated spectra of the efficiency of absorption (red dashed), scattering (black dotted), and extinction (green solid) for gold nanospheres with $R= 30$ nm [7].

Melting temperature of gold nanoparticles is about 150 degrees centigrade. It also has a desorption temperature between 150 to 300 $^{\circ}C$ which desorption temperature is the temperature that when the gold nanoparticles reaches to it, a layer of polymer that is attached to the nanoparticles, separated and placed on the substrate. Gold nanoparticles have the highest absorption at the wave length of 532 nm[6]. By applying a pulse laser with 530 nm wavelength on the soluble of gold nanoparticles, the temperature of gold nanoparticles increases and reach the melting and desorption temperatures and finally the process of deposition is done[8].

2. THE THEORETICAL MODEL

For study the thermal behavior of gold nanoparticles that soluble in polymer which interaction with pulsed laser, we use the Fourier heat transfer equation that as follows [12]:

$$\nabla^2 T - \frac{1}{a} \frac{\partial T}{\partial t} = \frac{1}{\rho c_p} Q \quad (1)$$

In this equation $Q = \alpha I$ amount of heat absorbed and a , ρ , c_p , α and I are defined thermal diffusion coefficient, density, specific heat capacity, coefficient of absorption of laser beam and intensity of laser, respectively. One of the methods to solve the differential equation is Green's function that in this paper through the boundary condition of problem, we have used this method to solve the heat transfer equation which it is a differential equation [4]. Green's function is to answer the following equation:

$$\nabla^2 G(x, \acute{x}, y, \acute{y}, t, \acute{t}) = \delta(r - \acute{r})\delta(t - \acute{t}) = \delta(x - \acute{x})\delta(y - \acute{y})\delta(z - \acute{z})\delta(t - \acute{t}) \quad (2)$$

After calculating the Green's function, the temperature T is obtained from the following equation:

$$T(r, \acute{r}, t, \acute{t}) = \int \int G(r, \acute{r}, t, \acute{t}) \frac{\alpha}{\rho c_p} I(\acute{x}, \acute{y}) d^3 \acute{r} d\acute{t} \quad (3)$$

Laser intensity I for the Gaussian pulse is as follows:

$$I \frac{2E_0}{t_0 \pi w^2(z)} \exp\left(-2 \frac{x^2 + y^2}{w^2(z)}\right) \exp(-\alpha z) \quad (4)$$

In this equation t_0 and E_0 are width and pulse energy lasers and ω_z is laser beam cross section on the surface of polymer and nanoparticles. If the height of the polymer and nanoparticles solution and polymer that we want it to deposition are L_1 and L_2 respectively and low pressure environment be considered, heat flux transferred in the $z = 0$ and $z = L_1 + L_2 = N$ will be zero, so:

$$\frac{dG}{dz}|_{z=0} = 0 \quad , \quad \frac{dG}{dz}|_{z=N} = 0 \quad (5)$$

In following for the calculation of Green's function, taking into account the above boundary conditions the solution of the nanoparticles into two areas $0 < z < \acute{z}$ and $\acute{z} < z < L_1$. With consider continuity and discontinuity of the Green's function and its derivative in $z = \acute{z}$ and continuity of Green's function and its derivative in $\acute{z} = L_1$, Green's function for the three regions, are as follows: (A) For the area

$0 < z < \acute{z}$:

$$\begin{aligned}
 G_1(x, \acute{x}, y, \acute{y}, z, \acute{z}, t, \acute{t}) &= 642 \times 10^6 \sqrt{\frac{\pi}{2}} a e^{-a(\acute{t}-t)(2.26 \times 10^{13})} \\
 &\cos[4753661.91z] \times \cos[4753661.91(L_1 - \acute{z})] \left[\frac{1}{2a(\acute{t}-t)} - \frac{(x - \acute{x})^2 + (y - \acute{y})^2}{8[a(t - \acute{t})]^2} \right] \\
 &- 27.3a \sqrt{\frac{\pi}{2}} \times 10^4 \times e^{-a(\acute{t}-t)(2.26 \times 10^{13})} \sin[4753661.91(L_1 - \acute{z})] \times \cos[4753661.91z] \\
 &\left[\frac{1}{2a(\acute{t}-t)} - \frac{(x - \acute{x})^2 + (y - \acute{y})^2}{8[a(t - \acute{t})]^2} \right]
 \end{aligned} \tag{6}$$

(B) For the area $\acute{z} < z < L_1$:

$$\begin{aligned}
 G_1(x, \acute{x}, y, \acute{y}, z, \acute{z}, t, \acute{t}) &= 642 \times 10^6 \sqrt{\frac{\pi}{2}} a e^{-a(\acute{t}-t)(2.26 \times 10^{13})} \\
 &\cos[4753661.91\acute{z}] \times \cos[4753661.91(L_1 - z)] \left[\frac{1}{2a(\acute{t}-t)} - \frac{(x - \acute{x})^2 + (y - \acute{y})^2}{8[a(t - \acute{t})]^2} \right] \\
 &- 27.3a \sqrt{\frac{\pi}{2}} \times 10^4 \times e^{-a(\acute{t}-t)(2.26 \times 10^{13})} \sin[4753661.91(L_1 - z)] \times \cos[4753661.91\acute{z}] \\
 &\left[\frac{1}{2a(\acute{t}-t)} - \frac{(x - \acute{x})^2 + (y - \acute{y})^2}{8[a(t - \acute{t})]^2} \right]
 \end{aligned} \tag{7}$$

(C) For the area $L_1 < z < N$:

$$\begin{aligned}
 G_2(x, \acute{x}, y, \acute{y}, z, \acute{z}, t, \acute{t}) &= 642 \times 10^6 \sqrt{\frac{\pi}{2}} a e^{-a(\acute{t}-t)(2.26 \times 10^{13})} \\
 &\cos[4753661.91\acute{z}] \times \cos[4753661.91(N - z)] \left[\frac{1}{2a(\acute{t}-t)} - \frac{(x - \acute{x})^2 + (y - \acute{y})^2}{8[a(t - \acute{t})]^2} \right]
 \end{aligned} \tag{8}$$

Now consider the equation (3) temperature for the above three regions are as follows:

(A) For the area $0 < z < \acute{z}$:

$$\begin{aligned}
 T_1(r, \acute{r}, t, \acute{t}) &= \frac{\alpha V E_0 a}{\rho c t_0 w^2 \sqrt{2\pi}} \times 10^6 \sum_j \cos[4753661.91z] \times \frac{Ei[-2.26 \times 10^{13}]a(\acute{t}_j - t)}{2a} + \\
 &\frac{(\acute{x} - x)^2 + (\acute{y} - y)^2}{8a^2} \times \frac{e^{-2.26 \times 10^{13}a(\acute{t}_j - t)}}{\acute{t}_j - t} + 2.26 \times 10^{13}aEi[-2.26 \times 10^{13}a(\acute{t}_j - t)] \times \\
 &(1284 \cos[4753661.91(L_1 - \acute{z}_j)]) - 54.6 \sin[4753661.91(L_1 - \acute{z}_j)]
 \end{aligned} \tag{9}$$

(B) For the area $\dot{z} < z < L_1$:

$$T_2(r, \dot{r}, t, \dot{t}) = 1284.12 \frac{\alpha V E_0 a}{\rho c t_0 w^2 \sqrt{2\pi}} \times 10^6 \cos[4753661.91(N - z)] \times \quad (10)$$

$$\sum_j \cos[4753661.91 \dot{z}_j] \left[\frac{Ei[-2.26 \times 10^{13}] a(\dot{t}_j - t)}{2a} + \right.$$

$$\left. \frac{(\dot{x} - x)^2 + (\dot{y} - y)^2}{8a^2} \times \frac{e^{-2.26 \times 10^{13} a(\dot{t}_j - t)}}{\dot{t}_j - t} + \right.$$

$$\left. 2.26 \times 10^{13} a Ei[-2.26 \times 10^{13} a(\dot{t}_j - t)] \right]$$

In this equations V is volume of gold nanoparticles. Figure 4 shows the temperature

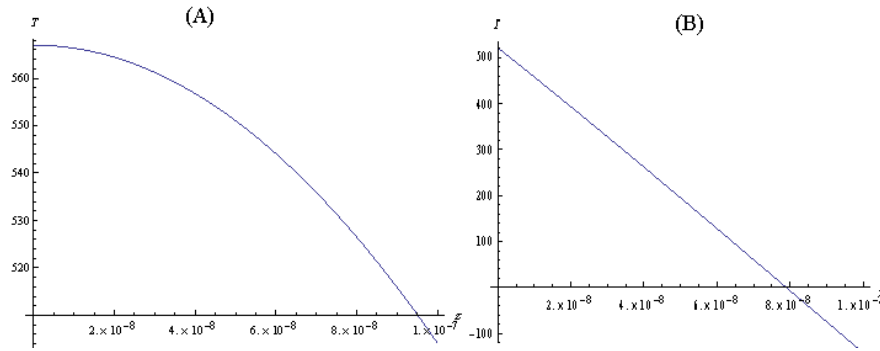


FIGURE 4. Temperature (K) profile of areas A) $0 < z < \dot{z}$ and B) $\dot{z} < z < L_1$ that they are interaction with laser pulsed with 532 nm wavelength.

variation of the medium polymer and nanoparticles that temperature equations are obtained by using the Green's function method. As can be seen, the temperature on the surface of a polymer and nanoparticles is about 280°C which that is useful temperature for deposition of polymer that use for OLED devices that confirmed by experimental results [8]. The $0.90.9\text{ mm}^2$ Alq3 square pattern from type I donor showed strong decrease in photoluminescence intensity when the temperature exceeds approximately 350°C [C in Fig. 5] while same sized, laser transferred pattern [B in Fig. 5] showed similar photoluminescence intensity with original Alq3 pattern [A in Fig. 5] Therefore, the temperature of Alq3 layer during the deposition process is not more than 350°C [8]. So the temperature created in this method should being about 300 centigrade degree and should not being more than 350°C

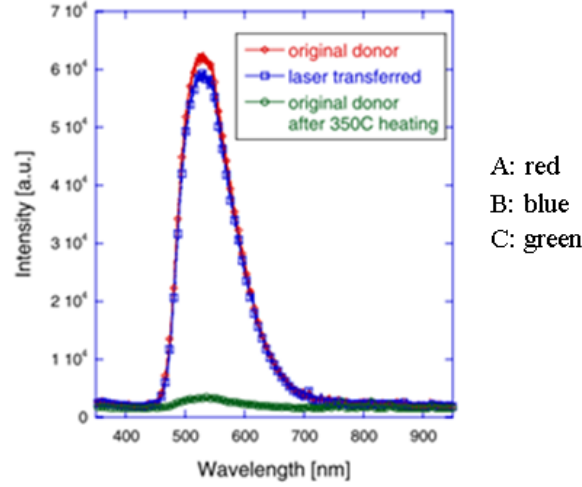


FIGURE 5. Photoluminescence spectral intensity of Alq3 patterns (A: original donor, B: laser transferred, C: original donor after 350 $^{\circ}C$ heating) [8].

centigrade degree that our calculations show this. In this paper we have considered the same as the radius of the nanoparticles (30 nm) Whereas in the general case and in experimental conditions nanoparticle radius can be considered variable (between 30 and 40 nm).

3. CONCLUSION

According to figure 4, by applying the laser light beam to the polymer solution and nanoparticles, the temperature that created due to absorption of laser light by gold nanoparticles is about 280 $^{\circ}C$ which that is the useful temperature for the deposition process that confirmed by experimental results that are in paper of reference [8] and also said in introduction of this paper (Desorption temperature between 150 to 300 $^{\circ}C$ which desorption temperature is the temperature that when the gold nanoparticles reaches to it, a layer of polymer that is attached to the nanoparticles, separated and placed on the substrate. By applying a pulse laser with 530 nm wavelength on the soluble of gold nanoparticles, the temperature of gold nanoparticles increases and reach the melting and desorption temperatures and finally the process of deposition is done). Heating caused by laser light beam to a solution of polymer

and nanoparticles, produce the temperatures needed to process of deposition for $z=120$ nm. Our calculations have been done without considering the interaction between gold nanoparticles. If the interaction between gold nanoparticles and heat transfer occurring between the nanoparticles also consider, this distance will be more height and thickness of the deposition by using this method will increase.

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