# Simulation of Laser Thermal Interaction with Titanium Dioxide /Polyvinyl Alcohol Nanocomposite Thin Films

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**Abstract**: The aim of this work is to use the computational simulation to define the operational conditions to achieve the desired process. The diagnostic tests were used to guide the experiment where PVA composites doped with Titanium dioxide nanoparticles were irradiated with nitrogen laser in order to modify its properties. The temperature of the samples with different laser fluencies were simulated using finite element method, in COMSOL program, to predict the fluencies that is suitable to use for modification before reaching the decomposition temperature of the nanocomposite sample to make sure not to cause any damage. The optical and thermal properties were experimentally studied, and the results were used to define the absorption coefficient and the thermal conductivity of the studied nanocomposites

**Keywords**: Polymer nanocomposite; Simulation ; pulsed laser ; heat equation .

## 1. INTRODUCTION

There are various chemical and physical changes caused when materials exposed to electromagnetic radiation. The ability to use the laser to affect a specific and small spot have a great advantage to use in manufacturing integrated circuits and control properties.[1] Many researchers deal with the interaction of laser irradiation with doped polymer films. Laser was used to change the optical structural and thermal properties of polymers and polymers composites like crystalinity and band gap [2,3]. Laser effect on thin films can be simulated by numerical methods to define the operational conditions. Which included minimizing heat effect zone, reaching the melting point ,or reaching ablation threshold.

Computer-assisted technologies for product design usually based on numerical methods, that are able to solve a set of algebraic equations to obtain desired results, in determined boundary conditions of process. Numerical programs are used to calculate tensions, shifts, vibration, heat transfer, fluid flow, and other process parameters [4]

In this work, the COMSOL program is used to build a numerical model capable of simulating the heat transfer and predict the temperature distribution on a thin film of TiO$_2$/PVA nanocomposited after irradiated by Nitrogen pulsed laser . The aim of this work is to define the Laser dynamic range for modifying the prepared nanocomposites before damaging (i.e the temperature of the nanocomposite does not exceed decomposition temperature of the nanocomposite)

## 2. THE PROPERTIES OF THE STUDIED NANOCOMPOSITES

The optical properties of the TiO$_2$ /PVA prepared nanocomposites with different doping percentage (1.25, 2.5, 5, 7.5, 10 % TiO$_2$/PVA) were studied. The PVA Pure films have absorption band of wavelength λ=198 nm 208 nm and at 281 nm assigned [25], theses three absorption bands are followed by transparency region. It can be understood that the absorption of the Nitrogen laser is neglected since PVA does not have an absorption peak around 337 nm which is the wavelength of the Nitrogen laser. But in the case of the doped PVA films with TiO$_2$, a new absorption peak can be noticed around 388 nm which correspond to the absorption of the TiO$_2$ nanoparticles.It can be seen that the absorption increases by increasing the dopant in the matrix .Table (1) illustrate the absorption coefficient for each nanocomposite film .

## 3. LASER ABSORPTION IN TIO$_2$ /PVA NANOCOMPOSITE

Doping PVA polymer with TiO$_2$ nanoparticles increase the composite absorption of the Nitrogen laser. As the laser is absorbed mostly by the nanoparticles and not by the PVA chemical bonds , we can neglect the photochemical effect and consider the laser effect thermally. The absorbed part of the laser energy in the nanocomposite depend on its properties including reflectivity and absorption which both depend on the wavelength of the laser wavelength .To study the laser thermal effect and temperature distribution we be consider the absorbed laser energy as heat source which is given by [5]:

$$Q(r, t) = \alpha I_0(r, t)(1 - R) \exp(-\alpha z) \qquad (1)$$

Where α and R are the absorption coefficient and the reflectivity of the nanocomposite film at the laser wavelength . I is the laser power intensity which depend on time and on the beam shape (which is Gaussian in this case).

The last part of the equation is related to the fact that the laser energy absorption decrease exponentially with depth from the sample surface (z)[6]

$$I(z) = I_0 e^{-az} \qquad (2)$$

The penetration depth of the laser is related to the skin depth for the electromagnetic field

$$\delta = \frac{1}{\alpha} = \frac{\lambda}{4\pi n'(\lambda)} \qquad (3)$$

Where, n′ (λ) is the imaginary part of the complex index of the refraction of the material. δ is the shield depth of the electromagnetic radiation. The thin film of the nanocomposites in our case has 50μm thickness which is much smaller than the

penetration depth of the laser, so we can neglect the variation of laser energy with depth.

## 4. HEAT EQUATION
We used the COMSOL 4.3 to solve the following heat equation:

$$\nabla^2 T(r,t) + \frac{1}{k} Q(r,t) = \frac{1}{\alpha} \frac{\partial T(r,t)}{\partial t} \qquad (4)$$

And find the temperature distribution in order predict the laser intensity that could cause damage in the nanocomposite film which means to reach its decomposition temperature.

The prepared nanocomposite films were found to have more stability as the doping ratio increased, as was found by thermal studying of nanocomposites , the decomposition temperature($T_d$) is found to increase as illustrated in table (1) Thermal conductivity is a very important factor in the heat equation which is equal to 0.2 W/(m. K) for PVA but increases for the composites because of the $TiO_2$ doping which has a thermal conductivity about (3.62) W/(m. K) Maxwell calculated the effective thermal conductivity (ETC) of a random distribution of spheres in a continuous medium for low filler concentration [7] as:

$$k_e = k_m \frac{k_f + 2k_m + 2\varphi(k_f - k_m)}{k_f + 2k_m - \varphi(k_f - k_m)} \qquad (5)$$

Where $k_e$, $k_m$ and $k_f$ are effective thermal conductivity ,matrix thermal conductivity and thermal conductivity of fillers , respectively ,and $\varphi$ is the volume fraction of inclusions . The calculated values of thermal conductivity of the nanocomposites is illustrated in table (1)

**Table 1. experimental values of thermal conductivity, decomposition temperature and absorption coefficient for (λ=337nm)**

| Sample TiO$_2$/PVA (wt/wt %) | k [W/(m. K)] | $T_d$ [C° ] | α [cm-1] |
|---|---|---|---|
| 0 | 0.2 | 288 | 36.54 |
| 1.5% | 0.208 | 290 | 201.66 |
| 2.5% | 0.213 | 302 | 391.57 |
| 5% | 0.2269 | 304 | 475.81 |
| 7.5% | 0.2413 | 306 | 1023.60 |
| 10% | 0.3412 | 319 | 1093.16 |

## 5. SIMULATION AND RESULTS
We can solve the equation using the COMSOL. The films are having the dimension (3cm radius and 0.05 cm thickness). The initial temperature is (300 K). The laser energy (0.375 J), the spot radius (2 cm) ,pulse duration (15 ns ) ,and repetition rate (0.5 Hz).

The laser is modeled as pulsed heat source and inserted in the heating equation as general inward heat

$$Q = \alpha * hf(x, y, t) * gf(t) \left[\frac{W}{m2}\right] \qquad (6)$$

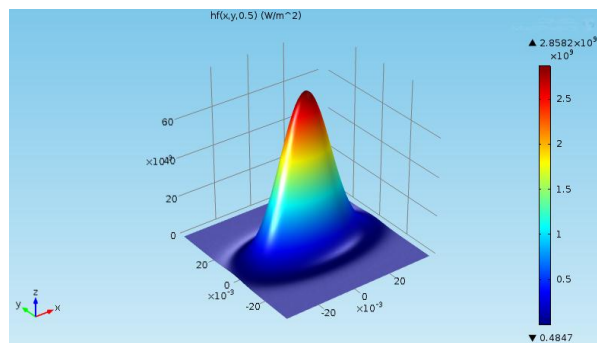Where α is the absorption coefficient,$hf(x, y, t)$ is the Gaussian laser beam as in figure (1)



Figure 1. Laser beam used in the simulation.

$gf(t)$ is the pulse function to represent the laser as pulsed train with pulse duration equals to 15 ns that represent the ON stage with the energy equals to 375mJ per pulse ,and pulse separation is 2 s which is the OFF stage


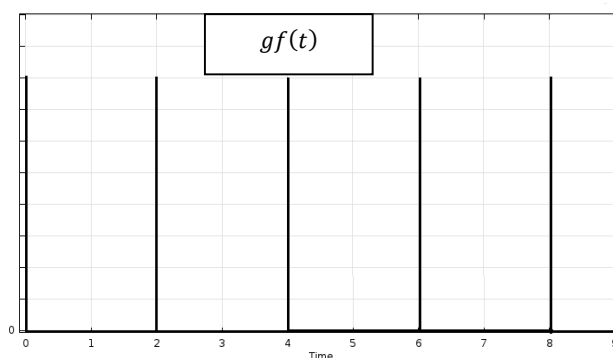
Figure 2.Pulsed function.

The simulations were performed for different number of pulses and for all the nanocomposite samples, until the maximum temperature reaches the decomposition temperature for the specific nanocomposite.
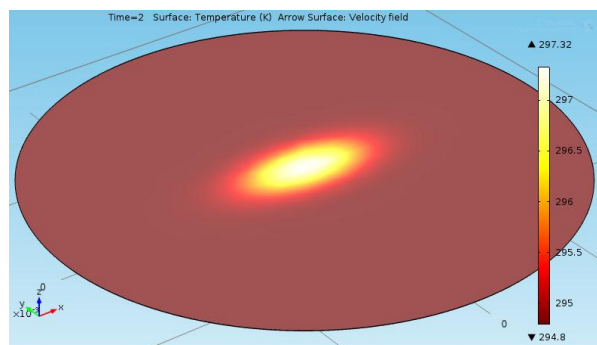


Figure 3. Temperature distribution within 2.5% sample after the first pulse.

Table (2) shows the simulation results. The maximum temperature after one pulse $T_{MAX}$ is found to increase as the nanocomposite doping is higher .As can be seen that after one pulse the maximum temperature increases from the initial temperature only (1°C) for PVA ,It is about (30° C) for the 10% nanocomposite sample.
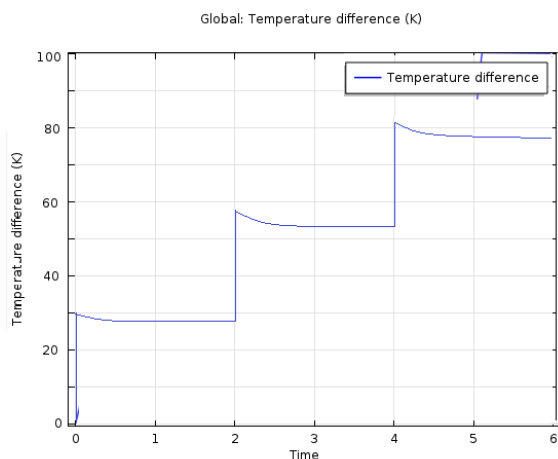
Figure 4. temperature change with time during simulation for sample 10%.

This can be understood since the absorption coefficient increases by increasing $TiO_2$ ratio. Heat diffusion in the thin film is faster for higher doped composites. It can be seen from the simulation that the PVA is hardly affected by the Nitrogen laser. Since the maximum temperature rose about 1°C and decreases before the next pulse .The laser gets more effective as the doping ration increases. And the decomposition temperature could be reached by lower fluencies as shown in table (2)

**Table 2. Simulation values for maximum temperature after one pulse and the damage threshold**

| Sample TiO₂/PVA (wt/wt %) | $T_{Max}$ [C] | Damage threshold [J ] |
|---|---|---|
| 0 | 1 | - |
| 1.5% | 5.5 | 1.611 |
| 2.5% | 11 | 0.836 |
| 5% | 13 | 0.716 |
| 7.5% | 28 | 0.328 |
| 10 % | 30 | 0.298 |

## 6. CONCLUSION

Laser heat effect on TiO2 /PVA nanocomposie thin films were simulated using COMSOL 4.3. The nanoparticles increases laser absorption in the nanocomposite thin films, which causes lower damage threshold for the nanocomposites by increasing doping percentage.

## 7. REFERENCES

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