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# The Effect of Temperature on the Optical and Analytical Properties of PET Polymer Used in Drinking Water Bottles

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**Abstract.** Polyethylene Terephthalate (PET) polymer has been utilized in many applications including, optoelectronics, radiology and food packaging due to its resistance to weak acid, organic solvents, and oils, in addition to low density and low cost. However, physical, mechanical and optical properties of PET are highly dependent on some ambient conditions like temperature since its thermal deformation temperature is 76° C. In this work, the effect of increasing the ambient temperature on the PET material used in the fabrication of plastic water bottles was studied optically and analytically. The optical attenuation coefficient was considered at different room temperature ranging from 25 °C to 45 °C emulating hot-sun-days ambient conditions in the laboratory. The elemental composition of the selected polymers was achieved using laser induced plasma spectroscopy (LIPS) technique showing Al emission line at 257.5 nm and CN emission line at 386.1nm in the sample-generated plasma. The optical attenuation coefficient has showed a dramatic increase with the temperature which may lead to leaching of some toxic elements existed in PET polymer into the bottle's water content during hot weather and cause health problems.

**Keywords:** PET; plastic water bottles; LIPS; optical attenuation

## 1. Introduction

Polyethylene terephthalate (PET) polymer has been conducted in variable applications including, optoelectronics [1], radiology [2] and food packaging [3]. It has been widely utilized in the fabrication of the containers produced for storing and carrying food and liquids due to its excellent thermal stability, low density and low cost [4]. In a very important study for Westerhoff, Paul, et al. [5], they showed that, Sb leaching from polyethylene terephthalate (PET) plastic used for bottled drinking water if the bottle exposed to the hot sun at a temperature above 22 °C. Therefore, it is essential to investigate the optical and structural properties of this type of polymers. The Pluta double-refracting computerized microscope



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and Opto-mechanical devices were the common methods to investigate the optical and structural characteristics of polyester fiber, e.g. the optical orientation, intrinsic birefringence and refractive indices. The obtained values were then compared with glycol-modified polyethylene terephthalate which showed less crystallinity [6].

Different spectroscopic techniques were employed to analyze the composition of the fumes resulting from combusted PET disposal at temperatures 500°C and 800 °C in airflow and in uncontrolled burning in air [7]. The results provided important information assessment of fire effluents danger effects on persons and the environment. The effect of menthol absorption by PET yoghurt drinks bottles was studied by Farhoodi et. al. [8] by using tensile test. The samples were initially immersed in 100 ppm menthol and stored for three months at 4°C, 25°C, and 45°C with periodic measurements of the modulus of elasticity, elongation and tensile strength. The investigated PET samples showed reduction in the modulus of elasticity and the tensile strength with increasing in the elongation at higher menthol concentrations.

In another study, the optical, chemical, and structural properties of PET polymer films were studied using UV-Vis, X-ray diffraction, and Fourier Transforms Infrared spectroscopy [9]. Their experimental observations suggested the potentiality of PET polymer as dosimeters using well reported protocols. The result of increasing the temperature and storage time of PET yoghurt bottles and their interaction with menthol was studied in [10]. The results showed increasing in the absorption levels with the storage time and temperature that affected the flavor stability of yoghurt drink.

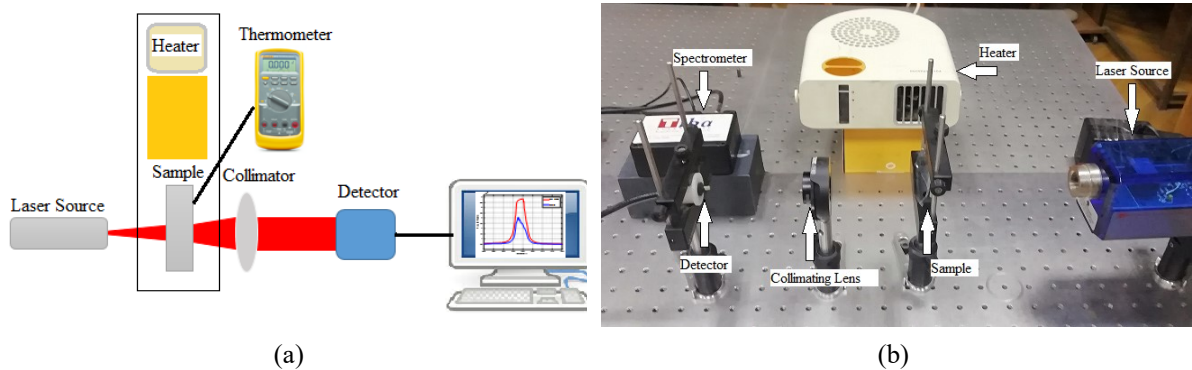
For elemental analysis of polymers, instead of conventional methods, the laser induced plasma spectroscopy “LIPS” technique has emerged as an efficient and non-destructive analytical technique that can provide multiple detection alternatives, non-contact measurement suitable for quick and online basic assessment of all material phases [11-14]. In LIPS technique, when a pulsed laser with high energy beam is focused on a material to create a plasma plume, several phenomena occur including: surface heating, vaporization, ablation, dissociation, and excitation [15]. Accordingly, subsequence processes occurred including: recombination processes of electrons with the created excited atoms, emissions lines for neutral atoms and atomic ions which are helpful to determine information about the plasma plume. A qualitative analysis is considered by spectroscopic investigation of the plasma spectral lines. By correlating the observed wavelengths of the plasma spectral lines with the NIST database, the identification of the examined sample elemental composition can be confirmed. The LIPS technique has also been widely used to investigate depth profile and to analyze the chemical mapping in common types of polymers. “High-density polyethylene “HDPE” and polycarbonate are examples” [16,17].

In this work, the effect of increasing the ambient temperature on the optical properties of PET polymer used in the fabrication of the commercial plastic water bottles has been studied. The elemental analysis of PET polymer has been considered using LIPS technique to detect trace elements in the sample. The optical attenuation coefficient is considered at different ambient temperatures.

## 2. Methods

### 2.1. The Optical Analysis

The examined sample is illuminated by a laser source model (IF VL08635) Industrial Fiber Optics, 8 mW output power and 635 nm wavelength, and the transmitted light is collected using a collimating lens. The output signal is then sent to a spectrometer (MSPM 1304) with a CCD based optical fiber detector (TOSHIBA TCD 1304 DG) then to a computer for processing. The collected data is then analyzed using Matlab 2017b program software. Figure 1 (a) shows a schematic draw of the experiment and (b) a lab photo of the optical setup.



**Figure 1:** Experimental setup for measuring collimated transmittance at different temperatures

Beer-Lambert law has been applied to calculate the decay in the optical intensity through the inspected sample. The optical attenuation through the studied material can be expressed as a function in its optical properties as [18][19].

$$I = I_0(1 - R_f)e^{-\mu_t d} \quad \dots\dots (1)$$

$$\text{where, } \mu_t = \mu_a + \mu_s \quad \text{and, } R_f = \left(\frac{n_1 - n_2}{n_1 + n_2}\right)^2 \quad \dots\dots (2)$$

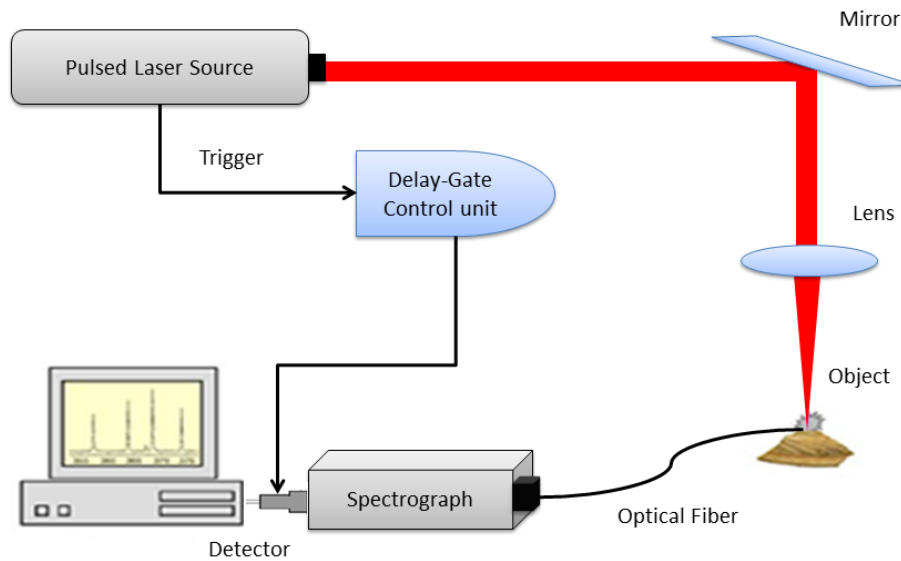
where,  $d$  is the sample thickness,  $I_0$  the incident light intensity,  $\mu_t$  is the total attenuation coefficient,  $R_f$  is the Fresnel reflection coefficient,  $n_1$  and  $n_2$  are the respective refractive indices of the two media.

Total attenuation coefficient  $\mu_t$  is the summation of both absorption and scattering coefficients. As the values of refractive index for PET and air are 1.575 and 1, respectively, then from eq. (1), the value of  $R_f$  will be 0.0499. Applying Beer-Lambert law shown in eq. (1) for the experimentally measured transmittance, the total attenuation coefficient  $\mu_t$  of the examined sample was  $0.0358 \text{ mm}^{-1}$ .

### 2.2. The LIPS Elemental Analysis

The schematic diagram of the LIPS setup used is shown in Figure 2. A nanosecond laser was used in the LIPS setup as described in details previously elsewhere [20-24]. In this work, Q-Switched pulsed Nd:YAG laser at 30 mJ pulse width of 10 ns and repetition rate of 20 has been employed to produce the plasma. Laser irradiation at 1064 nm is produced by the master oscillator with adjustable energy up to 500 mJ and 4% pulse energy stability.

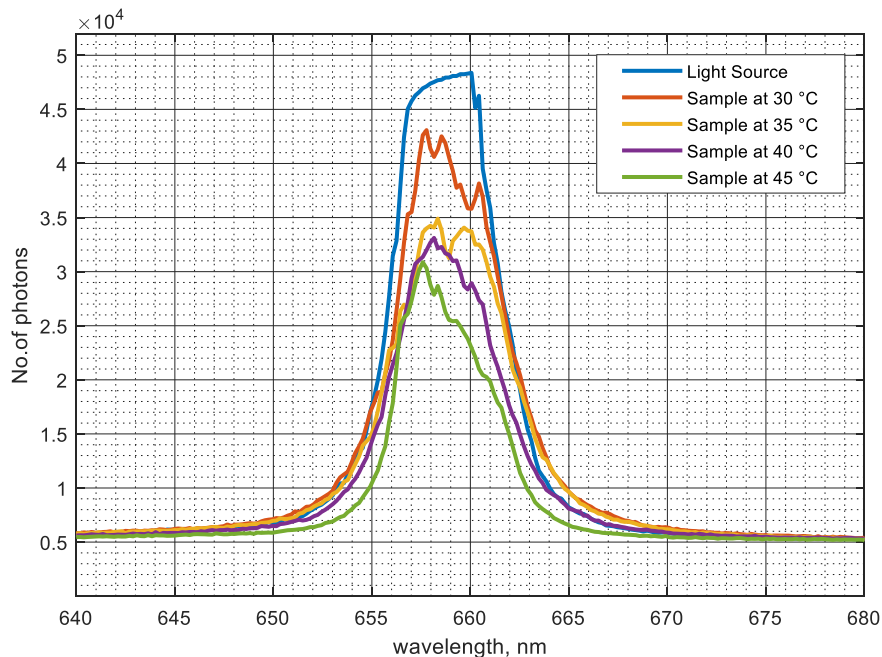
The spectra generated by the plasma plume was collected by a plane-convex quartz lens with a focal length of 10 cm on the optical fiber head, which was positioned at an angle of approximately 90° to the laser beam axes, then the spectra transfer via the optical fiber to the spectrometer input slit then to an ICCD camera which capture the spectra as illustrated in Figure 2. The delay time between the laser pulse Q-switch and the spectrometer detection was adapted to 1 μs as stated previously [20] [24].



**Figure 2:** Laser induced spectroscopy (LIPS) experimental setup.

### 3. Results and discussion

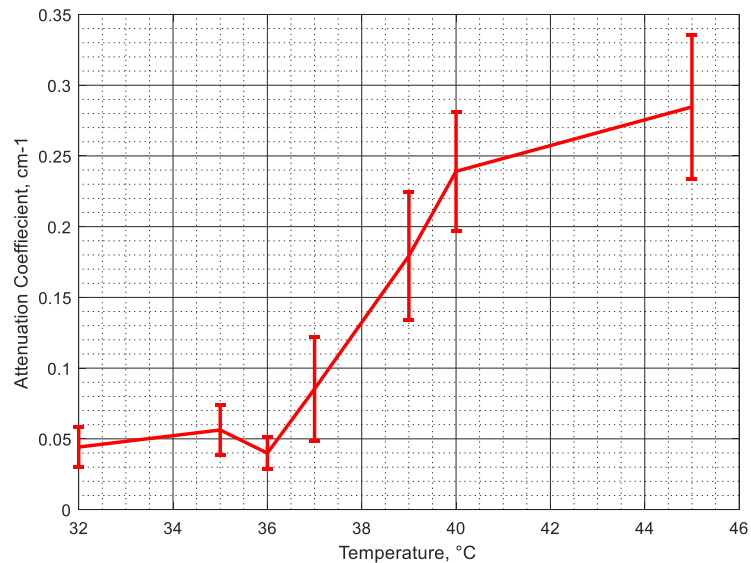
Samples of PET from commercial plastic water bottles were illuminated with 5 mW, 650 nm laser diode at different temperatures. Figure 3 shows examples of the light attenuation at different temperatures.



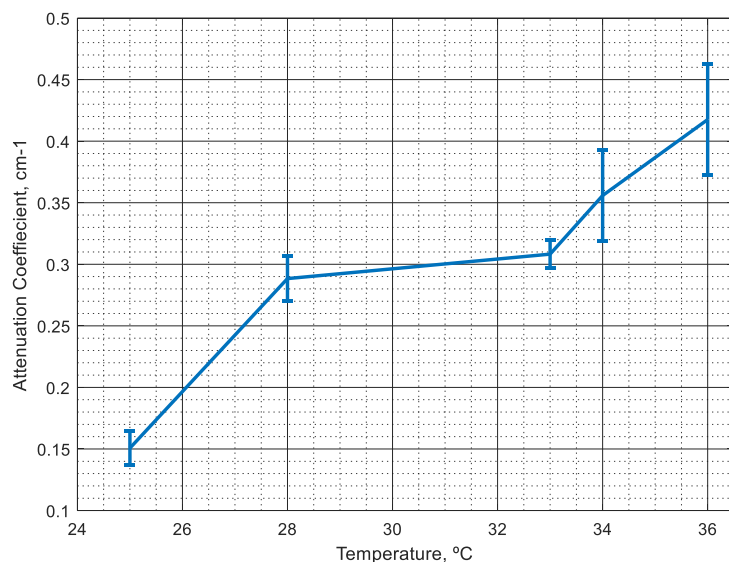
**Figure 3:** Laser Power Attenuation in the PET sample at different temperatures

As illustrated in Figure 3, by increasing the temperature, the transmitted intensity decreases leading to increasing in the total attenuation coefficient according to Beer-Lambert law.

The total attenuation coefficient of the examined samples was then calculated at different temperature as illustrated in Figure 4. Two laser wavelengths are employed in this experiment; 635 and 650 nm and the measurements were obtained as a function of the applied temperatures.



(a)



(b)

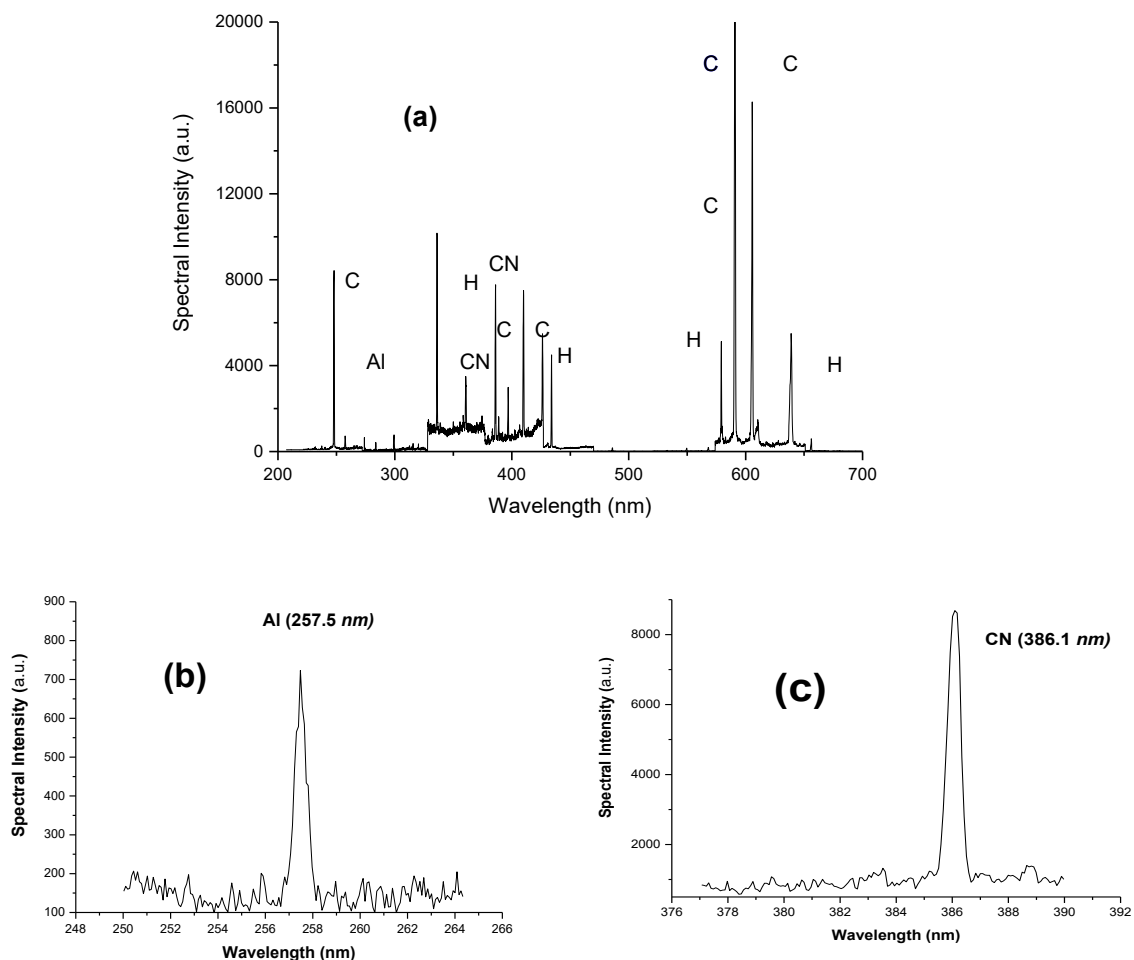
**Figure 4:** Variation of the PET attenuation coefficient with the temperature, (a) 635 nm, (b) 650 nm

Figure (4), represents the values of the optical attenuation coefficient at different room temperature ranging from 25 °C to 45 °C simulating hot-sun-days ambient conditions in the laboratory. As illustrated in fig. (4), the total attenuation coefficient increases dramatically starting from 36 °C to 40 °C. Unlike biological tissues, polymers have lower scattering properties than absorption. Therefore, the observed increase in the attenuation coefficient in the examined samples is mainly due to increasing in the absorption properties [25].

LIPS spectrum obtained from PET in the range of 200-700 nm is shown in Figure 5(a). This spectrum was analyzed using NIST data [26]. In the LIBS spectrum of the sample shown in Figure 2, some impurities are observed which are Al, and CN in PET polymer sample. The prominent lines of the impurities detected in the sample are shown in Figure 5(b) and Figure 5(c) for Al and CN at 257.5 nm and 386.1 nm, respectively. The characteristics of the produced plasma controls the resultant LIPS spectrum and the intensities of the emission lines

The plasma is assumed to be in the state of local thermal equilibrium (LTE) and the nominated spectral lines are considered under optically thin plasma conditions [27]. When the excited atoms relaxed to their lower energy configurations through radiating photons, spectral lines associated to the transitions between these different levels can be obtained in emission spectra.

Even though, aluminium and cyanide may exist as trace elements in PET but they are considered to be toxic elements according to the United States food and drug administration (FDA) [28]. The experimental results prove that the attenuation coefficient of PET increases with the temperature i.e. heat will accumulate very fast in the PET under high ambient temperature conditions during hot-sun-days. The later may result in leaching of some aluminium and cyanide existed in PET polymer into the bottle's water content and cause health problems. To confirm these studies, we are planning to do spectroscopic LIPS elemental analysis of the bottled water along with the above-mentioned experiment to monitor these heavy elements in water under ambient hot-sun-days temperature conditions.



**Figure 5:** (a) LIBS spectrum of PET from 200 to 700 nm, (b) Aluminum impurity line detected at 275.5 nm, (c) Cyanide impurity line detected at 386.1 nm .

#### 4. Conclusion

In the current study, LIPS technique has been applied for elemental analysis of polyethylene terephthalate (PET) plastic used for bottled drinking water. The observed results showed the exitance of Al and CN as impurities in PET. While the optical analysis showed that, the optical absorption properties of this type of plastic increases at temperatures above 25 °C during hot-sun-days temperature. Therefore,

this study supposed that, Al and CN may leach into the water content in the bottle if the temperature exceeds 25 °C and their concentrations in the water may increase gradually at higher temperature due to the increase in the absorption coefficient of PET. In the future work, we intent to analyse the bottle's water as well to measure the concentration of these contaminations in water during hot weather.

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