

## A Comparative Study on the Influence of IR Radiations to Some Polymers

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In the last decade, many efforts have been made in modifying the surface and bulk properties of polymers by the use of various radiations such as UV and IR radiations, plasmas, flame, corona, electron beams and ion beams etc. The present work deals with the changes induced to CR-39 and PET polymers by IR irradiation. The modifications induced in the polymers due to IR irradiation have been analyzed with the help of XRD and UV-visible spectra of the pristine and IR irradiated polymers and a brief mechanism has been suggested, where ever possible. It has been found that CR-39 is more sensitive towards the radiations as compared to PET.

**Key Words:** X-ray diffraction, Crystallite size

### INTRODUCTION

Irradiation is an established tool for modifying the structure and properties of polymers<sup>1-2</sup> and has attracted growing attraction<sup>3-4</sup> for potential technological application due to the increased uses of these materials. Irradiation of the polymers generally leads to a radiation damage, which modifies the properties of the surface and bulk of the polymers<sup>5-6</sup>. These modifications are the consequence of irreversible reaction mechanisms in polymers owing to processes like main-chain scission, intermolecular cross-linking, and creation of unsaturated bonds and emission of atoms, and molecules etc<sup>1</sup>.

The present work has been carried out to study the comparative influence of IR radiation on the crystalline and optical properties of CR-39 and PET polymer, so that their use in the environment of IR radiations can be checked. The effects induced by IR radiations have been investigated through the measurement of band gap energy, Urbach's energy and Crystallite size.

### EXPERIMENTAL PROCEDURE

Small pieces of PET and CR-39 have been cut from a sheet of average thickness of 100µm and 230 µm, respectively. The samples were washed and

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time period varying from 1 to 72 h with the interval of 12 h using an IR lamp cleaned with sodium hydroxide and then under running water to remove the adsorbed impurities. Irradiation was carried out in air at room temperature for (Philips infra phil HL4311) of 150 W at 210 V, at a distance of 6cm from the source output. The X- ray diffraction measurements were carried out with Panalytical's X'Pert Pro working at 40 KV and 25mA to measure the grain size. The nature of Optical modifications was analyzed using UV-VIS Spectrophotometer (ELICO SL159) in the wavelength range 200-600 nm.

## RESULTS AND DISCUSSION

The UV-Vis spectra of the unirradiated and irradiated samples for different exposure times are presented in Fig 1. It is evident from the fig that there is a red shift in the absorption edge with exposure time and has been correlated with the optical band gap  $E_{opt}$  given by  $E_{opt} = hc/\lambda$ , where  $h$  is Planck constant and  $c$  is the speed of light is reported in table 1. The wavelength  $\lambda$  is determined according to Tauc's expression<sup>7</sup>. Such a shifting may be due to the formation of free radicals, cations, anions, double bonds, triple bonds etc. Other possibility for shifting can be the increase in conjugation with increasing dose resulting in a decreased HOMO-LUMO gap<sup>8</sup>.

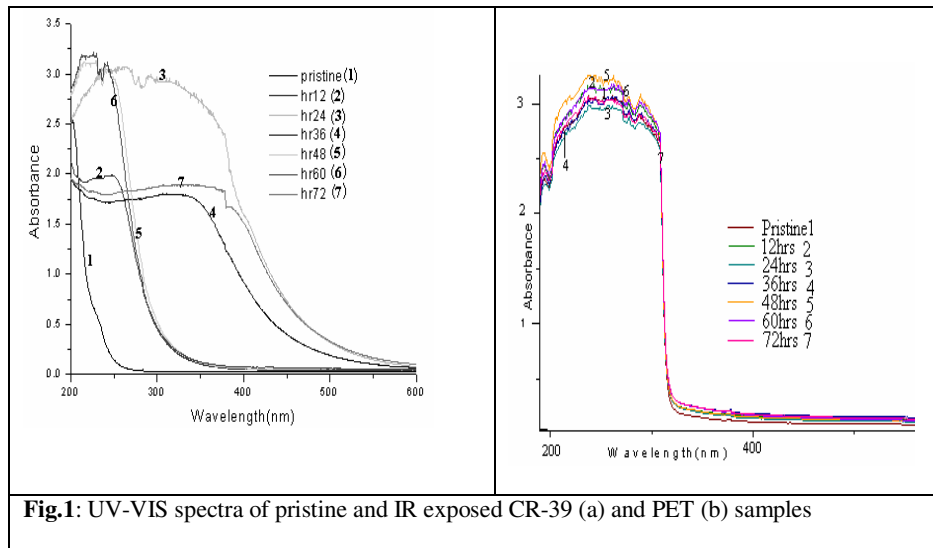
The  $E_{opt}$  has been found to decrease with the IR radiations exposure of CR-39 with some exception at 48 hr and 60 hr, whereas it remains same for PET, which indicates the stable behavior of PET due to the crystalline nature of the presence of benzene ring as aromatic carbohydrates provides more stability to polymers as compared to that of aliphatic compounds.. The decrease at higher doses has been observed to some extent that may be attributed to the already existing reactive species or hot molecules, which break up due to the gain of small amount of energy. In case of CR-39 the population of the free radicals produced at lower exposures may have been increased to a greater extent and it causes the free radicals to react with each other and caused a higher degree of cross-linking at 48 and 60hrs exposure. The Urbach's energy  $E_0$  has been calculated for the two polymers from the inverse of the slope of the linear part of the curve between  $\ln\alpha$  and energy (eV), where  $\alpha$  is the absorption coefficient<sup>9</sup> and are reported in Table 1.

It can be seen from the table that no particular trend could be applied to the Urbach's energy; however there is an overall increase in the Urbach's energy for CR-39, but a decreasing trend seems to be followed by PET. The increase in the Urbach's energy for CR-39 may accounts for the increase in the high diffusion of  $\pi$  electrons to the forbidden gap of the polymer and vice versa.

To analyze the changes in the crystalline properties of the polymers X-ray diffraction studies have been performed. The main diffraction peak for PET

**Table -1.** The variation of Band gap and Urbach's energy alongwith the crystallite size for CR-39 and PET with IR exposure time

IR exposure time (h)	Band gap energy <b>a</b> (eV)		Urbach's energy (eV)		crystallite size( $\text{\AA}$ ) <b>b</b>	
	CR-39	PET	CR-39	PET	CR-39	PET
0	5.2	3.93	0.27	0.26	10.58	51.22
12	3.9	3.93	0.42	0.15	10.58	51.56
24	2.6	3.93	0.33	0.17	10.66	53.17
36	2.5	3.92	0.39	0.17	10.58	54.42
48	3.9	3.91	0.37	0.18	11.30	53.82
60	4.0	3.91	0.41	0.17	11.64	51.93
72	2.3	3.91	0.36	0.18	10.42	--

**Fig.1:** UV-VIS spectra of pristine and IR exposed CR-39 (a) and PET (b) samples

occurs at  $2\theta = 26.15^\circ$  alongwith two other peaks at  $2\theta = 23.07^\circ$  and  $2\theta = 17.91^\circ$ . The overall intensity of the first two peaks has been found to decrease indicating the decrease of crystallinity of PET whereas the third peak found to get dissolved after 48 h of exposure. At 12h the intensity increases showing the increases in crystalline nature and the decrease of intensity at 24h to 60h shows that the amorphous nature of the polymer is increasing. The highest peak intensity peak has been found to shift towards greater angle at an exposure time of 60h. This implies that the lattice parameters change during irradiation of PET under the studied conditions.

The peak at  $2\theta = 21.11^\circ$  in case of CR-39 in diffraction pattern of the pristine sample indicates the amorphous nature of the polymer. The intensity has been found to decrease after 24 hrs exposures with exceptions at 12 and 72 hrs.

The decrease in the intensity indicates an increase in the amorphous nature of the polymer. For the quantitative analysis of the data the crystallite size of the irradiated and pristine sample have been calculated from the Scherrer's formula given below.

$$\text{Crystallite size}(L) = \frac{K\lambda}{d \times \cos \theta}$$

The observed values of  $2\theta$  and crystallite size (L) calculated at the different exposures are given in table 1 alongwith band gap and Urbach's energy. The increase in the crystalline size for CR-39 may be perhaps due to the increase in the Vander-waal bonding of more polymeric species in the crystallite. The crystallite size of the prominent peak of PET has been found to follow an increasing trend except at an exposure time of 60 hrs. The decrease in the grain size of the prominent peak at 60 hrs may be due to the increase in some repulsive forces over the attractive weak Vander-waal's forces.

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