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Effect of Thermal Annealing on the Structure of Ultra-High MW Polyethylene: Principal Component Analysis of FTIR Spectra

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ABSTRACT:

Using chemo metric analysis of FTIR spectra for the industrial selection of PE (UHMW), the viability of evaluating the variation in IR active band was investigated. The specimen of UHMWPE were prepared and spectroscopic technique applied on specimen before and after annealing i-e Fourier transform infra-red. To extract the Principe components and their related Eigen values from spectroscopic data PCA has been performed. By using the Eigen values, Entropy has been calculated and compare before and after annealing. In contrast to what we have anticipated, no significant difference were seen between the Eigen values derived from UHMWPE of annealed and unannealed specimen. Zero Eigen values and zero entropy have seen in both situations, indicating no obvious changes in the molecule structure or proof of major annealing damage. These findings imply that UHMWPE is not significant altered or damaged by annealing at particular conditions examined in this work. The impact of irradiation or other variable such as various annealing parameters that may affect a material response to thermal treatment must be explore further.

Keywords: Polyethylene (UHMW), Chemo metric analysis, FT-IR Spectroscopy, Principle-Component Analysis

1. INTRODUCTION

Orthopedic implants can be made from ultra-high molecular weight polyethylene (UHMWPE), a biomaterial that is often utilized. It has excellent mechanical and biocompatibility features, making it a good choice for many applications. The structural integrity of implants could be jeopardized, nevertheless, if UHMWPE is used over an extended period of time and is exposed to environmental conditions. For determining the remaining usable life of implants and guaranteeing patient safety, accurate and dependable methods for evaluating deterioration in UHMWPE are essential. . UHMWPE is just one type among the family of polymers, some other kinds of polyethylene are low-density polyethylene (LDPE), linear-low-density polyethylene (LLDPE), high-density polyethylene (HDPE), and ultimately ultra-high molecular weight polyethylene (UHMWPE) [1-6]. UHMWPE is a very versatile polymer having excellent physical, chemical and mechanical and structural properties [7]. It is odorless, tasteless, and white in color and nontoxic [8]. The melting point of UHMWPE is around 130°C to 136°C [9]. One of the elements that can have an impact on the characteristics and functionality of UHMWPE is radiation. Medical devices, such as implants made of UHMWPE, are frequently sterilized using irradiation, such as gamma or electron beam radiation. The material's chemical and structural changes brought on by radiation exposure, however, could affect its mechanical strength, resistance to wear, and fatigue qualities. A vital component of determining the structural integrity of UHMWPE is quantifying damage. Traditional approaches to damage assessment sometimes include destructive testing, which necessitates sample sacrifice and might not be appropriate for evaluating the state of implants while they are in use. For assessing UHMWPE deterioration, non-destructive methods are preferred. When analyzed using spectroscopy-based techniques, such as Fourier Transform Infrared Spectroscopy (FTIR), the molecular structure and chemical composition of UHMWPE have shown to be quite accessible[10-16]. FTIR offers details on the vibrational modes of molecules in addition to identifying specific functional groups and detecting changes in chemical bonds. But the quantitative data from FTIR spectrum analysis alone on the level of damage or degradation in UHMWPE might not be enough. In order to overcome this limitation, chemo metric analytical methodologies and FTIR spectroscopy are used for the goal of measuring damage in UHMWPE. Chemo metrics employs statistical and mathematical methods to decipher complex spectroscopic data and extrapolate important information. When spectroscopic information and UHMWPE's level of damage are connected, chemotherapy. A strong and non-destructive method for quantifying damage in UHMWPE is provided by the combination of spectroscopy-based approaches and chemo metric analysis. By using chemo metric models, it is now able to precisely assess the degree of damage in UHMWPE based on the data from FTIR spectra. In this research study, we explore the use of spectroscopy-based chemo metric analysis for quantifying damage in UHMWPE. We will investigate how radiation exposure affects UHMWPE samples in particular and analyze the chemical alterations brought on by radiation using FTIR spectroscopy. The chemo metric analysis of the spectroscopic data will be used to establish quantifiable connections between the spectrum features and the degree of damage.

2. Material and Methods

2.1 UHMWPE

2.1.1 Preparations

Throughout the course of this research UHMWPE in powder form possessing an average molecular weight 3 to 6 million grams/mole were used and was acquire from Sigma Aldrich. Micron film of UHMWPE powder is prepared, for this, the heat exchanger obtained from PIEAS (Pakistan Institute of Engineering and Applied Sciences, 45650, Islamabad, Pakistan) is used with increasing with a fall of 10ºC / min. The powder of PE with ultra-high molecular weight is hold down with 200 bar pressure, for 12-15 minutes at 140 ° C, 160 ° C and 190 ° C, respectively.

After sample characterization by FTIR spectroscopy, now following all standard procedures, sample aging was performed. For this reason, the samples were thermally annealed by keeping them in the furnace of the JSOF-050 model in the UET taxila lab for 21 days at a steady temperature of 80°C. During the process of heating, sample is constantly checked and the direction of the sample is changed every day. The oven is used as a heat sink, and its interior has two trays to hold the sample

2.2 Chracterization

2.2.1 Fourier Transform infra-red Analysis

IR spectra were recorded in full focus mode and measured in mode of transmission using a Nicolet 6700 FT-IR spectrophotometer (Thermo Electron Corporation, Waltham, MA, USA). The required spectrum is collected after obtaining 216 scans from (4000cm^{-1}to 400cm^{-1}) with a resolution of 2cm^{-1}. Spectra for each sample were averaged from three to four locations in order to lower the signal-to-noise ratio (SNR).

3. Results and Discussion

FTR Analysis

In the visible range of the electromagnetic spectrum (i.e. 400-800nm), the absorption behavior of UHMWPE has been studied. There is no significant changes before and after annealing

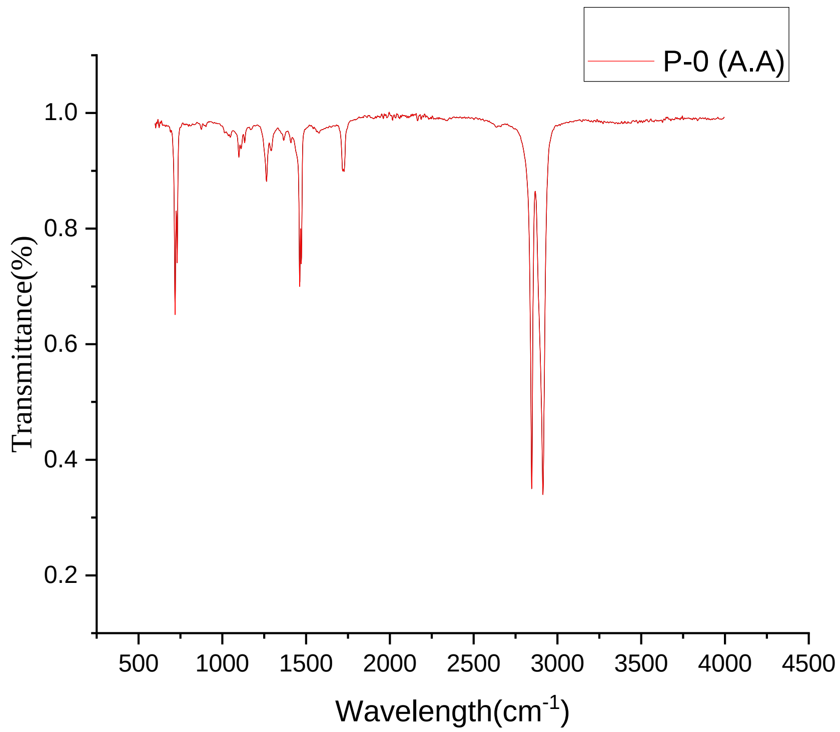

Figure 1. FT-IR spectra of UHMWPE sample before and after annealing

Chemo metric Study

Principal Component Analysis (PCA)

A valuable tool is altering the data and the new axis arrangement to show the data while keeping in mind the processes with the highest percentage of variance. The analysis can minimize the number of significant changes to a new modified PC with significant differences using this new set of axes, known as the principal component (PC). Using scree charts, the initial step is to establish how many CP are required to expose the hidden object patterns/spikes/occur in a given dataset. To determine which PCs are required for more investigation, a scree plot, a linear depiction of each PC's eigenvalue in many studies, is utilized. Identifying the necessary number of PCs is the first and most crucial step

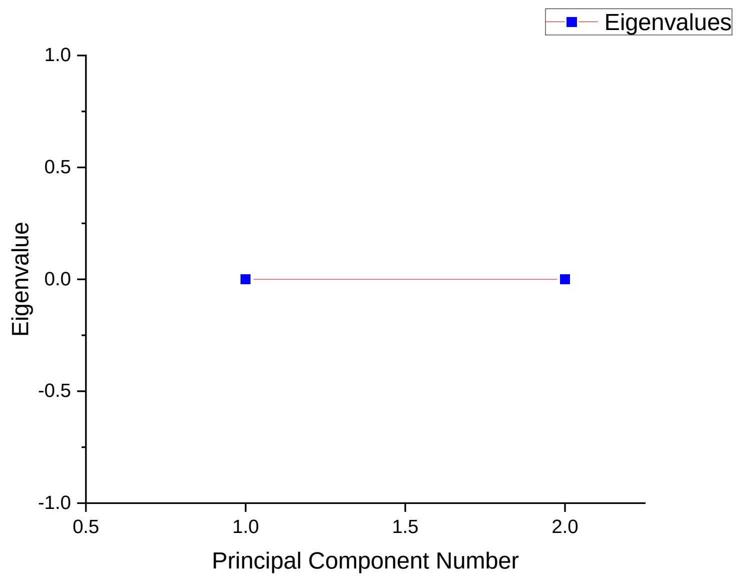

Figure 2. Screen plot of FT-IR data obtained from Principle Component Analysis PCA.

This screen plot of FT-IR data acquire from principle component analysis shows zero Eigen values which means there is no significant effect of annealing on UHMWPE.

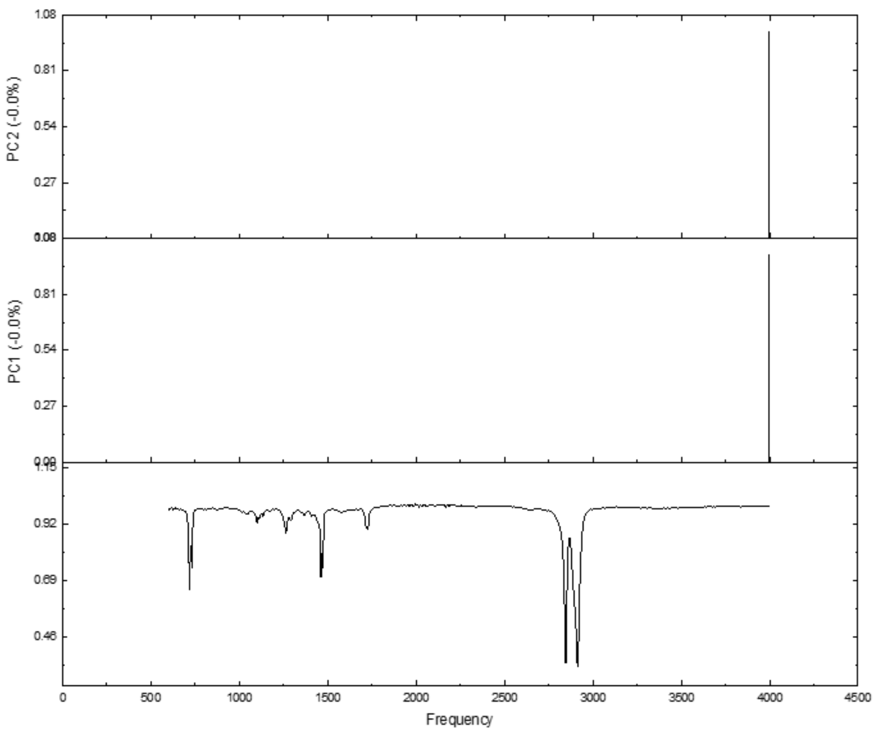

Figure 3. Factor loading graph for defining PCs

This factor loading graph of PC 1 shows no variance after annealing.

Entropy

By using the FT-IR data we have performed the principle component analysis PCA and find the Eigen values. After that we used the entropy formula given below to find the entropy

$$H = -\sum_{i=1}^{n}(x_i \log x_i)$$

Where

$$x_i = \frac{\lambda_i}{\sum_j^n \lambda_j}$$

The entropy of the PCA given in the following table

SAMPLE	**ENTROPY**	
	Before Annealing	After Annealing
P0	0	0

Conclusion

The molecular makeup and structure of UHMWPE were clearly revealed by our FTIR research. The annealing procedure did not, however, cause any appreciable modifications in the material's FTIR spectra. This shows that the annealing process did not appreciably change the chemical bonds or molecular arrangement. Additionally, the multivariate dataset might be examined to find any patterns or connections between the variables thanks to the chemo metric analysis, more specifically PCA. Surprisingly, the PCA yielded 0 eigenvalues, demonstrating that none of the principle components effectively represented the variance. Additionally, the dataset's entropy score was zero, indicating a lack of diversity or information content.

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