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Chemo-Metric Based Raman Spectroscopic Analysis for the Classification of Orthopedic Biomaterial

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ABSTRACT:

In this research work, we used Raman spectra analysis to examine the structural alterations in ultra-high molecular weight polyethylene (UHMWPE) caused by gamma irradiation and heating operations. We were able to investigate the molecular composition and configuration of the materials by examining the vibrations of their chemical bonds courtesy to the accurate method of Raman spectroscopy. By closely examining these spectra, we were able to identify shifts and modifications in the distinctive peaks that were indication of molecular structural changes brought on by heating and gamma irradiation. Furthermore, we used chemo-metric analysis, Principal Component Analysis (PCA) to classify these spectral fluctuations, which improved our understanding of how external interventions affect the structural integrity of biomaterials. This research advances the development of biomaterials and manufacturing quality assurance procedures, enabling a wider range of applications.

Keywords: Polyethylene (UHMWPE), Chemo-metric analysis, Raman Spectroscopy, Principle Component Analysis (PCA)

1. Introduction:

Orthopedic biomaterials—Ultra-High Molecular Weight Polyethylene, or UHMWPE—are essential to many medical applications, such as orthopedic implants and joint replacements. The effectiveness and durability of these biomaterials are essential components in ensuring the success of orthopedic surgeries and the general health of patients.[1] But oxidative degradation, which is a natural tendency of theirs, poses a serious problem because it frequently results in early failure and makes revision surgeries necessary[2, 3]. Growing interest has been seen in the development of sophisticated analytical methods for the evaluation and characterization of orthopedic biomaterials in recent years.[4, 5] Among these techniques, Raman spectroscopy is one of these methods that has shown to be very effective in revealing details about the molecular composition and structural characteristics of materials. Raman spectroscopy provides special benefits by using the scattering of monochromatic light. These benefits include high sensitivity, non-destructiveness, and the capacity to analyze samples in a variety of states, including liquid, solid, and gas[6, 7] .Principal component analysis, which finds recurrent patterns in the data with little information loss, is a popular technique for turning complex spectral datasets into easily understood information while Spectroscopy quickly gathers a large amount of data that is not directly interpretable[8].

Using chemo-metric based Raman spectroscopic analysis, we examined the effects of gamma irradiation and heating on ultra-high molecular weight polyethylene (UHMWPE). Our analysis revealed shifts in characteristic Raman peaks, changes in peak intensity, and peak broadening, indicating structural alterations such as bond length changes, reduced double bond concentrations, and increased molecular disorder .[9, 10].The intensity of the peaks in the Raman spectra linked to free radicals will be significantly reduced after the thermal treatment of UHMWPE. Principal Component Analysis (PCA) classified the spectral data into distinct groups, highlighting differences between untreated, gamma irradiated, and heated samples. These findings provide valuable insights into the structural integrity of UHMWPE, aiding in the development of improved orthopedic biomaterials and establishing benchmarks for quality control in manufacturing processes [11, 12]. The removal of radicals enhances the chemical stability of UHMWPE, making it more suitable for long-term use in orthopedic applications.

2. Material and Method:

2.1 UHMWPE

2.1.1 Methodology

Ultra-high molecular weight polyethylene (UHMWPE) samples were heated and exposed to gamma irradiation in the present study. The heated samples were treated for a specific period of time at a controlled temperature, whilst the gamma-irradiated samples were exposed to a specific dose of gamma radiation. Using a high-resolution Raman spectrometer, Raman spectra were acquired for the heated and gamma-irradiated samples and these spectra were then examined to look for structural alterations brought on by the treatments. Utilizing Principal Component Analysis (PCA) on the gathered Raman spectra, spectral data was classified in order to comprehend how the treatments affected the molecular structure of UHMWPE. Before applying PCA, the Raman spectra were pre-processed through baseline correction and normalization using specific software such as origin-lab.By emphasizing the primary distinctions between the heated and gamma-irradiated samples, PCA assisted in reducing the dimensionality of the data, enabling the identification of patterns and classification based on the structural changes brought about by the treatments.[10].

3. Results and Discussion

3.1 Raman Spectrum Analysis:

In the visible range electromagnetic spectrum (i.e 1400-1600nm) , the absorption behavior of UHMWPE has been studied.

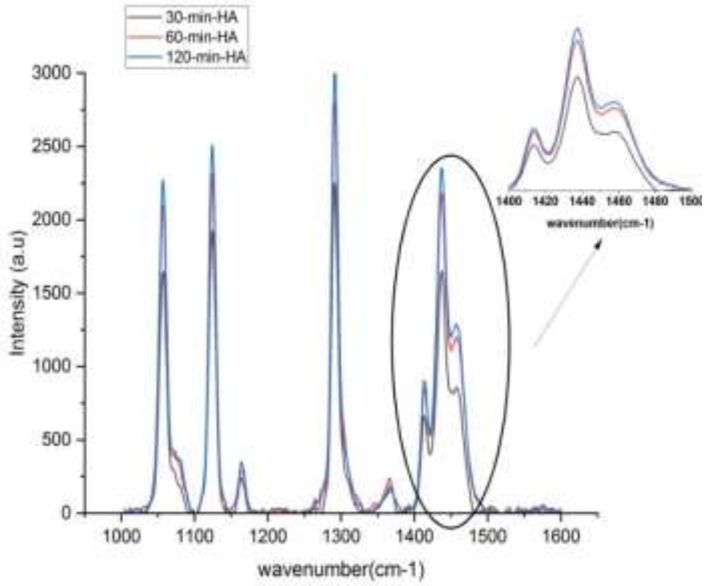

Figure 1 A Raman Spectrum of heated control sample of UHMWPE (no-vitamin E) .

Sample	%Crystalline (I_{1416}/I_{1295})	%Amorphous (I_{1080}/I_{1295})	% Inter-phase = [100-(%Crystalline+ %Amorphous)]
30 min heated	37.50	11.46	51.16
60 min heated	36.95	14.34	48.71
120 min heated	35.50	13.08	47.42

Table 1 Percentage Crystalline, amorphous and inter-phase for heated alone samples of UHMWPE.

The table analyzes how radiation exposure affects UHMWPE's crystalline, amorphous, and inter-phase regions.. Heating induces a gradual decrease in crystalline regions due to polymer chain breakage, while the inter-phase region's percentage rises with UHMWPE concentration, correlated with crystallite size[13, 14]. Radical migration within the material, initially trapped in crystalline regions, leads to chain scission at inter-phase boundaries, expanding the amorphous region. This dynamic inter-phase region serves as a critical site for morphological changes, influencing material properties like rigidity..Heat treatment in a nitrogen-filled open air environment alters the structure of UHMWPE, most notably by reducing the amount of interphase regions in the material. The breakdown of polymer chains close to crystalline boundaries and subsequent interactions with oxygen in the environment are thought to be the cause of this reduction.As a result, radicals go from the material's core to the inter-phase areas, where they then react with oxygen to produce more structural changes.[15] Optimization of the characteristics and performance of UHMWPE in orthopedic applications is made possible by these additional insights into the composition and structure of the material due to heat treatment.Orthopedic implants produced from heat-treated UHMWPE can provide greater mechanical strength, resistance to wear and degradation, and better tissue integration by customizing processing techniques to increase durability and bio-compatibility. Ultimately, this understanding facilitates the development of orthopedic implants with extended lifespan and enhanced functionality such as stiffness and durability, benefiting patients and health care providers alike.

Chemo-metric Analysis

Principle Component Analysis (PCA)

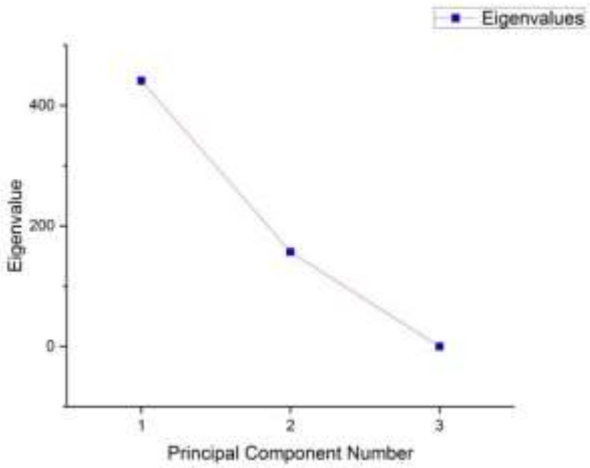

Figure 2 Screen plot of Raman spectrum data obtained from Principle Component Analysis PCA

In this figure 2 Ultra-High Molecular Weight Polyethylene (UHMWPE) is a commonly used biomaterial in orthopedic implants due to its remarkable mechanical properties and bio-compatibility. UHMWPE experiences molecular changes during heating that may have an impact on its structure and characteristics. Eigen values in Raman spectroscopy indicate the variation in molecular structure or composition that each principal component is able to capture. The heated UHMWPE samples exhibit a decrease in Eigen values across the Raman spectrum components, indicating a reduction in the molecular complexity or diversity of the polymer. Heating can cause polymer chains to undergo change and lose some of their crystallinity, resulting in a more ordered molecular structure. This could show up as a reduction in the variety of chemical structures that Raman spectroscopy can identify. Heating may cause changes in chain conformation, such as increased polymer chain alignment or orientation.This may result in a decrease in the range of molecular conformations found in the sample, as indicated by a decrease in Eigen values. Extreme heating may cause chain scission or cross-linking reactions in UHMWPE, although these are less likely under normal processing conditions. Reduced variance in the Raman spectra could be the result of these processes, which could drastically change the polymer's molecular structure and composition.

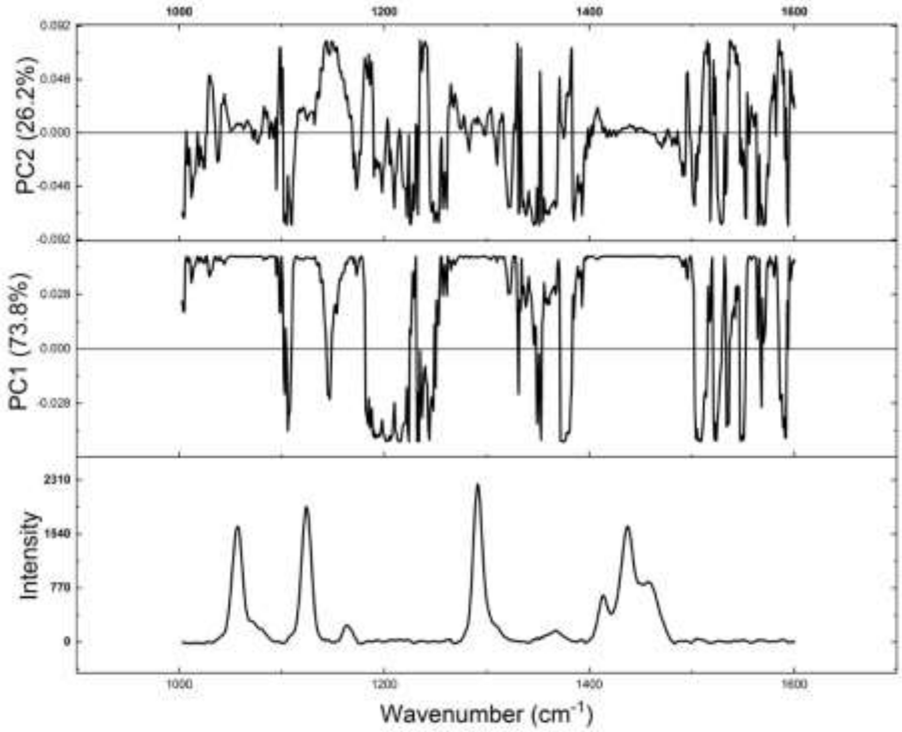

Figure 3 Factor loading graph for defining PCs

Principal Component Analysis (PCA) helps with noise reduction, classification, and data interpretation for a variety of applications by simplifying complex Raman spectroscopy data by lowering dimensionality and emphasizing important spectral properties. It is an important tool in material characterization and biomedical analysis because it improves signal-to-noise ratio and permits efficient sample discrimination and classification based on spectrum differences[16, 17].

PC1 is primarily responsible for capturing changes in the spectra caused by radiation-induced oxidation and cross-linking. PC1 is important in Raman spectroscopy because it clarifies changes these activities make to the UHMWPE spectra. Radiation exposure-induced oxidative and cross-linking processes in UHMWPE can cause changes in its molecular structure, which might show up as alterations in peak intensities or positions in the Raman spectrum.

Conversely, PC2 examines changes in the polyethylene (PE)-specific characteristic bands by using Raman spectroscopy, PC2 provides information about changes in the molecular characteristics of PE that are different from those PC1 recorded.These alterations may be the result of modifications brought about by external agents like gamma radiation, which could alter the chemical, physical, or structural attributes of PE. The spectral properties unique to polyethylene are altered as a result of these adjustments, and this information is useful for classifying and characterizing UHMWPE and other orthopedic biomaterials.

4. Conclusion:

The removal of radicals from UHMWPE through thermal treatment provides a more uniform and stable molecular structure, as confirmed by the PCA analysis of Raman spectroscopy data. Reliable classification is ensured and the treatment procedure is validated by the distinct separation of treated and untreated samples in PCA score plots. Furthermore, identifying the critical spectral characteristics affected by the treatment offers insightful information for quality control and additional optimization in the manufacturing of orthopedic biomaterials. The effectiveness of integrating Raman spectroscopy and PCA to improve the quality and functionality of UHMWPE in medical applications.

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