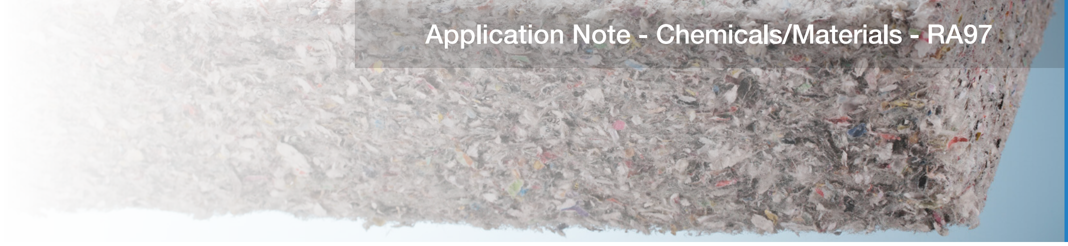


Chemometrics-Driven Chemical Characterization of Cellulose Sheets using Raman Microscopy

Background and Challenges

Cellulose crystallinity is a key property influencing the physical, mechanical, and chemical behavior of renewable, biodegradable materials. The crystalline-to-amorphous ratio, along with specific crystalline forms, directly affects material performance. Therefore, assessing these critical parameters is essential for optimizing material functionality and ensuring consistent quality in industries such as bioplastics, textiles, packaging, and sustainable composites.

In this study, we demonstrate the capabilities of Raman microscopy for the chemical analysis of cellulose sheets, focusing on the determination of crystalline and amorphous cellulose content using chemometric tools. Additionally, we highlight its effectiveness in distinguishing between crystalline cellulose I and II forms.

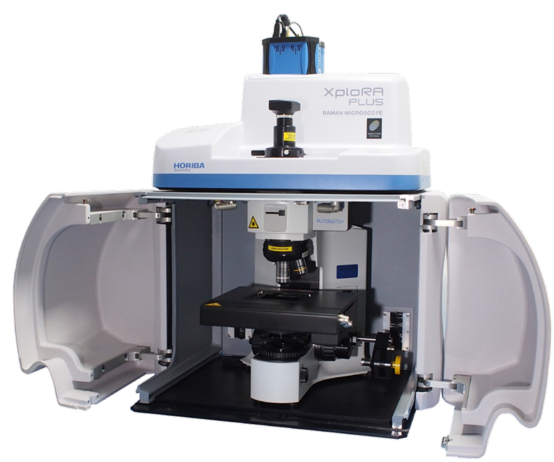
Using high-resolution Raman imaging, combined with multivariate analysis, we achieve detailed chemical mapping of cellulose structure and composition, supporting efficient, non-destructive quality control of bio-based materials.

Cellulose Sheets characterization: How?

This study was conducted using our HORIBA XploRA™ PLUS Raman microscope, which features an optimized, compact design with advanced automation to enable accurate, full chemical analysis with maximum ease of use and efficiency. Its user-friendly setup allows seamless integration into R&D and QA/QC laboratories, delivering fast compound identification and high-resolution chemical imaging at low operational cost.

The analysis was performed by running several mappings on cellulose sheets using a 785 nm excitation laser wavelength and a 600 gr/mm grating, covering a spectral range of 50 - 1800 cm^{-1}.

All data acquisition, processing and modeling were performed using our LabSpec 6 software.

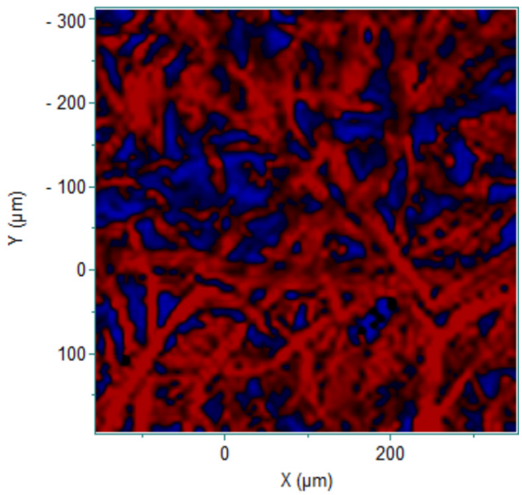


XploRA™ PLUS

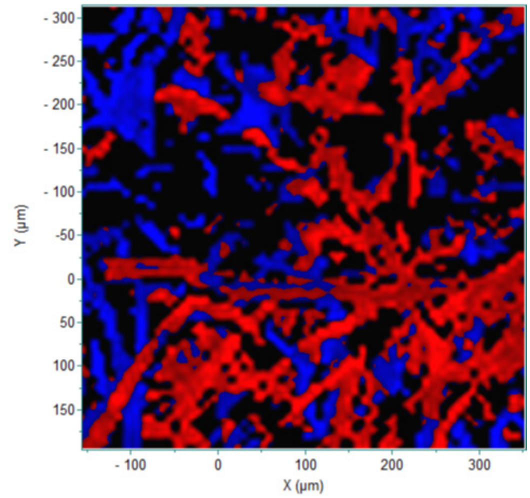
Solution from HORIBA

Raman imaging was performed using a point-by-point acquisition approach, with an integration time of 5 seconds and 1 scan. Due to significant surface topography variations in the sample, automatic autofocus adjustment was applied along the Z-axis. Spectra were then preprocessed using baseline correction, followed by Standard Normal Variate (SNV) normalization. To quantify the proportions of amorphous and crystalline cellulose, as well as distinguish between crystalline cellulose I and II forms, a Multivariate Curve Resolution (MCR) analysis was conducted.

HORIBA



■ Amorphous Cellulose
■ Crystalline Cellulose



■ Crystalline Cellulose II
■ Crystalline Cellulose I

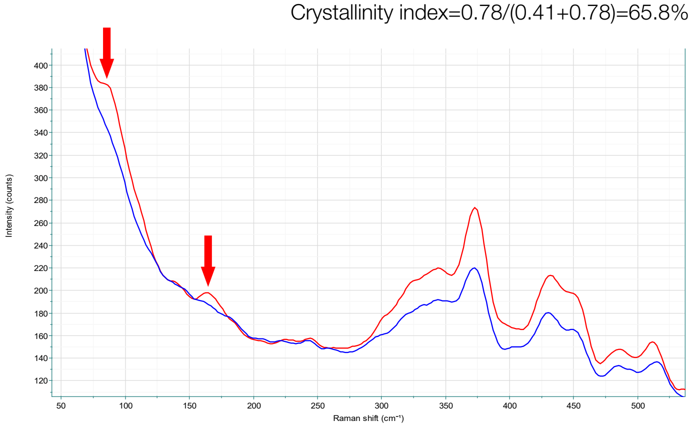
Score statistic

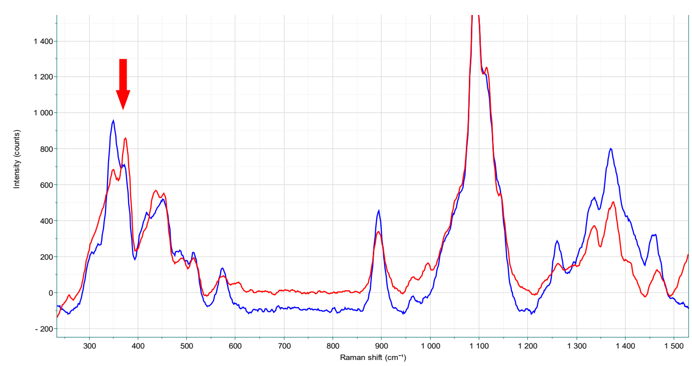
	Mean	%
Crystalline	0.779173	65.8
Amorphous	0.405249	34.2

Crystallinity index=0.78/(0.41+0.78)=65.8%

Score statistic

	Mean	%
Cellulose I	0.250219	56.9
Cellulose II	0.189557	43.1





The Raman images clearly distinguish between amorphous and crystalline cellulose, with their proportions were accurately extracted and the crystallinity index calculated using score statistics automatically generated by the MCR model, built with our LabSpec 6 software's chemometric module, MVAPlus. The same approach was applied to quantify both Cellulose I and Cellulose II after the automatic subtraction of amorphous cellulose from the Raman map.

Summary

- We were able to detect, differentiate, and quantify the proportions of multiple components within cellulose in its various forms, with high spectral and spatial resolution.
- The XploRA™ PLUS offers excellent sensitivity, and combined with a user-friendly interface and powerful built-in chemometric modeling tools, enables efficient data processing and precise identification and quantification of products.

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