Application note

Rapid identification and quantification of textile fibers via ATR-IR spectroscopy

Author

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Industry/application

Textile fiber identification, quantification, and quality control.

Products used

Thermo Scientific™ Nicolet™ Summit™ FTIR Spectrometer with Diamond ATR Accessory.

Thermo Scientific™ OMNIC™ Paradigm Software's Multi-Component Search

Goals

To demonstrate the application of ATR-FTIR spectroscopy for the rapid, non-destructive identification and quantification of textile fibers using the Thermo Scientific™ Nicolet™ Summit™ FTIR Spectrometer. To show the advantages of Thermo Scientific™ OMNIC™ Paradigm Software's Multi-Component Search functionality and validate its accuracy against known standards.

Key terms

ATR-FTIR, Textile analysis, Fiber quantification, OMNIC Paradigm, Spectral libraries.

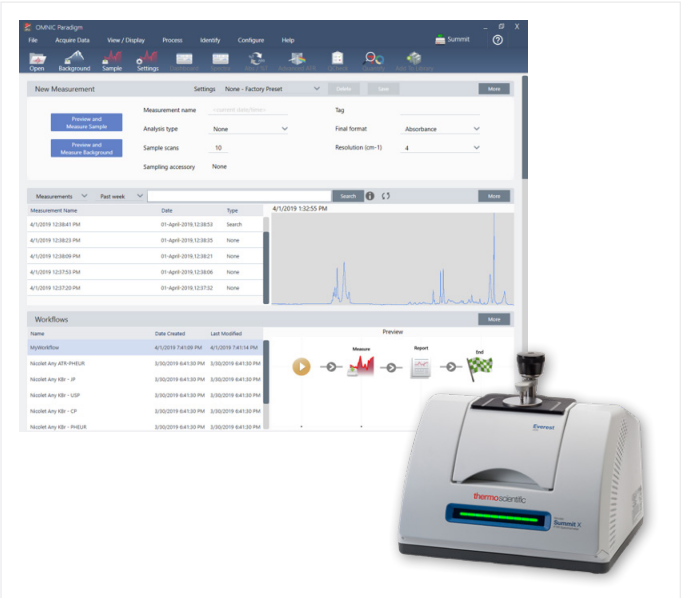
Key benefits

- Fast, non-destructive fiber analysis with minimal sample preparation.
- Accurate quantitative estimation for multi-component blends (error <3%).
- Automated analysis using OMNIC™ Paradigm's Multi-Component Search algorithm.
- High reproducibility and robustness using the Summit FTIR diamond ATR design.
- Reduced analysis time and improved workflow efficiency for textile QC.

Introduction

The identification and characterization of textile fibers are essential tasks in industries ranging from quality control and manufacturing to forensics and heritage conservation. Traditionally, fiber analysis has relied on optical microscopy and chemical solubility testing. These conventional methods, while long established, are often labor-intensive, time-consuming, and destructive. Microscopic observation allows basic morphological differentiation—a useful method for distinguishing natural fibers such as cotton, wool, or linen—but provides little insight into the chemical composition of modern regenerated and synthetic materials. Similarly, chemical dissolution and staining techniques require significant sample handling and may permanently alter or destroy the specimen. Compared to conventional approaches, vibrational spectroscopy, especially the Fourier Transform Infrared (FTIR) technique, provides a rapid, non-destructive, and reliable approach to textile analysis. The technique measures the interaction between infrared radiation and the molecular vibrations of polymers, providing a unique spectral fingerprint for each fiber type—whether natural (cotton, wool, silk, linen), regenerated (viscose, cellulose acetate), or synthetic (polyester, nylon, acrylic). When coupled with Attenuated Total Reflection (ATR) sampling, FTIR achieves superior surface sensitivity and reproducibility. The use of a diamond ATR crystal provides unmatched durability, chemical inertness, and a wide spectral range. The Thermo Scientific™ Nicolet™ Summit™ FTIR Spectrometer, in conjunction with Thermo Scientific™ OMNIC™ Paradigm Software, automates the identification and quantification process,making it indispensable for applications such as quality control, product authentication, and textile research. Recent research supports these findings. Peets et al. (2019) demonstrated that both ATR-FTIR and reflectance FTIR provide accurate classification of textile fibers. Their study confirmed that amide-based fibers such as wool, silk, and polyamide can be effectively differentiated using IR spectral features near 1700 cm^{-1}, reinforcing the robustness of ATR-FTIR for textile analysis applications.

This application note summarizes the methodology, results, and benefits of using ATR-FTIR spectroscopy with the Nicolet Summit FTIR spectrometer for rapid, reliable, and non-destructive textile fiber analysis.



Material and method

The textile samples were analyzed using a Nicolet Summit FTIR spectrometer equipped with a diamond ATR crystal accessory, operating at a spectral resolution of 4 cm^{-1} across the mid-infrared range (4000-500 cm^{-1}), with each spectrum representing the average of 20 scans to ensure optimal signal-to-noise ratio while maintaining reasonable acquisition times of approximately 30 seconds per measurement.

A diverse collection of textile samples was analyzed, including the following:

- Pure fiber samples: cotton, wool, silk, polyester, nylon, linen, viscose, and cotton
- Binary blends with known compositions (e.g., cotton/polyester blends at 50/50, 70/30 ratios)
- Tertiary and quaternary blends with known compositions

The analytical workflow consisted of collecting a fresh background spectrum before each sample measurement, carefully positioning the textile sample on the diamond ATR crystal with uniform pressure application via the integrated pressure tower to ensure optimal contact. In woven textiles, fibers are typically organized as threads of distinct materials rather than as mixed fibers within a single filament. As the ATR sampling area of the diamond crystal is small (~2 mm diameter), it is important to ensure representative measurements. In practice, the heterogeneity of fabrics does not significantly affect accuracy when measurements are made at several points on the sample surface. The statistical distribution of sampling across different fibers ensures consistent and representative results.

Spectral data were processed using the Multi-Component Search function in OMNIC Paradigm software, which uses a sophisticated search algorithm to compare sample spectra against a library of pure fiber spectra. The overall workflow combines spectral library development with automated analysis as follows:

1. Library creation: Pure component spectra are first collected and stored in a reference library.
2. Automated analysis and estimation of the quantification: Estimation of the quantification of components in textile blends is performed using the Multi-Component Search function in OMNIC Paradigm software. This sophisticated algorithm automatically determines the optimal linear combination of reference spectra weighted by their proportional contributions that best reproduces the measured sample spectrum. The user does not need to predefine the mixture composition, only the number of components expected.
3. Validation: Quantitative results were validated using known binary, tertiary, and quaternary blends, with typical prediction errors below 1% for binary blends.

While the results from the Multi-Component Search function provide numerical composition values, these should be interpreted as semi-quantitative estimations rather than absolute quantitative determinations derived from chemometric calibration models. The algorithm uses linear combination fitting of pure-component spectra to approximate blend composition based solely on 100% reference spectra. Unlike full chemometric methods (e.g., Partial Least Squares regression), this approach does not involve empirical calibration with multiple concentration levels. Therefore, although the compositional estimates demonstrate excellent agreement with known values, they are best regarded as accurate spectral proportion estimations, not formal quantitative analyses.

Results and discussion

Spectral identification of pure fibers

The ATR-IR analysis revealed distinctive spectral features for each fiber type (Figure 1):

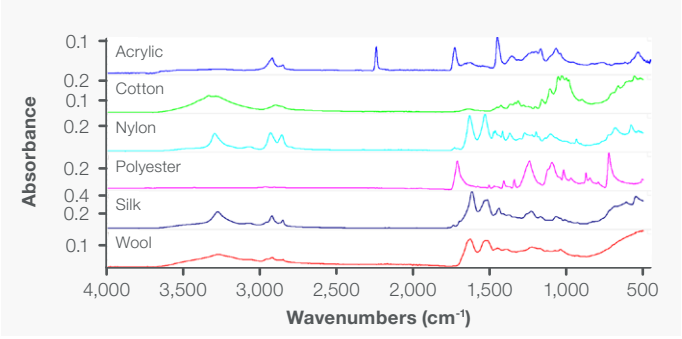


Figure 1. Example of ATR-IR spectra of pure fibers.

The main characteristic infrared absorption bands observed for each fiber type are summarized in Table 1, highlighting the distinctive vibrational modes used for material identification.

Fiber	Key vibrations
Cotton	O–H (3300 cm^{-1}), C–H (2900 cm^{-1}), C–O (1030 cm^{-1})
Wool / silk	Amide I (1650 cm^{-1}), Amide II (1550 cm^{-1})
Polyester	C=O (1720 cm^{-1}), C–O (1240 cm^{-1})
Nylon	Amide I (1640 cm^{-1})
Acrylic	C≡N (2240 cm^{-1})

Table 1. Characteristic vibrations of common textile fibers.

The spectral library created from these pure components served as the foundation for quantifying components in blended textiles.

Quantitative analysis of blended textiles

The Multi-Component Search algorithm produced highly accurate results across a range of sample compositions. Figure 2 illustrates the excellent agreement between the experimental spectrum of a 50/50 cotton/polyester blend and the composite spectrum calculated by the algorithm. The cumulative match value represents the combined contribution of each reference spectrum to the overall fit, while the overall match value quantifies the total similarity between the measured and reconstructed spectra. These indicators confirm the strong correlation and reliability of the algorithmic model.

Table 2 summarizes the quantification results for binary, tertiary and quaternary blends, comparing the known compositions with those determined by ATR-FTIR analysis:

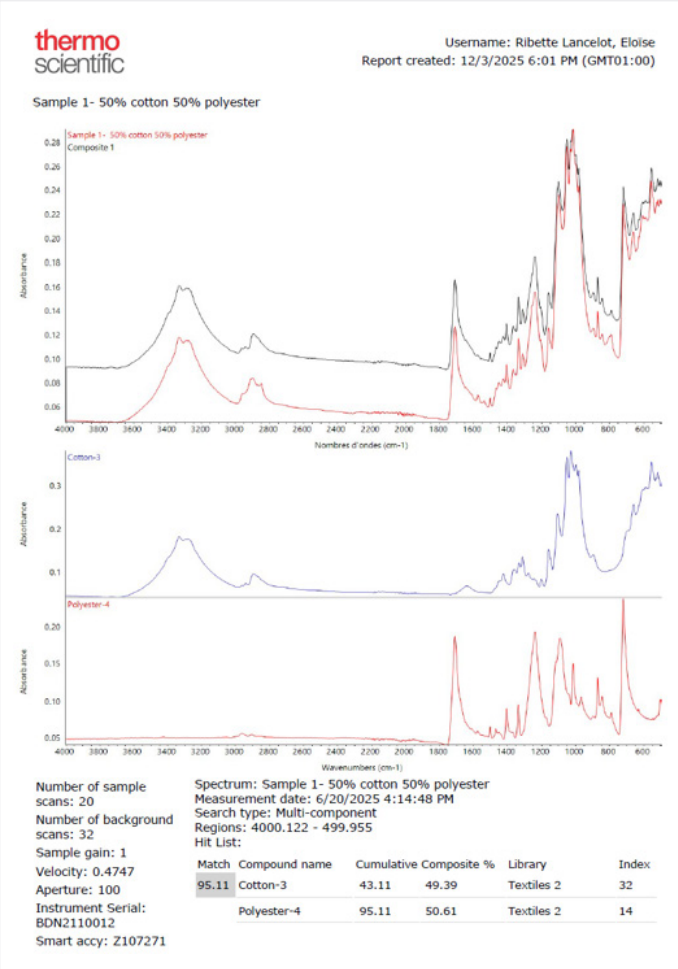


Figure 2. Example of Multi-Component Search.

Sample	Known composition	Measured component 1 (%)	Measured component 2 (%)	Measured component 3 (%)	Measured component 4 (%)
Sample 1	50% Cotton - 50% Polyester	49.39	50.61	-	-
Sample 2	70% Wool - 30% Polyester	71.00	29.00	-	-
Sample 3	50% Viscose - 50% Polyester	49.84	50.16	-	-
Sample 4	70% Viscose - 30% Polyamide	69.17	30.83	-	-
Sample 5	40% Acrylic – 30% Wool – 30% Polyamide	39.89	29.25	30.86	-
Sample 6	45% Acrylic – 35% Polyester - 20% Polyamide	45.22	37.53	17.25	-
Sample 7	45% Acrylic – 35% Viscose – 10% Wool – 10% Polyamide	42.44	32.39	11.48	13.69

Table 2. Quantification of known blends using the Multi-Component Search.

For simple binary blends (Samples 1-4), the measured compositions show exceptional agreement with the known values, with deviations typically less than 1%. This level of accuracy is particularly impressive considering the non-destructive nature of the technique and minimal sample preparation. While the deviations were slightly higher for complex mixtures (typically below 3%), the overall composition determination remained within acceptable limits for quality control applications. The method also demonstrated consistent accuracy across various fiber combinations, including natural/synthetic blends (cotton/polyester), protein/synthetic blends (wool/polyester), and regenerated/synthetic blends (viscose/polyester, viscose/polyamide). Although silk and wool exhibit similar amide absorption bands due to their proteinaceous structures, no blended samples containing both fibers were analyzed in this study. Silk was always tested as a pure component, and therefore direct assessment of potential misclassification between silk and wool was not performed. However, given the spectral differences in the amide I and amide II regions and the algorithm's demonstrated accuracy across other challenging blends, it is expected that the method would reliably distinguish between these two fibers when analyzed under similar conditions.

Conclusion

This study demonstrates the value of ATR-FTIR spectroscopy across the textile industry, from manufacturing quality control to product authentication and scientific research. The Multi-Component Search functionality enhances analytical capabilities by providing reliable composition estimates for complex textile blends with minimal user intervention, making it an ideal solution for modern textile analysis needs.

The approach offers several desirable features:

- Rapid measurements (<1 min)
- Minimal sample preparation
- High repeatability and accuracy
- Compatibility with natural, synthetic, and blended fibers

The methodology's combination of speed, ease of use, and precision makes it a powerful solution for quality control, product authentication, and research applications in the textile industry.

References

Peets, P., Kaupmees, K., Vahur, S., & Leito, I. (2019). Reflectance FT-IR spectroscopy as a viable option for textile fiber identification. Heritage Science, 7(93). https://doi.org/10.1186/s40494-019-0337-z

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