



Application Note AN-RS-001

用拉曼光谱仪识别聚合物

Rapid, nondestructive determination of colored plastics

Despite its precision in analyzing polymers, Raman spectroscopy struggles to accurately identify colored plastics due to fluorescence interference from pigments and additives. Polymer identification results may be less reliable under these conditions.

Utilizing multiple excitation wavelengths, comprehensive reference libraries, and employing advanced techniques all improve the reliability of Raman analysis. Metrohm's Raman solutions encompass all of these capabilities and

provide fast, accurate polymer identification. This Application Note focuses on Metrohm's advanced XTR® technology which improves identification of substances by eXTRacting the Raman signal from spectra with strong, occluding background fluorescence. Several types of colored polymers are examined, showing the benefits of using 785 nm Raman spectroscopy with the novel XTR fluorescence rejection technique.

INTRODUCTION

This Application Note describes the identification of poly(ethylene-vinyl acetate) – also known as PEVA, polystyrene (PS), and polypropylene (PP) in colored plastics with Raman spectroscopy.

Measurements with the handheld MIRA XTR

Raman spectrometer require no sample preparation and provide immediate and unambiguous results. Rapid and nondestructive determination takes place through application of the XTR algorithm followed by an automated library search.

EXPERIMENTAL

All spectra were measured using MIRA XTR, at a wavelength of 785 nm and with Orbital Raster Scan (ORSTM), in auto-acquisition mode. Occluding fluorescence initiates XTR algorithms automatically, returning a high-resolution, baselined spectrum of the material.

All samples in this study were common household and office materials, tested through direct contact using the intelligent Universal

Attachment (iUA).

Metrohm's Illicit and General Chemicals Library is a comprehensive spectral database of common materials for accurate identification of mixed samples. Each sample was identified using this library in MIRA Cal software. A range of polymer standards is displayed in **Figure 1**, illustrating their distinct fingerprints in the Raman spectrum.

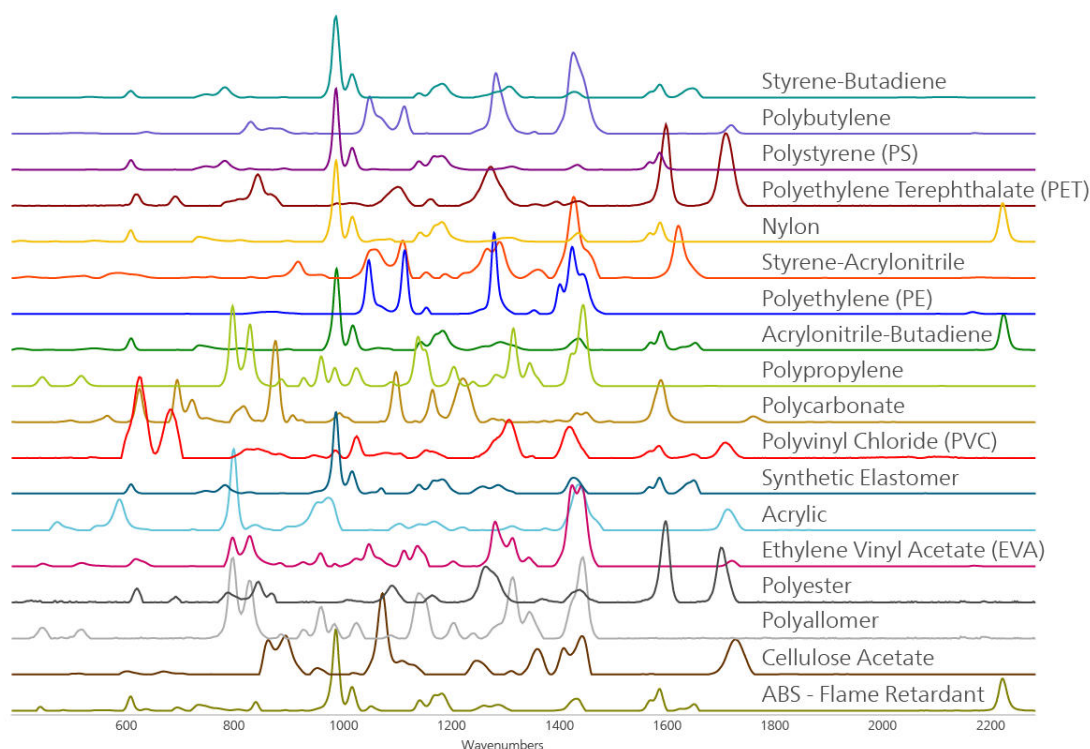


Figure 1. Stacked Raman library spectra for a wide range of polymer samples demonstrate how distinct the Raman fingerprint peaks are for each material.

RESULTS

The Raman spectra of various items composed of unknown polymers in different colors were

collected (**Figure 2**) and checked against the MIRA Illicit and General Chemicals Library.

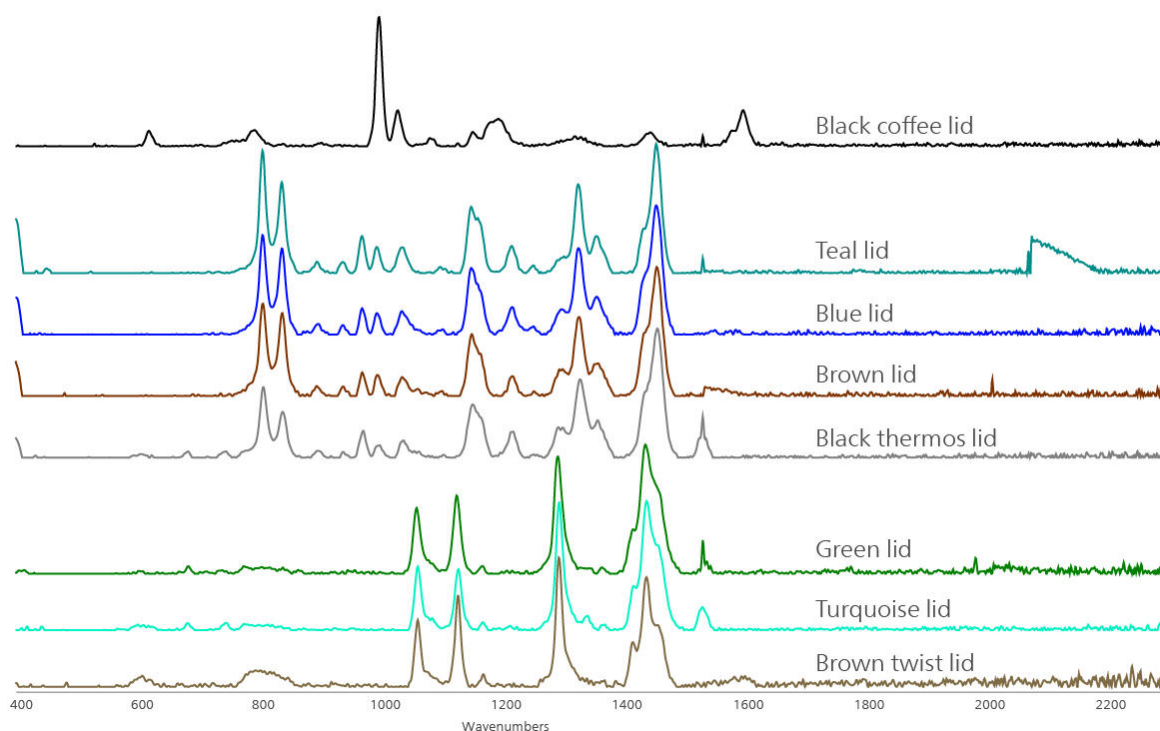


Figure 2. Resolved, stacked Raman spectra of various strongly colored plastics.

Results display on the device within seconds and include the name, CAS number, and HQI (Hit Quality Index) – a measure of the strength of correlation between sample and library spectra.

Figure 3 demonstrates the accuracy of data collected from even strongly colored samples by comparing sample and library spectra.

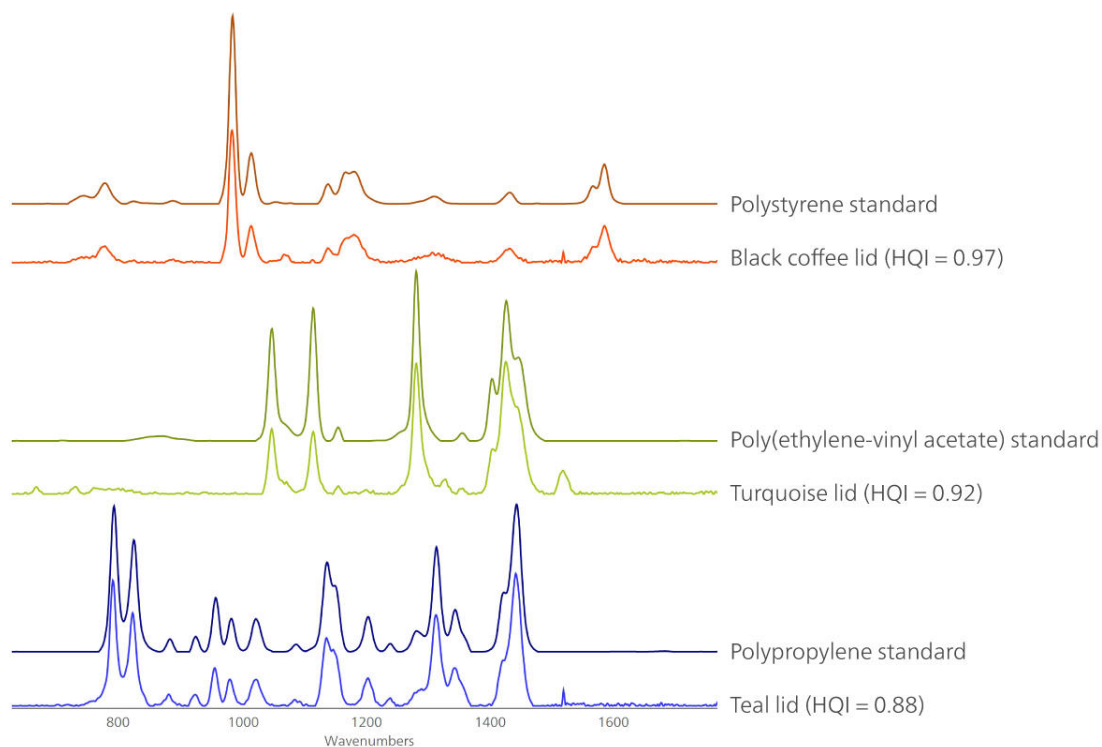


Figure 3. A direct comparison of experimental and library spectra demonstrates the accuracy and resolution of both spectra and results. Each plastic sample matched to a single library spectrum with high HQI values.

CONCLUSIONS

Metrohm has unique solutions that overcome the problem of fluorescence while retaining all the benefits of 785 nm interrogation — fast,

accurate, nondestructive identification of colored polymers.

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CONFIGURATION



MIRA XTR Advanced

MIRA XTR 是高功率 1064 nm 系统的替代品。在先进的计算处理的支持下,MIRA XTR 使用更灵敏的 785 nm 激光器和 XTR 算法从样品荧光中提取 Raman 数据。MIRA XTR 还配有轨道光栅扫描 (ORS) 技术,可更好地覆盖样品,从而提高结果的准确性。

MIRA XTR Advanced 套件包括校正标准件、智能通用附件、直角附件、样品瓶附件和 Mira SERS 附件。适用于任何类型分析的完整套件。3B 类操作。MIRA XTR 支持瑞士万通手持式拉曼功能库。



iUA

iUA 是一款 MIRA 系统用智能 3 位置采集光学附件。iUA 综合了通用附件的灵活性,以及 MIRA SmartTip 附件的只能操作模式。每个位置都显示了该位置的理想用途,即,表面、袋子或水瓶。



MIRA

MIRA(Metrohm Instant Raman Analyzer)非法材料库,包括药物、TIC、TIM、前身和常规化学品。