Identifying polymers with Raman spectroscopy

This Application Note describes the Raman spectroscopy identification of polymers such as ABS, PE, PS, PET and PMMA in various dyes. Rapid and non-destructive determination takes place after a suitable spectrum database has been created. Measurements with the Raman spectrometer Mira M-1 require no sample preparation and provide immediate and unambiguous results.

INTRODUCTION

Today's industry, but also daily life, cannot be imagined without polymers. Handheld Raman spectroscopy is uniquely suited for the identification of commonly used polymers, because evident results are obtained within seconds. Furthermore, because Raman analysis is nondestructive, later use or recycling of the sample remains unrestricted.

In this study, a library of widespread polymers of different colors was built and subsequently used for the identification of unknown polymer samples.
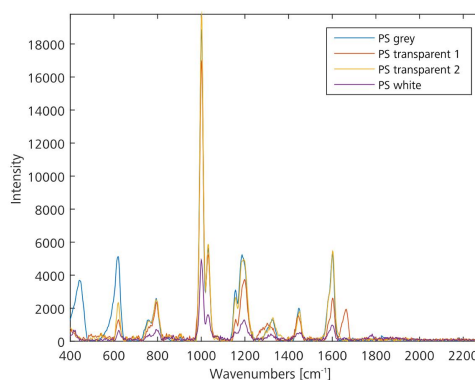

Figure 1. Raman spectra of differente polystyrene samples

EXPERIMENTAL

All spectra were measured using the Mira M-1 handheld Raman spectrometer in auto acquisition mode, i.e., integration times were determined automatically. A laser wavelength of 785 nm and the Orbital-Raster-Scan (ORS) technique were used. As many of the polymer samples were very thin, spectra were recorded with the point-and-shoot adapter which is suitable for a short working distance (SWD).

An extensive collection of ABS (Acrylonitrile butadiene styrene), PA (Polyamide), PC (Polycarbonate), PE (Polyethylene), PP (Polypropylene), PS (Polystyrene), PET (Polyethylene terephthalate), PVC (Poly(vinyl chloride)), and PMMA (Poly(methyl methacrylate)) polymer standards and samples of different colors was used to build a comprehensive library with the Mira Cal software.

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RESULTS AND DISCUSSION

For each polymer kind, one spectrum (i.e., one color) was chosen, and these spectra were superimposed. The overlay (Figure 2) shows that each of the polymers has a unique spectrum that differentiates it from the other analyzed plastics. The spectral area containing the majority of peaks reaches from 600 to 1800 cm^{-1}; proving that the spectral range of Mira M-1 is appropriate for the studied polymer samples.
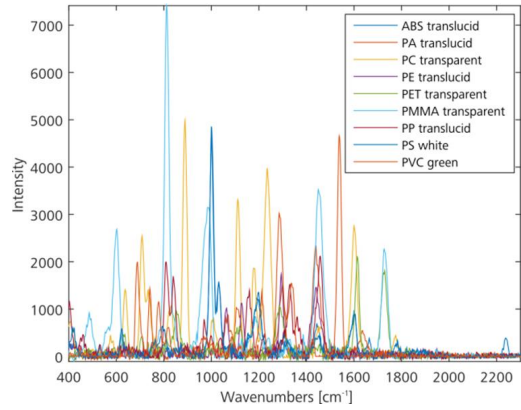

Figure 2. Overlay of the spectra of selected polymer samples (plot made with MATLAB)

The spectra of various everyday and laboratory items of unknown polymers and different colors (Figure 3) were checked against the library. The library, which had been built using polymer standards of different colors, was helpful in identifying the test samples: Opaque samples were identified color-specifically, while transparent and translucent samples were, in many cases, identified only as such.
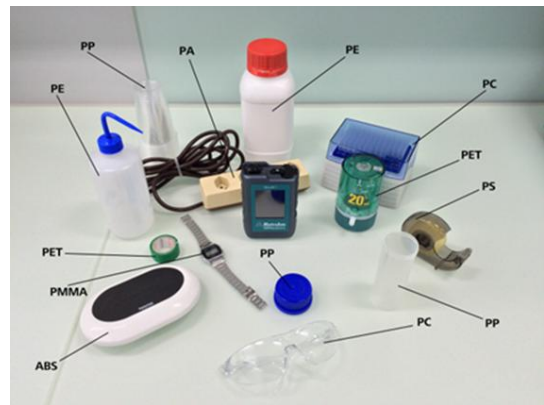

Figure 3. Items measured against the library

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As can be seen in **Figure 4**, the signals of dark samples, such as black, grey, and dark blue ones, were very low in intensity and no polymer specific peak could be observed. This is a phenomenon found in many spectroscopic techniques and is due to the absorption of the laser light by carbon black.

Because identification of the dark samples (mainly dark grey and black) was not possible, they were excluded from the library, and only transparent, translucent, and light-colored samples were kept in the library.

The spectral correlation values, which indicate how well the sample spectrum matches the reference spectrum in the library, were higher than 0.90 for all measured samples (including, but not limited to, the ones shown in **Figure 3**). All polymer samples were thus unambiguously identified using the Mira M-1 spectrometer.

Figure 4. Overlay of the spectra various dark-colored polymers

CONCLUSIONS

This study shows that Mira M-1 can be used to identify unambiguously various polymers of different colors by measuring their spectra and matching them with a library. The identification takes just a few seconds.

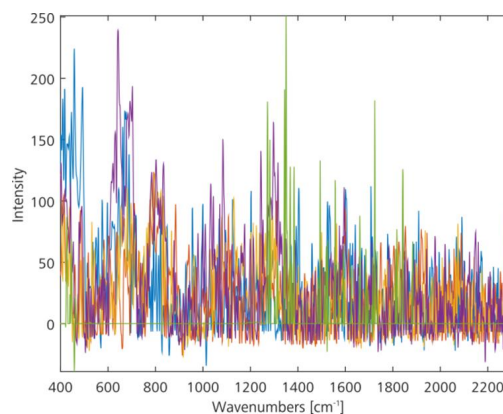Problems arise only when dark-colored polymers have to be analyzed. Such samples strongly absorb the spectrometer's laser light and thus, some polymer-specific peaks don't appear in the spectrum. Dark-colored samples, therefore, cannot be identified by Raman spectroscopy.

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CONFIGURATION

MIRA P Advanced

Le Metrohm Instant Raman Analyzer (MIRA) P est un spectromètre Raman portable performant qui s'utilise pour les déterminations rapides et non destructives et le contrôle des matériaux les plus divers, comme les principes actifs pharmaceutiques et les excipients. De très petite taille, le MIRA P est pourtant très robuste et dispose d'une structure de spectrographe haute efficacité, équipée de notre technologie « Orbital Raster Scan » (ORS) inédite. MIRA P satisfait aux prescriptions FDA 21 CFR partie 11.

Le Advanced Package comprend une lentille avec laquelle les matériaux peuvent être analysés directement ou dans leur conditionnement (classe de laser 3b), ainsi qu'un support de flacon pour analyser les échantillons dans des flacons en verre (classe de laser 1).

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