

筑路材料的拉曼光谱分析

Various solid materials used in road construction were analyzed using a handheld Raman spectrometer. The investigated materials are commonly used pigments and resins such as CaCO_3 , TiO_2 , and DEGALAN®. The measured

spectra differed remarkably from each other. To evaluate the main differences in the chemical structures, the peaks of the different spectra were assigned to the functional groups causing them.

INTRODUCTION

Different materials such as paints, (white) pigments, and resins are commonly used in the construction of roads. Together with glass beads (used for night-visible road marking) and various other materials, they help us to get safely from A to B.

In this study, different roadmaking materials

were analyzed using the Mira M-1 handheld Raman analyzer. The gathered spectra were compared with each other to see the main differences in the functional groups. The analysis proved that Mira M-1 is suited for the differentiation of such materials.

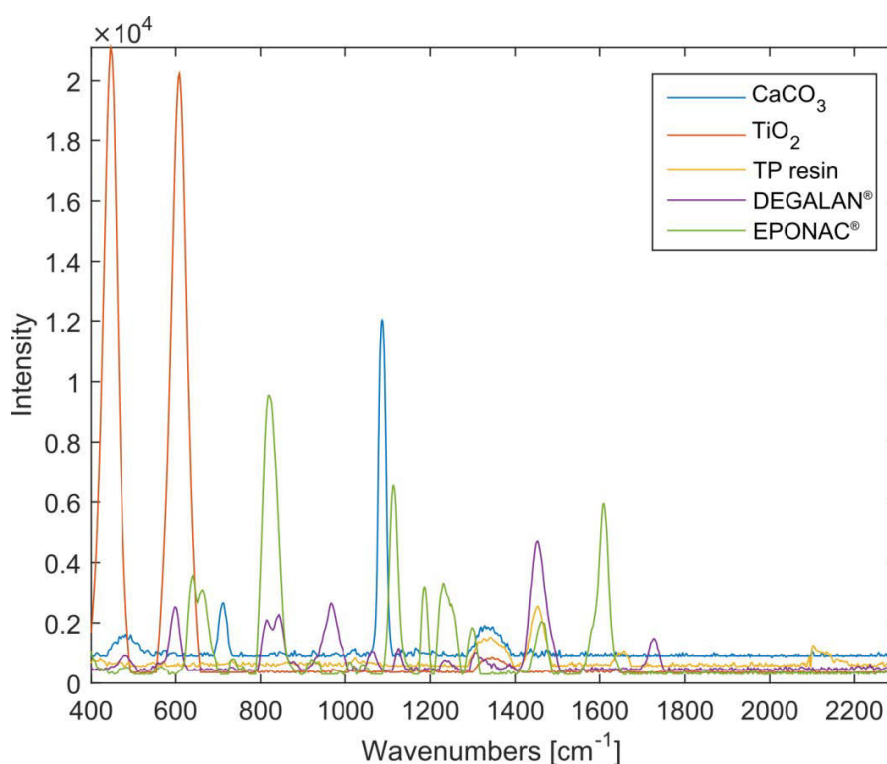


Figure 1. Overlay of spectra of different roadmaking materials

EXPERIMENTAL

All spectra were measured using the Mira M-1 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 applied. The measurements were done in small sample vials with the vial holder adapter.

The following samples were investigated:

1. Chalk (CaCO_3)

2. Titanium dioxide (TiO_2)

3. EPONAC® resin

4. TP resin

5. Pigment yellow

6. Pigment blue

7. Pigment red

8. DEGALAN® resin

RESULTS AND DISCUSSION

The measurement of calcium carbonate furnished a clear spectrum with two main peaks at 712 cm^{-1} (symmetric O–C–O bending

vibration) and 1087 cm^{-1} (symmetric stretching vibration).

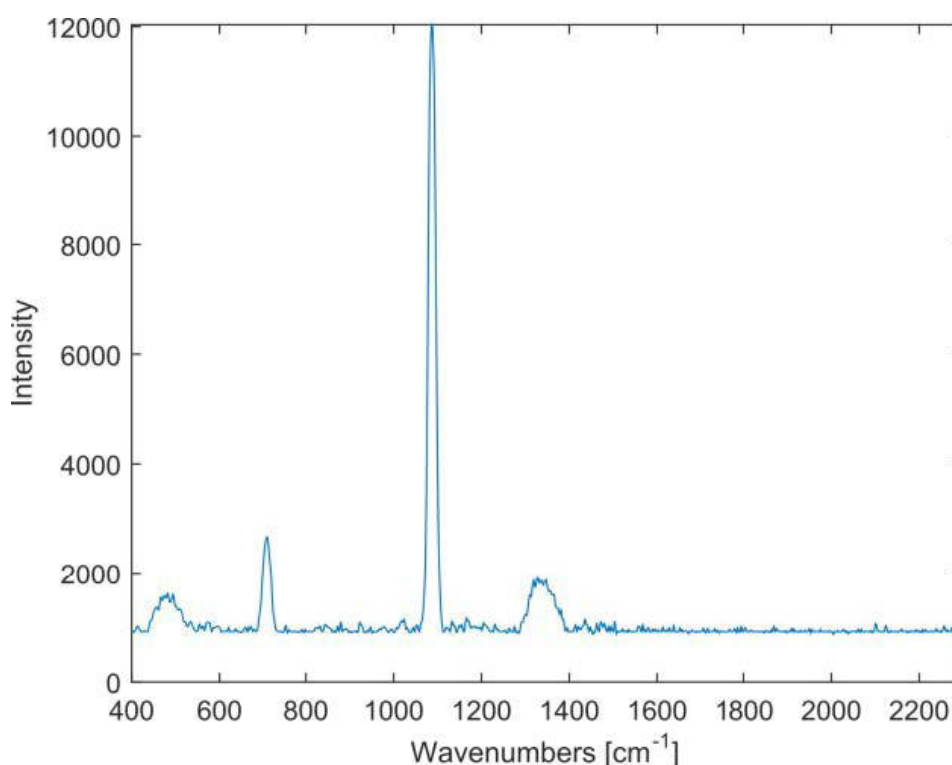


Figure 2. Spectrum of calcium carbonate.

Looking at the titanium dioxide spectrum, one can see two main peaks which give information on the present crystal modification (rutile or

anatase). Two peaks represent rutile, while three peaks are typical for anatase because of its crystal symmetry.

Both peaks are symmetric stretching vibrations and belong to O–Ti–O (446 cm^{-1}) and Ti–O (609 cm^{-1}). In the case of anatase, the peak at 446 cm^{-1}

¹ is split in two. This makes it easy to differentiate between rutile and anatase.

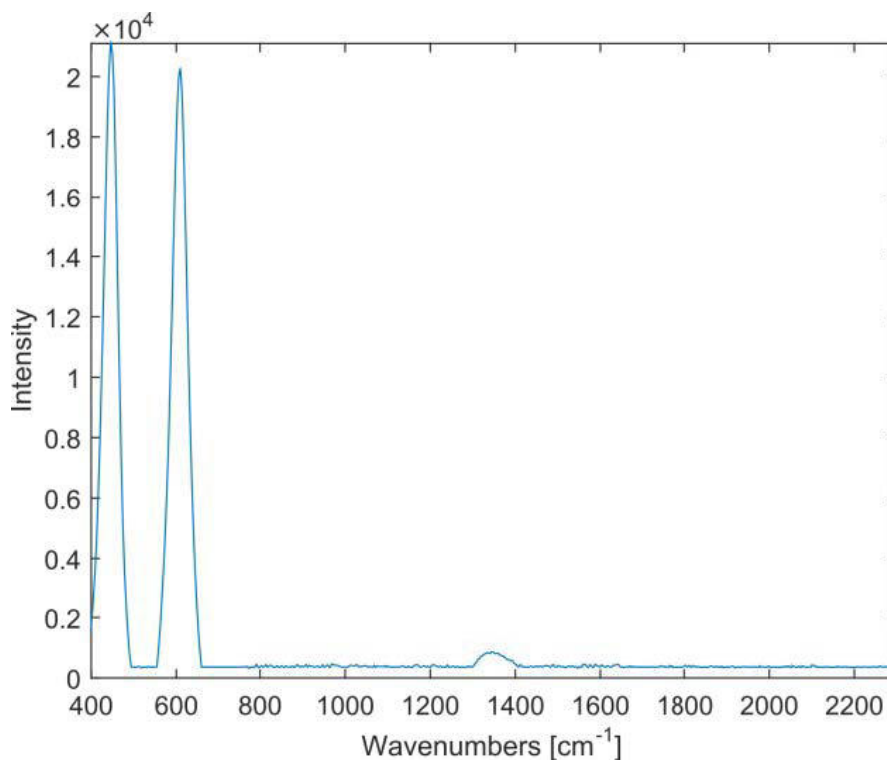


Figure 3. Spectrum of TiO₂ (rutile).

A glance at the spectra of typical resins such as EPONAC® or DEGALAN® reveals nicely separated

peaks which can be assigned to their corresponding functional groups (see below).

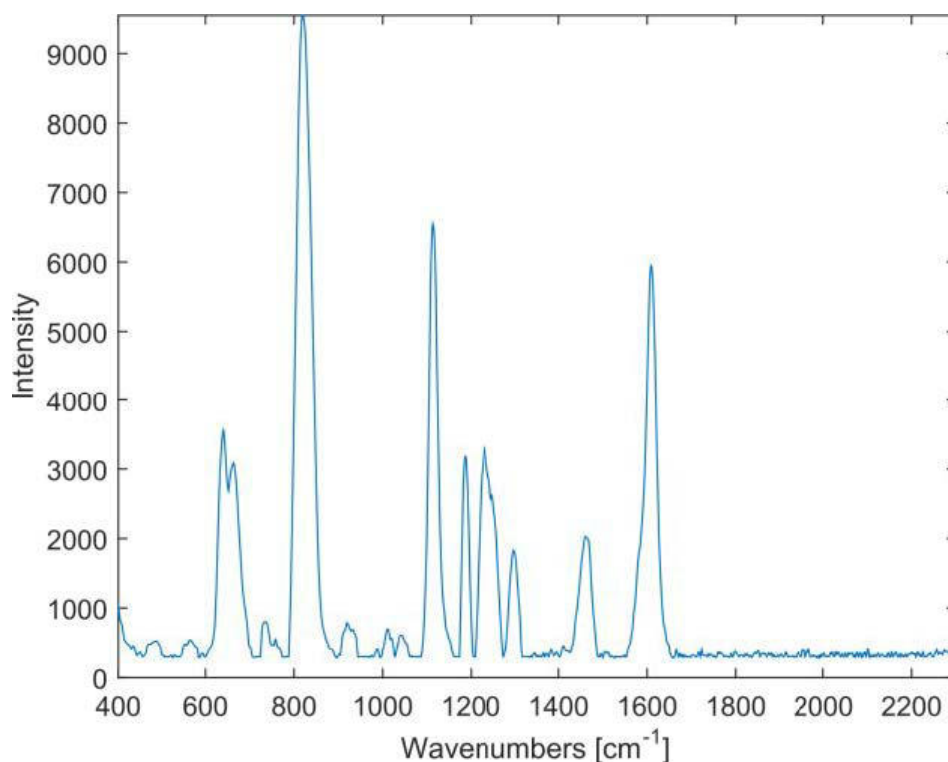


Figure 4. Spectrum of the EPONAC® resin.

Table 1. Peaks observed in the EPONAC® spectrum.

Peak [cm ⁻¹]	Description
640	Cyclic vibration (para-substituted benzene)
819	C–H bending vibration (para-substituted benzene)
1000	Various C–C stretching vibrations
1113	C–OH stretching vibration
1189	C–(CH ₃) ₂ stretching vibration
1231	C–O
1248	C–H (benzene)
1298	–CH ₂ – twisting vibration
1461	–CH ₂ – bending vibration
1609	C=C

RESULTS AND DISCUSSION

The peaks are very characteristic for para-substituted benzene and confirm that EPONAC® is a copolymer of bisphenol A (BPA) and another component.

When comparing the EPONAC® spectrum with the DEGALAN® spectrum (see **Figure 5**), it is

obvious that the peak of the benzene at 1600 cm^{-1} is missing. The peak around 1700 cm^{-1} , together with the peaks slightly below and above 1200 cm^{-1} , is characteristic for carbonyl groups. In addition to that, the C–C peaks are more distinct for EPONAC® than for DEGALAN®.

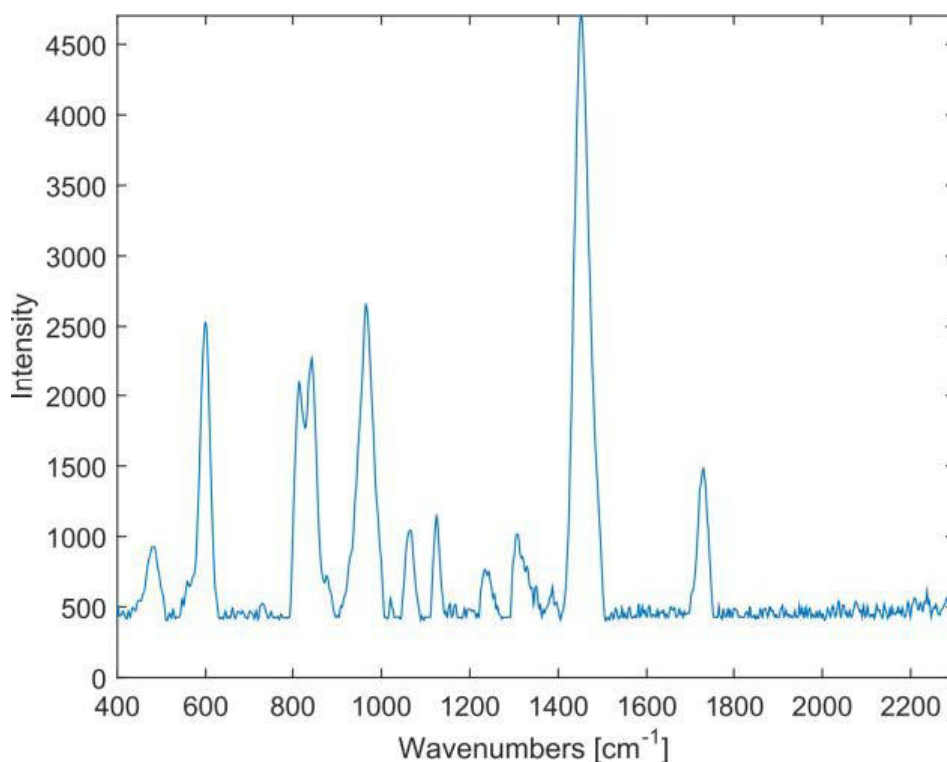


Figure 5. Spectrum of the DEGALAN® resin

Table 2. Peaks observed in the DEGALAN® spectrum.

Peak [cm ⁻¹]	Description
599	–COO bending vibration
814	Propionate bending vibration
843	C–CH ₃ stretching vibration
965	C–C stretching vibration
1065	C–COO stretching vibration
1125	C–O
1234	C–O
1308	–CH ₂ – twisting vibration
1452	–CH ₂ – bending vibration
1728	C=O carbonyl group, ester

Using these differences, it is easy to discriminate between the resins and also between resins and

pigments (see **Figure 6**).

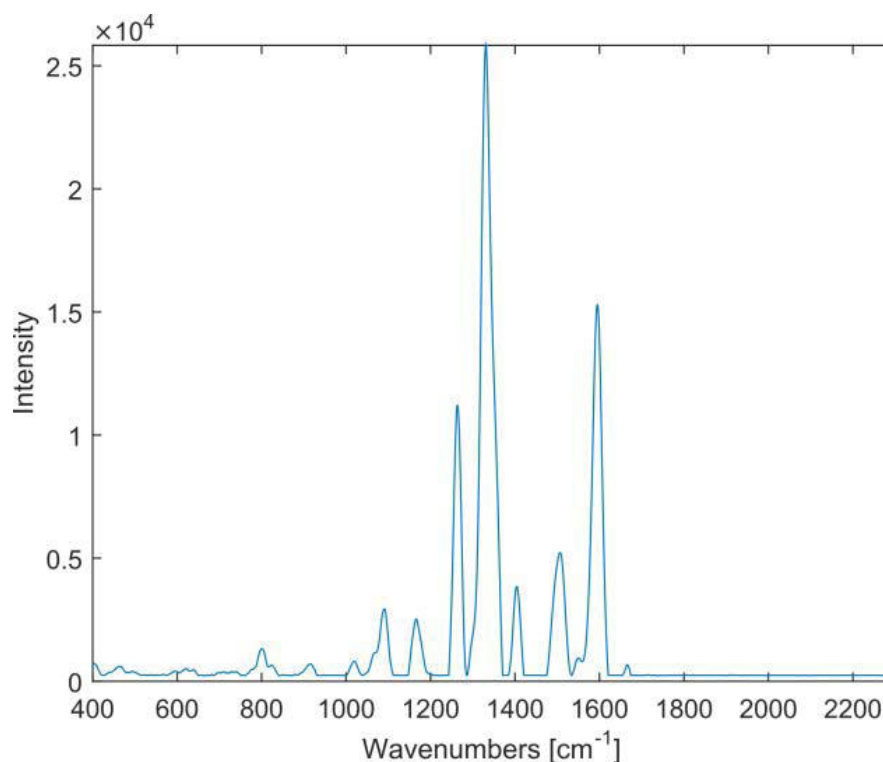


Figure 6. Spectrum of the yellow pigment «Hansa®-Brilliantgelb»

CONCLUSIONS

Because of the great differences in their spectra, handheld Raman spectroscopy is ideally suited for the analysis of materials used in road construction. The investigation of the spectra

showed that there are significant differences in the functional groups of the materials, thus allowing the identification with handheld Raman systems such as Mira M-1.

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CONFIGURATION



MIRA P Advanced

瑞士万通快速拉曼分析仪 (MIRA) P 是一款性能强大的手持式拉曼光谱仪,可用于各种材料的快速无损测定和验证,例如药物有效成分和赋形剂。MIRA P 小而坚固,配备了瑞士万通的ORS技术。MIRA P 符合 FDA 联邦法规 21 章第 11 款的规定

。Advanced Package 包含一个附加透镜,可用它直接分析材料或者在材料容器分析(3b 级激光器),还有一个小管支架套筒用于分析玻璃小管中的样本(1 级激光器)。