Application Note 410000029

See-through ID with Raman technology

Through-package identification with 1064 nm Raman

Raman spectroscopy is widely used for rapid, nondestructive identification in scientific, medical, and law enforcement settings. Traditionally, it is used to sample materials directly or through transparent/translucent barriers, which limits its practicality in the field. A new and unique advancement—Raman identification through opaque packaging—overcomes this limitation. Through-package analysis permits easier, safer, and faster material identification and avoids contact with unknown substances for warehouse inspections, first responders, and customs agents.

INTRODUCTION

See-through Raman spectroscopy (ST) is a recently developed technology that expands the capability of Raman spectroscopy to measure samples through packaging materials. The technology is available on the Metrohm TacticID-1064ST (TID1064ST) handheld Raman system with 1064 nm laser excitation. This design enhances the relative intensity of the signal from deeper layers, increasing the effective sampling depth and permitting measurement of materials inside visually opaque containers.

ST technology also incorporates a large sampling area. The larger sampling area has the additional advantages of preventing sample damage through reduced power density and improving measurement accuracy of heterogeneous materials.

ST AND COMMON CONTAINERS

Through-package identification of materials in white polyethylene (PE) bottles (a common packaging for solid chemicals) and other opaque packaging such as white and manila envelopes is demonstrated with 1064 nm Raman spectroscopy. The container contribution is removed with advanced identification algorithms, and the sample is correctly identified. Identification through colored plastic, multiple opaque layers, and thick glass can be made with TID1064ST. Identification of sodium benzoate inside a white PE bottle is given in **Figure 1**.

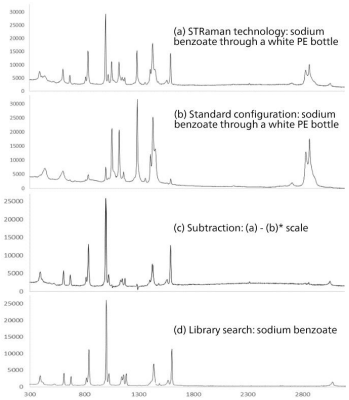

Figure 1. ST identification of sodium benzoate through a white polyethylene bottle: (a) ST scan, (b) standard Raman scan, (c) subtraction: (a) - (b)* scale, and (d) library sodium benzoate spectrum.

Coated tablets can also be identified. ST technology penetrates the coating layer and measures the Raman spectrum of the underlying tablet. This allows the instrument to effectively sample through colored and dark materials, enabling reliable analysis without being obscured by surface effects. **Figure 2** shows the Raman spectrum of a tablet with a very dark coating. Despite interference from the coating, signature peaks are still apparent.

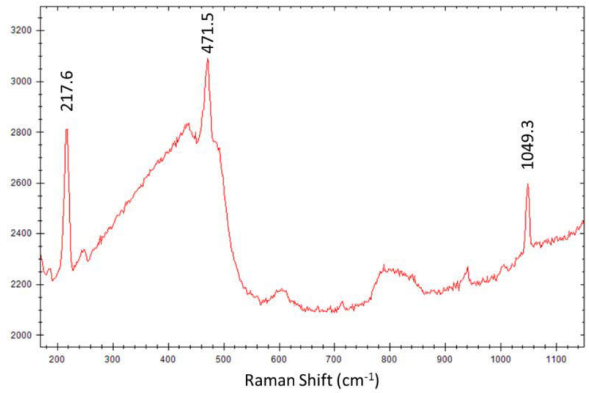

Figure 2. Example of a 1064ST spectrum of a tablet with very dark coating.

APPLICATIONS OF ST TECHNOLOGY

Many raw materials are packaged in single- or multi-layer kraft paper sacks, often with a plastic lining. Brown kraft paper exhibits strong fluorescence under 785 nm Raman excitation, which can hinder material identification. However, with ST and 1064 nm Raman technologies, accurate identification is possible even through such challenging packaging.

To demonstrate, we evaluated the ability of ST Raman at 1064 nm to identify several common excipients—varying in Raman scattering strength—through multi-layer paper bags used in pharmaceutical raw material packaging. As shown in Table 1, even trisodium phosphate, a notoriously low Raman scatterer, was correctly identified. A positive ID requires a hit quality index (HQI) above 85 that exceeds the second-best hit by at least 2 points. In contrast, trisodium phosphate could be identified only through white kraft paper using 785 nm excitation.

Figure 3 shows the spectrum of trisodium phosphate as measured through a two-ply bag of white and brown kraft paper, with a positive library search result. Although the spectrum is dominated by spectral features from the paper bag, TID1064ST is capable of reliably identifying trisodium phosphate.

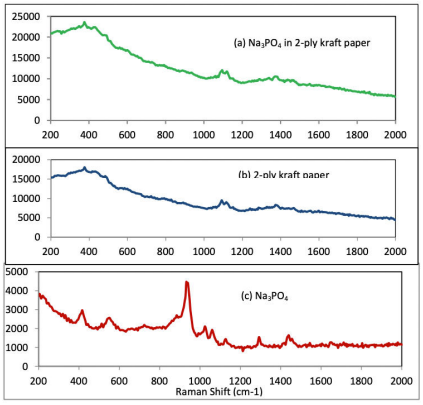

Figure 3. Identification of trisodium phosphate in bilayer bag of white and brown kraft paper layers: (a) ST technology, (b) standard Raman configuration, and (c) pure spectrum of trisodium phosphate.

Table 1. Positive identification of samples in kraft paper bags using 1064 nm ST technology.

Packaging material and # layers	Calcium carbonate ($CaCO_3$)	Dextrin	Cyclodextrin	d-Maltose H_2O	Trisodium phosphate (Na_3PO_4)
1 white kraft + 1 brown kraft	97.7	96.7	95.6	93.8	93.2
2 layers of brown kraft	97.6	92.2	91.6	90.9	88.7
2 layers of white paper	96.8	98.025	95.2	95.0	94.9
1 white kraft paper with blue bands + 1 brown kraft paper	95.1	92.8	91.4	91.35	89.0
1 white paper + 1 woven fiber	96.2	95.7	93.2	92.6	91.1
1 white kraft + 1 plastic film + 1 brown kraft	96.1	91.8	92.0	90.7	88.4
1 white kraft + 2 brown kraft	97.4	94.6	94.0	92.9	93.0

CONCLUSION

The ability to measure samples inside packages, eliminating the need for sample contact, is one of the major advantages of Raman spectroscopy. Metrohm's ST technology permits measurements through opaque materials: from white plastic bottles to fiber and kraft paper sacks, envelopes, and even skin. This supports easy adoption of this spectroscopic tool in many working environments, from the laboratory to the field. The combination of ST technology and 1064 nm laser excitation addresses even dark and highly colored packaging materials. This makes Raman suitable for many new potential users, for whom it has not previously been a viable tool.

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CONFIGURATION

TacticID-1064 ST

TacticID®-1064 ST 是一款 1064 nm 手持式拉曼分析,用于快速炸、毒品和其他可疑材料。TacticID-1064 ST 的透功能可以穿不透明和透明的包装品行非破坏性分析,同可着示品威,以便急救人、安全人、法部、炸小、海和境保局以及危物品理小迅速采取行,并保持品接触最小。

TacticID-1064 ST 利用成熟的拉曼光技,合得利的 STRaman® 技,使用能地未知化学品、毒品、物、炸和多其他物行可行的(甚至可穿不透明的障碍),从而大大降低了操作不定性和。

TacticID-1064 ST 配有 1064 nm 激光激功能和用于透用的 ST 配器,可描大的品区域,生无光光,从而使用能直接穿包装硬的街品、不均匀的混合物和材料。

此防等 IP68 的系配有触摸屏和/或硬件按界面的高亮度示屏,使用方便,甚至可穿防装。

瑞士万通 TacticID-1064ST 基本版套装包括透附件、通用附件、聚乙附件、固的手提箱、、源和激光目。

TacticID-1064 ST Advanced

TacticID®-1064 ST 是一款 1064 nm 手持式拉曼分析,用于快速炸、毒品和其他可疑材料。TacticID-1064 ST 的透功能可以穿不透明和透明的包装品行非破坏性分析,同可着示品威,以便急救人、安全人、法部、炸小、海和境保局以及危物品理小迅速采取行,并保持品接触最小。

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瑞士万通 TacticID-1064ST Advanced 套装包括透附件、通用附件、SWD 附件、品瓶支架、LWD 附件、直角附件、聚乙附件、透反射探、固的手提箱、、源和激光目。