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See Through Raman Technology: Expanded capabilities for through package identification using 785 nm and 1064 nm excitation Raman

Raman spectroscopy is a form of molecular spectroscopy that gives specific molecular information of materials. Raman is used widely for rapid, non-destructive, non-invasive identification testing in chemical, material, pharmaceutical and biomedical research, in medical diagnostics, and increasingly by law enforcement. A limitation of Raman spectroscopy is that samples can only be measured directly, or through transparent containers. Though this is not really a limitation in a laboratory environment, for field-deployed handheld instrumentation the preference is to identify samples as they are, with minimal sample handling and opening of packages. Raman identification through opaque packaging would make the technology easier to use for incoming raw materials in warehouses and for first-responders, customs agents and others who need to rapidly identify materials without touching them.

See through Raman Spectroscopy (STRaman™) is a newly developed technology that expands the capability of Raman spectroscopy to measure samples beneath diffusely scattering packaging material. Conventional Raman typically has a very small sampling area with a high power density at the laser focal point on the sample, which means that only a limited portion of a sample is measured, and samples may heat or burn. The ST technology has been designed to overcome these issues. The technology is available on portable and handheld Raman system with 785 nm and with 1064 nm laser excitation laser. The STRaman™ technology features a much larger sampling area than the confocal approach. This design enhances the relative intensity of the signal from the deeper layers, thereby increasing the effective sampling depth, allowing the measurement of material inside visually opaque containers. The larger sampling area has the additional advantage of preventing sample damage by reducing the power density, as well as improving measurement accuracy by eliminating heterogeneous effect.

We have demonstrated the abilities of the 785 nm STRam for through-package identification (1,2) such as white polyethylene bottles, a common packaging for solid chemicals, and other opaque packaging such as white and manila envelopes. A spectrum of material underneath opaque layers is collected because of the technology's increased sampling depth. Coupled with advanced identification algorithms, the package Raman signal contribution is removed and the sample correctly identified. Identification through colored plastic, multiple opaque layers and thick glass can be made with the STRaman™technology with 785 nm excitation. An example of identification of sodium benzoate inside a white PE bottle is given in Figure 1. Coated tablets can also be identified as the See-through technology penetrates the coating layer and measures the Raman spectrum of the underlying tablet. And because the power density of the system is lower than the highly focused signal used in conventional Raman, even colored tablet coatings and dark samples can be measured without laser burning of the surface. Figure 2 shows the Raman spectrum of a black powder collected with the STRam at full laser power without suffering any burning.

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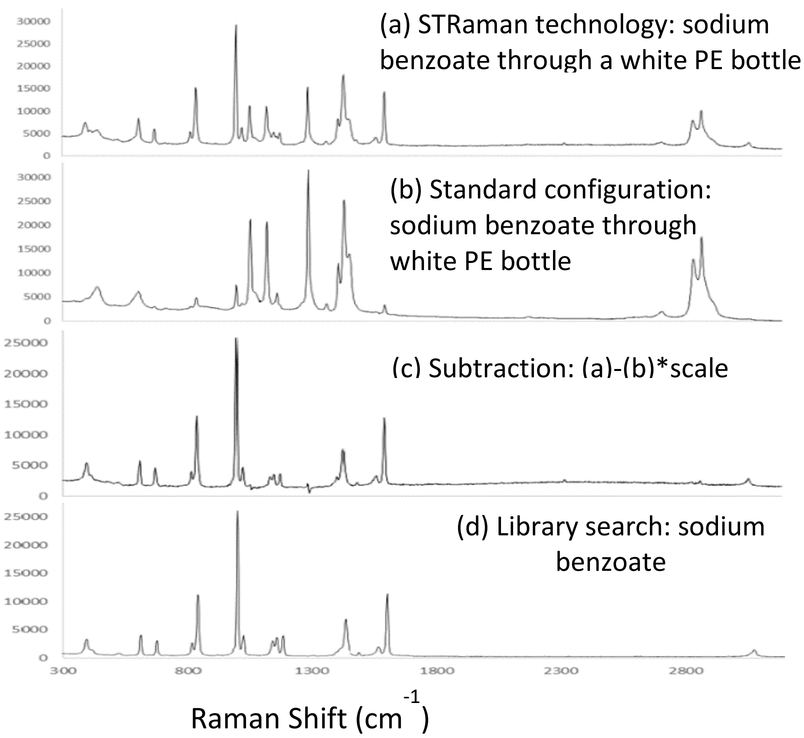

Figure 1: STRam identification of sodium benzoate through a white polyethylene bottle: (a) Spectrum measured through the bottle using the STRaman™technology; (b) spectrum measured with a standard Raman configuration; (c) the result of scaled subtraction of (b) from (a); and (d) pure spectrum of sodium benzoate.

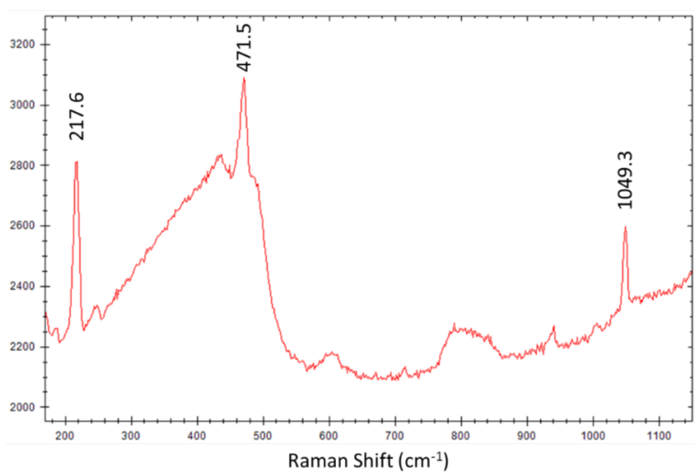

Figure 2: STRam spectrum of dark powder.

Many raw materials are supplied in kraft paper sacks of single or multiple layers, sometimes with a plastic lining layer as well. Brown kraft paper, as well as many other dark colored materials, has a strong

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fluorescence when measured with 785 nm Raman. Applying the STRaman technology to our 1064 nm Raman systems enables material identification even through such challenging packaging materials. To illustrate, we obtained a number of different multi-layer paper bags used as containers of raw material at pharmaceutical companies, selected several commonly used excipients with varying Raman scattering strengths, and tested the ability of STRaman™ at 1064 nm to identify them through the paper bags. As table 1 shows, even the weakest Raman active material trisodium phosphate, which is roughly 40 times weaker than calcium carbonate, is positively identified (a positive ID means the correct chemical is listed as the top hit, with a hit quality index above a set threshold, and higher than the 2nd hit by a set margin. The HQI threshold is set to 85, and the margin is set to 2 in these tests). At 785 nm excitation, however, trisodium phosphate can only be successfully identified through the white kraft paper bag.

Packaging Material	Calcium Carbonate ($CaCO_3$)	Dextrin	Cyclodextrin	d-Maltose H_2O	Trisodium Phosphate (Na_3PO_4)
2 layers: 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
2 layers: 1 white kraft paper with blue bands + 1 brown kraft paper	95.1	92.8	91.4	91.35	89.0
2 layers: 1 white paper + 1 woven fiber	96.2	95.7	93.2	92.6	91.1
3 layers: 1 white kraft + 1 plastic film + 1 brown kraft	96.1	91.8	92.0	90.7	88.4
3 layers: 1 white kraft + 2 brown kraft	97.4	94.6	94.0	92.9	93.0

Table 1: Positive identification of samples in kraft paper bags using 1064 nm STRam system.

Figure 3 shows the spectrum of trisodium phosphate as measured through a two ply bag of white and brown kraft paper, with positive library search result. Although the spectrum is dominated by fluorescence and Raman features from the paper bag, the algorithm used in STRaman is capable of extracting from it the signature of trisodium phosphate and reliably identify it.

Additional advantages of the STRam technology are its greater sampling area. Due to this design Raman can be used more widely and give more repeatable results for heterogeneous samples, such as mixed powders or natural products.

The ability to measure samples inside packages, eliminating the need for sample preparation, is one of the major advantages of Raman. The advancements brought forth with STRaman technology take that a step further to measuring through opaque packages – from white plastic bottles to fiber sacks, to kraft paper sacks, envelopes and even skin – allows easy adoption of this spectroscopic tool in many working environments, in the laboratory or in the field. The development of the technology for both 785 nm and 1064 nm laser excitation addresses even dark and highly colored packaging that are influenced by fluorescence. This opens Raman to many new potential users, for whom it has not previously been a viable tool.

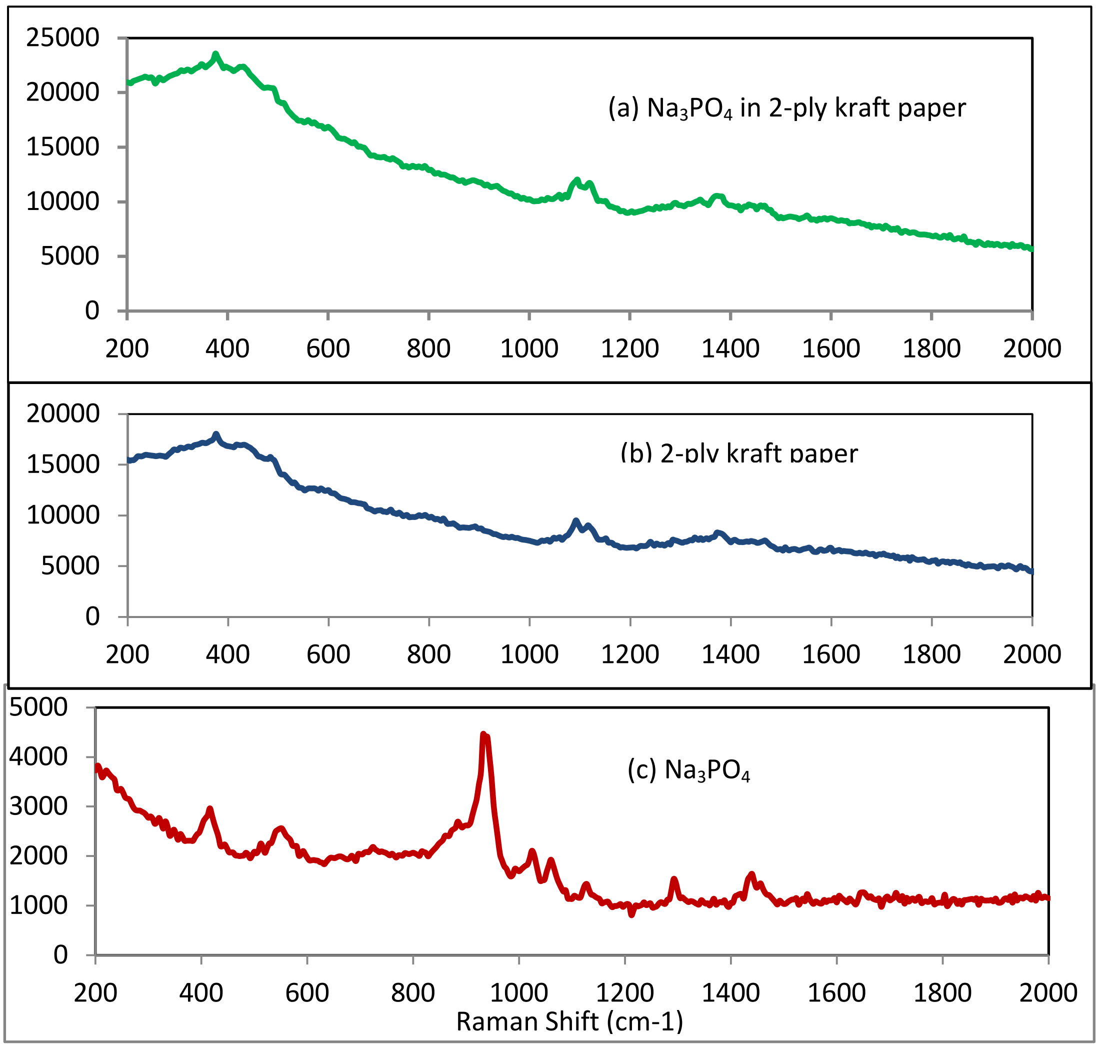

Figure 3: 1064 nm STRam identification of trisodium phosphate in bilayer bag of white and brown kraft paper layers (a) Spectrum measured through the bilayer bag using the STRaman™technology; (b) spectrum of the bilayer bag measured with standard Raman configuration; (c) pure spectrum of trisodium phosphate .

1. J. Zhao, K.A. Bakeev, J. Zhou, "Raman Spectroscopy Peers Through Packaging ", Photonics Spectra, February 2018, https://www.photonics.com/a62932/Raman_Spectroscopy_Peers_Through_Packaging.

2. K.A. Bakeev, "See-Through Science", The Analytical Scientist, May 2018, https://theanalyticalscientist.com/issues/0518/see-through-science/.

Additional Resources

- STRam product information
- STRam Product Video
- TacticID-1064 datasheet

Further Reading

- Introduction to Raman Spectroscopy
- STRaman Technology

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