Technical Overview

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Verifying Raw Materials by Spatially Offset Raman Spectroscopy

Introduction

The Agilent RapID Raman system uses a powerful technology, called spatially offset Raman spectroscopy (SORS), for identifying materials inside unopened packaging. SORS enables Raman analysis of materials through thick or opaque containers such as paper sacks, plastic tubs, and bottles. This Technical Overview explains how SORS works, and how it is used for raw materials identification (RMID) verification to improve QC speed and workflow.

Raw Material Identity Verification Through Containers

To avoid manufacturing errors, accepting incoming materials for pharmaceutical manufacture requires verification that the material's identity is correct. The resources needed to do this testing can be high, particularly where 100 % testing is mandatory or desirable. RMID testing by Raman spectroscopy is commonplace due to its speed and convenience; however, Raman requires a clear line of sight to the raw material, which is not the case with most packaging. Sacks, tubs, bottles, and FIBCs are often made of opaque or fluorescent materials, which means that testing by conventional spectroscopy requires the containers to be opened. Opening containers requires a powder-handling booth, protective clothing, and cleanup, and significantly increases cost and resources.

SORS

Spatially offset Raman spectroscopy (SORS) is a derivative of Raman spectroscopy that enables high-quality Raman spectra of the contents of opaque packaging to be measured in seconds for an effective noninvasive material identification. Figure 1 shows the SORS measurement of sucrose through a 1.5 mm thick polypropylene (PP) pot. Nontransparency and fluorescence from packaging defeats conventional Raman instruments. SORS produces a high-quality spectrum through several millimeters of opaque plastic, multiple layers of paper, or many millimeters of colored glass, allowing positive identification where it would otherwise be impossible (see Figure 1A and B). The SORS spectrum in Figure 1C is a clear match for the sugar reference spectrum shown in Figure 1D.

How SORS Works

In SORS, two spectra are measured at different laser excitation positions on the container (Figure 2). The zero offset spectrum is collected at the same place the light is detected, then the offset measurement is collected after redirecting the laser some millimeters away. A scaled subtraction of the two spectra allows the container spectrum to be removed, leaving only the contents spectrum for analysis. The SORS spectrum, which is free from background or container spectrum, is then matched against a reference for identification verification.

Example containers.

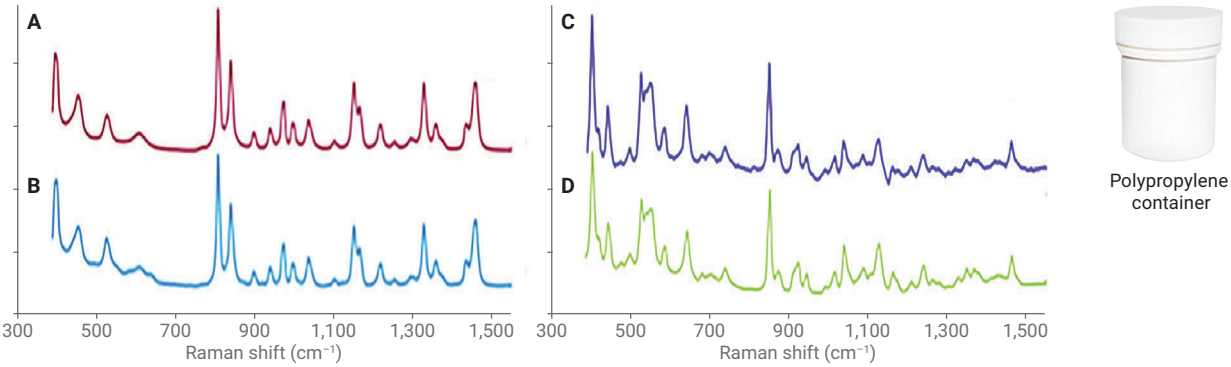

Figure 1. A) Conventional Raman spectrum through a white PP container without sucrose inside; B) with sucrose; C) SORS spectrum through the same white PP container, t = 8 s; D) reference sucrose spectrum.

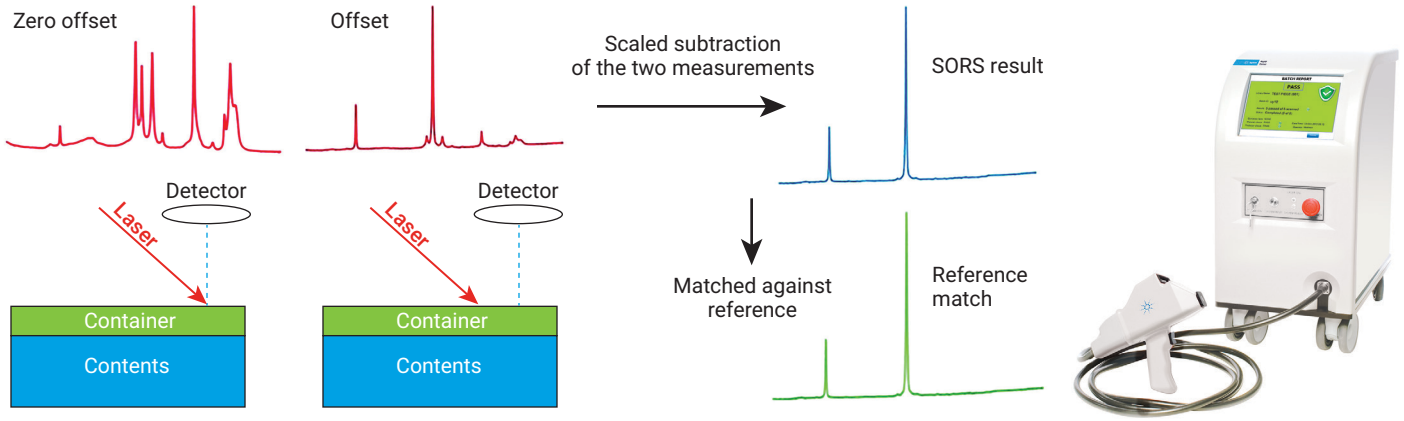

Figure 2. SORS measurements through a container. Zero offset geometry (left), with spatial offset (right). Scaled subtraction retrieves the contents spectrum only, which is matched with a reference for identification.

Library Training

The RapID system includes a straightforward means to add new materials to the production library by measuring a few reference spectra through the original packaging. This is to optimize the measurement conditions of a given container; a clear plastic is different from a multilayered paper sack. Spectra are measured at several points around the container to build up a representative sample of the container/contents SORS spectra. The software builds a library model, then runs standard validation checks against the model before it can be released for routine testing. Automatic crosschecking against other models ensures that spectra from existing models do not match the new model.

Production Use

Once released into production, the user can select the material using the bar code scanner on the RapID probe head, or by manual selection, to begin the batch analysis. Each SORS measurement typically takes 10 seconds, and the result is reported immediately as a pass or fail (Figure 3). One hundred sacks can be ID-verified in less than 30 minutes total analysis time in the warehouse area. The batch report is automatically generated, and can be output to a network or LIMS system.

Raw material identity verification through a white plastic sack.

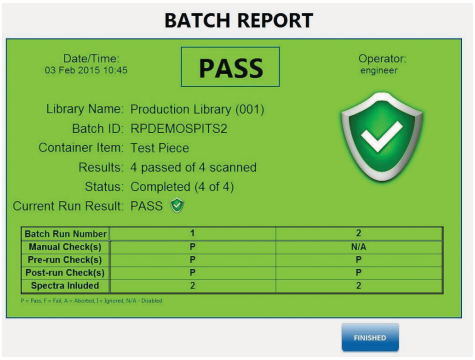

Figure 3. Batch report pass screen.

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