Raw Materials Identification through Multiple Polyethylene Bags

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Introduction

Raman technology is known for its fast speed and convenience for material identification and verification. Raman measurements can be conducted through transparent containers without any sample preparation, as shown in the photos of the NanoRam for raw material identification in Figure 1.

Figure 1. NanoRam in action for raw material identification

This technical note showcases the NanoRam handheld Raman spectrometer for raw material identification through multiple polyethylene (PE) bags. The PE bags used in the test was a Whirl-Pak 4oz bag, with the thickness of 2.25 mil (~0.06mm).

A pharmaceutical active ingredient (API) in powder form from three different lots was used for testing. Tests were completed through a single layer bag, 5 PE bags, and 9 PE bags.

Experimental

Two methods were created:

- “5PE” using material from lot#1 in 5 layers of PE bags
- “9PE” using material from lot#2 in 9 layers of PE bags

Each method was created with 20 scans, using the same API material. Method "5PE" was generated with a sample from lot #1in 5 layers of PE bags, and method "9PE" was generated with a sample from lot#2 in 9 layers of PE bags. No method was created for the single layer PE bag sample.

Identification tests were run using materials from lot#1, lot#2, and lot#3 in the single layer PE bag, 5 layers of bags, and 9 layers of bags against both methods. A point-and-shoot sampling adaptor was used for all tests. Materials from different lots were used in the test to make sure that normal lot-to-lot variation, if existing, would not have a negative impact on the material identification results.

Test Result and Discussions

The method used in the NanoRam is a multivariate analysis approach, which is based on principal component analysis (PCA) models for materials classification. The method utilizes a minimum of 20 Raman spectral scans and therefore can be developed to include possible variations of the material within itself, from different vendors, or associated with material uniformity such as uniformity from different lots and batches. The "Pass" or "Fail" test results are based on a calculated p-value on a 95% confidence level. When p-value ≥ 0.05, the result is "Pass", meaning the sample cannot be excluded from the acceptance space established by the 20 scans of the method and that the sample is highly likely to be the material represented by the method. When the p-value is less than 0.05, the result is "Fail", meaning that the measured sample is not the material represented by the method.

The test results are summarized in Table 1. "Pass" results were obtained for all identification tests using the "5PE" and "9PE" methods for samples through different layers of bags, and from different lots as well.

Table 1.

Method	Raw Materials						
	Lot#1 in 1 layer PE bag	Lot#1 in 5 layers PE bags	Lot#1 in 9 layers PE bags	Lot#2 in 5 layers PE bags	Lot#2 in 9 layers PE bags	Lot#3 in 5 layers PE bags	Lot#3 in 9 layers PE bags
5PE (Lot#1)	**Pass** p = 0.4689	**Pass** p = 0.9945	**Pass** p = 0.6257	**Pass** p = 0.9717	*	**Pass** p = 0.9733	*
9PE (Lot#2)	**Pass** p = 0.3436	**Pass** p = 0.5270	**Pass** p = 0.9997	*	**Pass** p = 0.8282	*	**Pass** p = 0.9749

* Experiments were not conducted as full factorial because of the comparable results shown among the three lots.

Figure 2 shows the overlay of the Raman spectra for the API material in 1 layer, 5 layers, 9 layers of PE bags, as well as the spectrum of the PE bag only. The PE material shows several prominent Raman peaks in the regions marked by the rectangular boxes. It can be observed that as the PE bag gets thicker with more layers, the Raman signatures of the PE material get more prominent, as seen with the PE peaks shown in the spectrum for material in 9 layers PE bags. On the other side, as the PE material gets thicker with more layers, the Raman signatures of the API material get less prominent, such as the API peaks shown in spectrum for the material in 9 layers PE bags. Nevertheless, because of the algorithm in constructing the PCA model using 20 scans in the NanoRam, the method generated on the NanoRam can be so robust that the method generated through several layers of PE bags can reliably identify samples through multiple layers of PE bags.

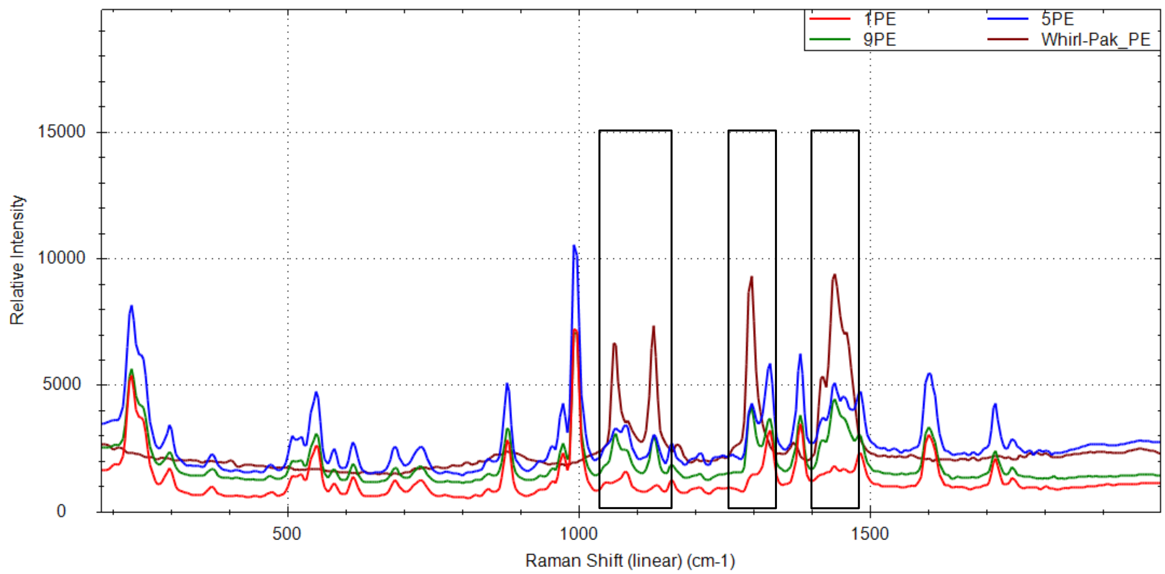

Figure 2. Spectra overlay of API material in 1 layer-, 5 layer-, 9-layer PE bags, along with spectrum of the PE bag

With more layers of PE bags, the PE material gets thicker, and the Raman signatures of the API material get less prominent while the interference from the PE material will affect more of the result. While the highest number of layers tested here is 9 layers, there will be limitations as to the layers of bags that can be applied. The applicable number of layers should be determined by a method validation process where the method is validated via positive tests, negative tests, as well as the robustness tests.

Conclusions

The NanoRam is able to test material through multiple layers of transparent plastic bags. The number of PE bags, varying from 1 to 9 layers, all gave “Pass” results for the materials inside the bag, demonstrating minimum interference from the PE bags on the material identification result. The method generated from the NanoRam can be so robust that the method generated through multiple layers of PE bags can reliably identify samples through equal or different numbers of layers of PE bags.

Other resources

NanoRam datasheet

Further reading: Using Handheld Raman Spectroscopy To Reduce Risks In Materials Used For Manufacturing

Further reading: Rapid Raw Material Identification for Formulation Compounds Using Handheld Raman Technology

If you have any questions about the application or would like to know how Raman would work for your application, please contact us at appnote@bwtek.com or call us at +1 (855) 297-2626 to speak with an expert.

