HORIBA Scientific

Technical Note

Raman

SO-TN05

ParticleFinder – Automated particle location and Raman analysis with LabSpec 6

Raman spectroscopy is increasingly used for routine screening, whether via automated wellplate measurements, tranmission Raman bulk analysis of turbid materials, or in situ remote analysis within reactors. The fast, non-destructive nature of Raman, coupled with its high chemical specificity makes it ideally suited for such applications.

The ParticleFinder module for LabSpec 6 offers a new tool for those analyzing particulate materials, allowing automated location of particles, analysis of key particle statistics (such as size and shape) and subsequent chemical characterization with Raman. In cases where the number of particles to be analysed is large, manually locating and marking each particle is time consuming, and the time spent can often outweigh the benefits that Raman can offer.

With ParticleFinder a video image with hundreds or thousands of particles can be quickly processed using light/dark thresholds to locate and mark the particles. Statistics for all of the particles are presented, and the user can choose to filter out specific particles based on these statistics – for example, particles outside of a specific size range can be excluded. Once the particle location exercise is completed, Raman characterization can begin, using the full capabilities of HORIBA Scientific's instruments, including the compact XploRA™ microscope, and flexible LabRAM HR Evolution.

Typical examples where ParticleFinder offers enormous advantages include the analysis of airborne particles and contaminants on filters, characterization of mineral grains for geological and mining exploration, and investigation of pharmaceutical ingredients and mixtures.

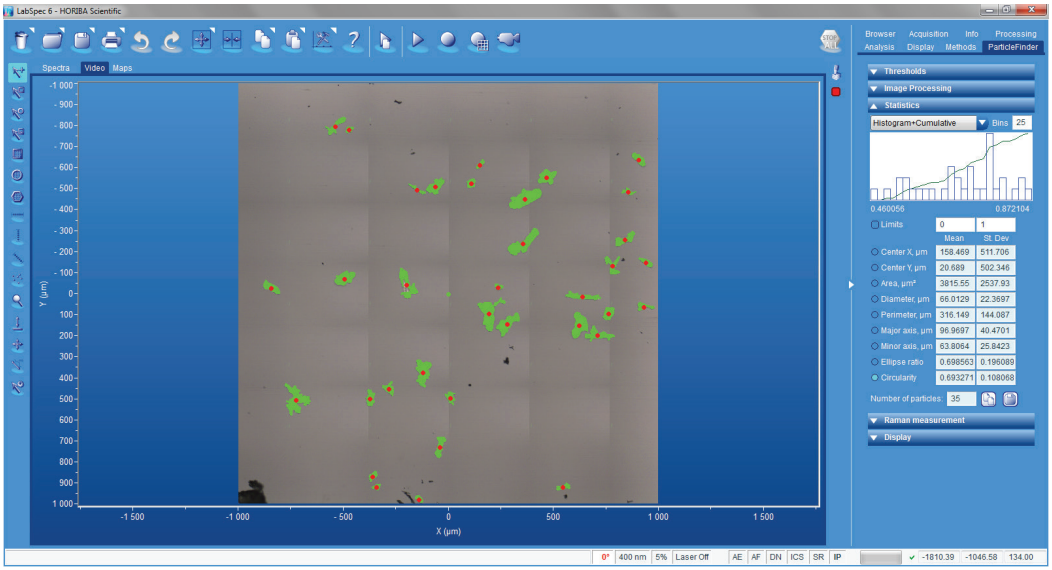

Figure 1 – LabSpec 6 screenshot, showing the ParticleFinder interface, with located particles

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Key Functionality

ParticleFinder offers a simplified work flow, through particle location, filtering, statistical analysis and finally Raman measurement.

Once a color video image has been captured (with unlimited field of view when using LabSpec's video montage function) fast threshold tools allow the user to quickly locate particles within the image.

The subsequent application of standard morphological filters (such as erode, dilate, open, close, majority) coupled with hole filling, edge particle exclusion, and minimum size exclusion ensure that only meaningful segmentation is performed. Statistical results from the located particles are presented in histogram form, with outputs for center positions (X and Y stage coordinates), area, diameter, perimeter, major and minor axes, ellipse ratio and circularity. Located particles can be filtered according to any of these statistics, allowing subsequent Raman analysis of only key particles of interest.

Finally, with the desired particles located and marked, Raman characterization can begin – high precision motorized sample stages will move each particle in turn beneath the laser spot. A suite of analysis functions are available to the user, including AutoFocus, AutoExposure, and FLAT correction, ensuring the very best results can be achieved.

Flexible instrument options include a wide range of excitation laser wavelengths (from deep UV through to infra-red), high sensitivity CCD, EMCCD and InGaAs detectors, the unique DuoScan™ optics for laser spot scanning, and high spectral resolution. With such capabilities, ParticleFinder is ideally suited for both routine particle chemical screening and high end research of particle material properties.

Application Example

Pharmaceutical crystals on a glass slide were analyzed via the ParticleFinder module, to identify their chemical composition.

A large area optical image was acquired using LabSpec 6's video montage tool, covering a 2 x 2 mm^2 area within which a number of crystals are observed. Thresholding of the image, with subsequent morphological filtering (dilate; fill; remove edge particles) allows a clear binary image of located particles to be created. It is these particles which are then automatically targeted for Raman chemical analysis.

Raman analysis was made at the center of each particle using a HORIBA Scientific LabRAM HR Evolution Raman microscope, using a 10x objective, 532nm laser, and approximately 3 cm^{-1} spectral resolution.

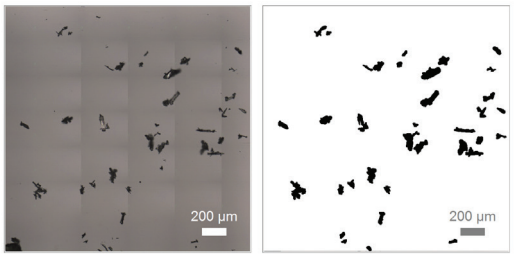

Figure 2 – video image of pharmaceutical crystals (left), and the resulting ParticleFinder binary image (right) created after morphological processing.

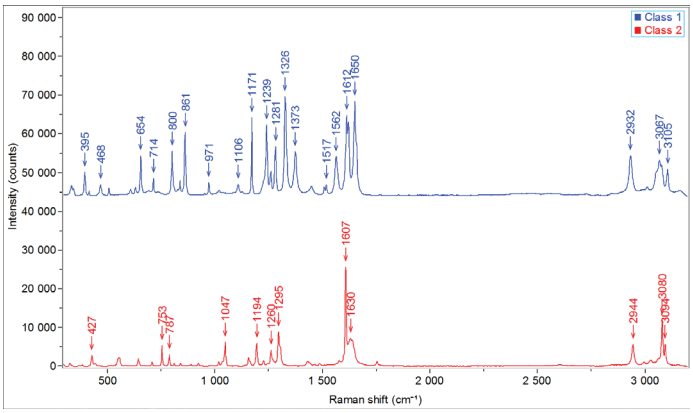

Figure 3 – average class spectra automatically calculated using the LabSpec 6 DCA multivariate analysis module.

The resulting 35 spectra were analyzed using the DCA clustering method of LabSpec 6's integrated MVA multivariate module. The average class spectra are displayed in Figure 3. Correlation with Raman spectral libraries, using the HORIBA Edition of the KnowItAll® Informatics Suite (Bio-Rad Laboratories, Inc.) provides fast identification of the spectra. The results indicate that out of the 35 particles just two are 4-acetylsalicylic acid (aspirin) – particles number 15 and 17; the remainder are N-(4-hydroxyphenyl)acetamide (more commonly known as paracetamol or acetaminophen).

Conclusion

HORIBA's ParticleFinder brings a new level of automation to the Raman analyst. By locating and automatically analyzing multiple particles presented to the microscope it can dramatically improve sample throughput in busy analytical laboratories focusing on particulate characterization. The detailed particle size/shape parameters also presented allow chemical information to be related to physical/structural properties with ease.

In combination with the extended capabilities of HORIBA Scientific's Raman system, LabSpec 6's ParticleFinder module provides the ultimate solution for chemical analysis of particles.

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HORIBA Scientific

info.sci@horiba.com www.horiba.com/scientific

USA: +1-866-562-4698
UK: +44 (0)20 8204 8142
China: +86 (0)21 6289 6060
France: +33 (0)1 69 74 72 00
Italy: +39 2 5760 3050
Brazil: +55 (0)11 5545 1500
Germany: +49 (0)89 4623 17-0
Japan: +81 (0)3 6206 4721
Other: +33 (0)1 69 74 72 00