THz-Raman® – The “Structural Fingerprint” of Raman

Ondax’s patented THz-Raman® Spectroscopy Systems extend the range of traditional Raman spectroscopy into the terahertz/low-frequency regime, exploring the same range of energy transitions as terahertz spectroscopy – without limiting the ability to measure the fingerprint region. This region reveals a new “Structural Fingerprint” to complement the traditional “Chemical Fingerprint” of Raman, enabling simultaneous analysis of both molecular structure and chemical composition in one instrument for advanced materials characterization.

See What You’ve Been Missing – More Data, Better Sensitivity & Reliability

Clear real-time differentiation of structural attributes of the material enables clear identification and analysis of polymorphs, raw material sources, defects & contamination, crystal formation, phase monitoring and synthesis methods.

One Sample, One System, One Answer

In-situ, real-time measurement of both composition and structural analysis eliminates the need for multiple samples and instruments, lowering capital, training and maintenance costs.

Benefits

• Both chemical composition + molecular structure from one Raman measurement
• In-situ, real-time structural monitoring + chemical analysis
• Higher SNR with inherent calibration reference
• Faster, more comprehensive and reliable measurements
• Compact, easy to use, and adaptable to existing Raman systems
Real-time, in-situ monitoring of both structure and composition

THz-Raman® measurements capture low-frequency lattice and phonon modes that are manifested by both inter- and intra-molecular vibrations. These modes are highly responsive to changes in molecular structure and can be used to monitor structural changes caused by polymorphic or isomeric shifts, lattice defects, contaminants, and changes in phase or crystallinity. The example below shows how THz-Raman can be used as a real-time monitor of polymorphic changes in Theophylline.

Reaction Monitoring of Polymorphism

The figure below shows low frequency spectra of anhydrous theophylline (Form II) before and after its transformation into a flocculated slurry (monohydrate, Form M). Spectra collected at the start and finish (T=2s red and T=200s blue) show the disappearance of peaks at 20, 35 and 85 cm\(^{-1}\) in the anhydrate spectrum and the appearance of a new peak at 96 cm\(^{-1}\) in the spectrum of the monohydrate.

The waterfall plot (above right) shows the transformation from Form II to Form M is complete in approximately 100 seconds. The spectrum of the suspended solids was resolved from the broad underlying boson peak and the profile shown above. The time profile shown at right was then generated, which shows the disappearance of Form II (red) and the appearance of Form M (blue).

Data courtesy Clairet Scientific, Ltd.

Sample Interface Accessories

A variety of sample interface accessories enable the TR-PROBE to be easily configured to match a broad range of applications. Immersion or Contact probe tips may be mounted with either a fixed SwageLok mount or, for longer probes that may need alignment, an adjustable tip/tilt probe mount. The Vial/Cuvette Sample Holder incorporates an adjustable steering mirror, interchangeable focusing lens, and safety shutter. And the Steerable Collimated Beam Mount allows for projection and steering of the collimated output beam with precision alignment, for applications requiring long-range collection paths.
# THz-Raman® Probe System Specifications:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wavelength</td>
<td>nm</td>
<td>532, 785, 850</td>
</tr>
<tr>
<td>Power at sample port (min)</td>
<td>mW</td>
<td>25 to 250, 60</td>
</tr>
<tr>
<td>Physical Dimensions (W x L x H)</td>
<td>in</td>
<td>3” x 8.5” x 2.3”</td>
</tr>
</tbody>
</table>

1 Specify power level at time of order
2 Probe head only, does not include sample accessory

## Spectrometer:

<table>
<thead>
<tr>
<th>Spectrometer Specification</th>
<th>Fixed Grating Spectrometer</th>
<th>Tunable Grating Spectrometer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spectral Range (typical)</td>
<td>-200 cm$^{-1}$ to +2200 cm$^{-1}$</td>
<td>400-1100 nm (w/Si Detector)</td>
</tr>
<tr>
<td>Spectral Resolution</td>
<td>2.5 cm$^{-1}$ to 4 cm$^{-1}$</td>
<td>0.7 cm$^{-1}$ or greater</td>
</tr>
<tr>
<td>Computer Interface</td>
<td>USB</td>
<td>USB</td>
</tr>
</tbody>
</table>

3 Spectrometer selection and specifications will be determined by application requirements and options ordered

## System Description and Configurations:

All THz-Raman® Series platforms are ultra-compact and simple to connect via fiber to almost any spectrometer or Raman system. Our patented SureBlock™ ultra-narrow-band Volume Holographic Grating (VHG) filters precisely block only the Rayleigh excitation with >OD8 attenuation, enabling simultaneous capture of both Stokes and anti-Stokes signals. A high-power, wavelength-stabilized, ASE-free single-frequency laser source is precisely matched to the filters to assure maximum throughput and exceptional attenuation of the excitation source.

The TR-MICRO mounts directly to a broad range of popular microscope platforms and micro-Raman systems, and can be easily switched in and out of the optical path. The system includes an Ondax SureLock™ 785nm, 850nm, or 976nm laser source, notch filters, and optional circular polarization (linear polarization is standard). A 532nm excitation source or a sample imaging camera are also available upon request.

The new TR-PROBE is a compact, robust THz-Raman® probe that enables in-situ reaction or process monitoring. The TR-PROBE can be configured with a variety of immersion or contact probe tips, a convenient vial holder, tablet holder, or a steerable collimated beam (see sample options on previous page).

The XLF-CLM is configured for Benchtop use and offers an optional vial/cuvette sample holder for fast, easy measurements. The system also comes with a standard cage mounting plate (centered on the collimated output beam) to allow for customized collection optics or easy integration into a customized system. The XLF-CLM includes a SureLock™ 785nm, 850nm, or 976nm laser source, notch filters, and optional circular polarization.

Model XLF-CLM with Integrated Laser Module and Sample Vial/Cuvette Holder

Model TR-MICRO with Integrated Laser Module
Compatible with Leica, Nikon, Olympus and Zeiss microscopes (shown mounted on Leica DM 2700 M)

Model TR-PROBE with fiber-coupled laser source and interchangeable probe tips and sample holders
Compatible with either fixed-grating or tunable grating spectrometers
Additional Applications

Pharmaceutical Applications

Key challenges for the pharmaceutical industry include polymorph identification, reaction monitoring, raw material quality control, and counterfeit detection. THz-Raman® reveals “structural fingerprints” that can rapidly differentiate polymorphs, isomers, co-crystals, and other structural variations of substances and compounds.

Explosives Detection, Forensics and Source Attribution

THz-Raman® goes beyond chemical detection to reveal a “structural fingerprint” that can be attributed to specific ingredients, methods of manufacture, and storage/handling of many popular home-made explosive (HME) materials, revealing clues about how and where they were formulated.

Semiconductor and Nanomaterials

Graphene and carbon nanotubes are just two of the many nanomaterials that exhibit strong low-frequency signals. For Graphene, THz-Raman® analysis can determine the number of monolayers, and for carbon nanotubes, the diameter of the structure. Differences in structural characteristics and defects in crystals can also be detected.

Crystallization and Reaction Monitoring

Low-frequency THz-Raman® signals undergo clear, rapid shifts corresponding to changes in molecular structure, enabling highly sensitive, real-time monitoring of crystal form, phase, or structural transformations.

Industrial and Petrochemical

THz-Raman® delivers additional sensitivity and information about molecular structure to control processes, improve yields, and monitor crystallization or structural transformation during formulation of chemicals and polymers.

Gas Sensing

Rotational modes of gases such as Oxygen provide signal intensities up to 10x those in the fingerprint region. Stokes/anti-Stokes ratios can also be used for remote sensing of temperatures in gases, plasmas, liquids and solids.