High Explosives (4)—Technology Data Sheet

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High Explosives (HE) Technology Name: Raman Explosive Identification System

Physical Principle/Methodology of Technology:

Raman spectroscopy is a spectroscopic technique used to observe vibrational, rotational, and other low-frequency modes in a molecular system. The technique is commonly used in chemistry to provide a fingerprint by which molecules can be identified. It relies on inelastic scattering, or Raman scattering, of monochromatic light, usually from a laser in the visible, near infrared, or near ultraviolet range. The laser light interacts with molecular vibrations, phonons, or other excitations in the system, resulting in the energy of the laser photons being shifted up or down. The shift in energy gives information about the vibrational modes in the system. Infrared spectroscopy yields similar, but complementary, information.

To be more specific, the Raman effect occurs when electromagnetic radiation impinges on a molecule and interacts with the polarizable electron density and the bonds of the molecule in the phase (solid, liquid, or gaseous) and environment in which the molecule finds itself. For the spontaneous Raman effect, which is a form of inelastic light scattering, a photon (electromagnetic radiation of a specific wavelength) excites (interacts with) the molecule in either the ground rovibronic state (lowest rotational and vibrational energy level of the ground electronic state) or an excited rovibronic state. This results in the molecule being in a so-called virtual energy state for a short period of time before an inelastically scattered photon results. The resulting inelastically scattered photon that is "emitted"/"scattered" can be of either lower (Stokes) or higher (anti-Stokes) energy than the incoming photon. In Raman scattering the resulting rovibronic state of the molecule is a different rotational or vibrational state than the one in which the molecule was originally, before interacting with the incoming photon (electromagnetic radiation). The difference in energy between the original rovibronic state and this resulting rovibronic state leads to a shift in the emitted photon's frequency away from the excitation wavelength, the so-called Rayleigh line. The main problem for Raman spectroscopy testing applications is that this Rayleigh line scattering can in many cases mask the weaker Raman signal.

Typically, a sample is illuminated with a laser beam. Electromagnetic radiation from the illuminated spot is collected with a lens and sent through a monochromator. Elastic scattered radiation at the wavelength corresponding to the laser line (Rayleigh scattering) is filtered out by either a notch filter, edge pass filter, or a band pass filter, while the rest of the collected light is dispersed onto a detector.

The Raman spectroscopy can be used as a highly specific, non-destructive, eye-safe monitor of molecular composition. It has been widely used for standoff explosive detection.

There are numerous advanced types of Raman spectroscopy, including surface-enhanced Raman, resonance Raman, tip-enhanced Raman, polarized Raman, stimulated Raman (analogous to stimulated emission), transmission Raman, spatially offset Raman (to minimize the contribution of Raman bands from the container walls), hyper Raman, deep UV Raman (to overcome the inherent weakness of normal Raman scattering and associated visible luminescence), and THz-Raman (to more deeply penetrate a material or "see through" external layers as container).

Potential Monitoring Use Cases (pre-dismantlement, dismantlement, post-dismantlement, storage stage):

Explosive measurement and identification.

Pre-dismantlement: Unlikely, due to heavy shielding between HE and experimental apparatus.

Dismantlement: Possible, with direct optical access or at most very light shielding (e.g., semitransparent plastics) at some point in time. Works for long distance measurement between HE and apparatus.

Post-dismantlement: As above.

Storage stage: As above.

For detection technologies, what does the method determine/measure:

Presence/absence and identification by comparison with a spectral library of all known explosives.

The vibrational modes can be regarded as a fingerprint that uniquely identifies the substance or substances in a sample. Thus, detailed molecule specific information can be determined.

Physical Description of Technology (e.g., approximate size, weight):

An instrumentation set-up could consist of a (pulsed) laser and optics to direct the laser beam, a fiber coupled telescope for detecting the Raman signal, and a spectrometer with gated Intensified Charged-Coupled Device (ICCD) for detection.

A few kg.

Time Constraints (e.g., measurement times including distance from object, time to install the equipment):

Set-up and calibrate equipment takes 15 minutes. Measurement time takes 1 minute/sample. Stand-off measurement (more than tens of meters) possible.

Will this method work in the presence of shielding? If so, what is the maximum amount of shielding that will still allow the method to work?

Normally Raman spectroscopy needs optical access to the sample but Spatially offset Raman spectroscopy (SORS) can measure trough semitransparent white or colored plastic containers. Works best for detection of explosives and not for absence.

Technology Complexity (e.g., hardware, software, and ease of use by personnel):

A finished system should be easy to set up and operate.

Infrastructure Requirements (e.g., electrical, liquid nitrogen, etc.):

Electrical power.

Technology Limitations (e.g., detection limits for HE, operational temperature range, differences in technology detector materials): Need optical or semitransparent access to the measurement objects.
Information Collected by the Technology (used to help determine if an information barrier (IB) is required for use): Presence/absence and identification. Detailed molecule specific information. Raman spectroscopy is commonly used in chemistry, since vibrational information is specific to the chemical bonds and symmetry of molecules. Therefore, it provides a fingerprint by which the molecule can be identified. An IB might be needed to prevent an inspector gaining inappropriate/unnecessary information regarding binders, etc.
Safety, Security, Deployment Concerns: The Raman spectroscopy commonly uses an eye-safe laser source.
Technology Development Stage (Technology Readiness Level, TRL): The technique is presently adapted and developed for trace detection. Commercial system exists but must be adopted and tested for this special case. Possibly TRL 5.
Where/How the Technology Is Currently Used (e.g., international safeguards, border protection): Has been used as a standard analytical tool for identification of chemical substances for many years. Well suited for use on many different substances, e.g., explosives and drugs.
Examples of Equipment: All handheld: • BRAVO (Bruker Corporation) • FIRSTDEFENDER RM (Thermo Fisher Scientific) • CBEx (Snowy Range Instruments) • CHEM 500 (Sci Aps Inc.) • FIRST GUARD (Rigaku Analytical Devices)