Determining Layer Properties in 2D Materials

Two Dimensional Materials

Few-layered materials have dramatically different properties from their bulk phase. Their tunable optoelectronic characteristics are largely governed by the interactions between the vertically stacked layers and are affected by the number and orientation of the layers. The vibrations corresponding to these interlayer interactions, known as shear modes, manifest as low frequency Raman peaks very close to the laser Rayleigh line, which are not detected by traditional Raman spectroscopy. Using low frequency/THz-Raman™ however, the shear modes have been easily measured for transition metal dichalcogenide (TMD) materials, enabling clear, unambiguous measurement of both the number and orientation of layers.

Figure 1. *Generalized chemical structure of TMDs, showing the metal (grey) and chalcogenide (yellow) atoms, adapted from S. Mouri, K. Matsuda et al., Nano Lett. 13, (2013) 5944. (Left) and Optical Micrographs (100x) of two-layer $MoSe_2$ substrates. Red dot indicates the approximate location of the Raman measurement (Right)**

The Attalon THz-Raman™ Solution

Attalon's THz-Raman™ systems extend the range of traditional Raman spectroscopy to the THz/low frequency Raman regime, where lattice modes that correlate to material structure are found and inter-layer modes can be clearly and quickly observed. While conventional Raman spectra might hint at similar information, the spectra are often indirect and not easily verified using ab-initio simulations. In this example, a sample of $MoSe_2$ with a distribution of two different relative orientations of the two layers was studied (*Figure 1*). The Raman spectral data presented here were collected with excitation at 532 nm using a Attalon TR-MICRO-532 THz-Raman™ system connected to a single-stage spectrometer with a spectral resolution of 1.5 cm. Normalized THz-Raman™ spectra of the two orientations of $MoSe_2$ are shown in *Figure 2*.

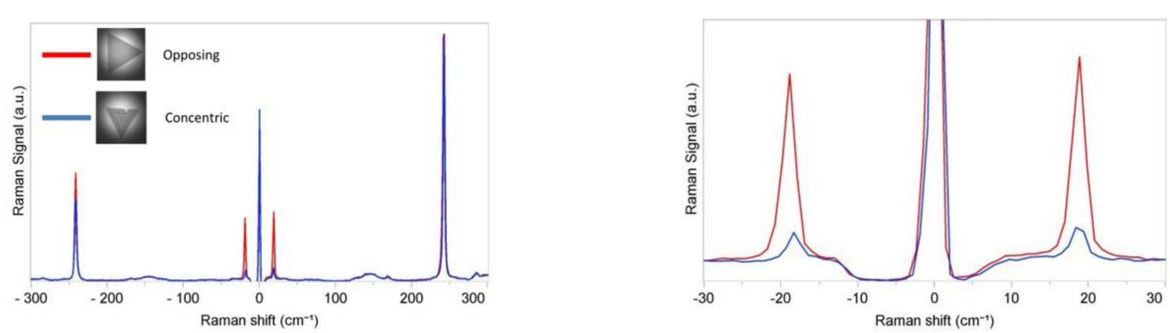

Figure 2. *Normalized THz-Raman™ spectra of two-layer $MoSe_2$ materials showing the corresponding shift and change in magnitude of the peak corresponding to the bulk mode at 242 cm^{-1} (Left) and the shear mode peak at 18 cm^{-1} (Right)*

**The $MoSe_2$ sample was synthesized and characterized at the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory (X. Li, A.A. Puretzky; see ACS Nano 9, 6333-6342 (2015) for details*

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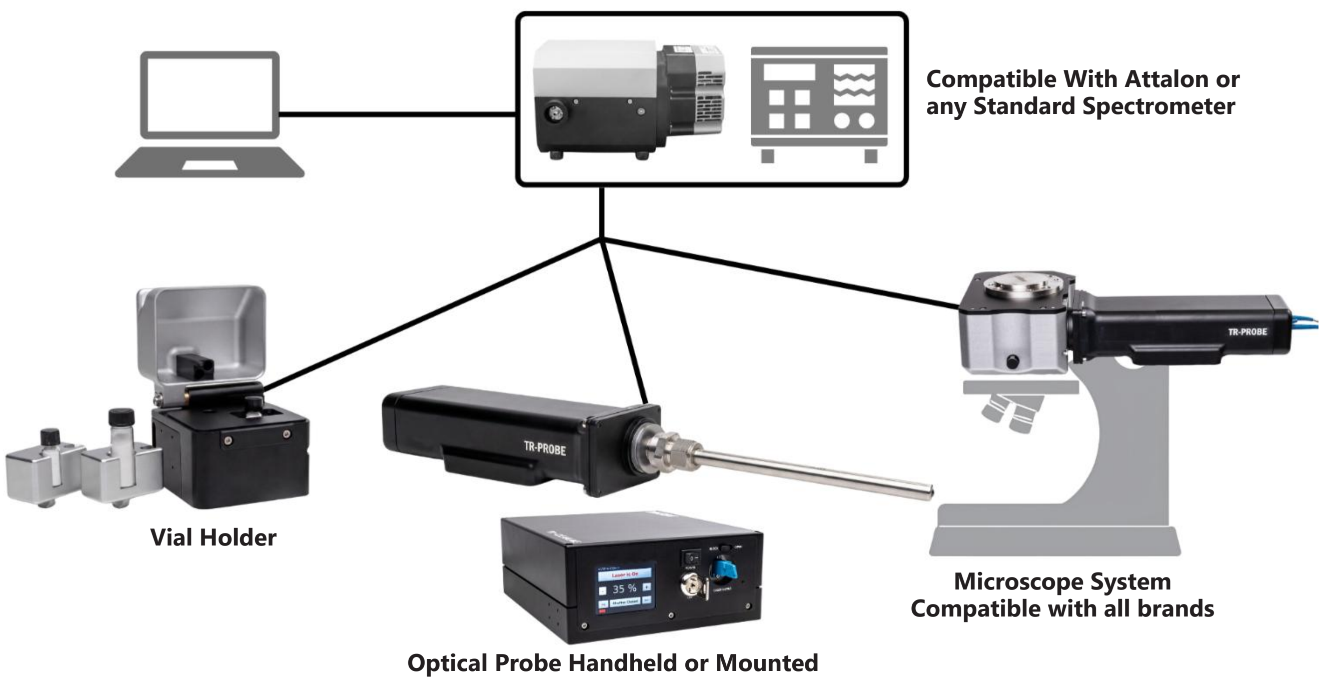
THz-Raman™ Analysis

The Raman spectra in *Figure 2* illustrate that regardless of orientation, both the two-layer $MoSe_2$ materials show an out-of plane bulk mode as a peak at 242 cm^{-1} in the Raman spectrum. The shear modes at 18 cm^{-1} are not present for single layer $MoSe_2$. The opposing two-layer $MoSe_2$ case has a shear mode peak at 18.9 cm^{-1} as determined by a center of mass analysis. When the $MoSe_2$ layers are oriented to be concentric, the peak undergoes a bathochromic shift to 18.4 cm^{-1} and a large change in the intensity of the peak. This demonstrates that THz-Raman™ spectroscopy provides direct information about the number and orientation of the layers in 2D materials. While atomic force and scanning tunneling microscopies can be used to determine the exact atomic registration between different layers, they are slow techniques and require expensive instrumentation and off-line analysis. For rapid prototyping of two-dimensional materials, THz-Raman™ provides a fast, non-destructive and cost-effective solution.

FEATURES

- Direct measurement of inter-layer vibrations in few-layered materials
- Quantitative analysis number of layers
- Direct correlation of orientation with peaks positions and magnitude
- Sensitivity to defects and dopants in the 2D material structure
- Simultaneous chemical and structural analysis
- Directly calculate THz-Raman™ spectra using ab-initio calculations



Attalon's patented THz-Raman™ spectroscopy systems extend the range of traditional Raman spectroscopy into the THz/low-frequency regime. This enables simultaneous analysis of both molecular structure and chemical composition for advanced materials characterization. All THz-Raman™ systems are compact, robust, plug-and-play platforms that deliver incredible speed, throughput and ease of use, all at an extremely affordable price. With a broad selection of excitation wavelengths from 488 nm to 1064 nm, optional polarization control and a wide variety of sample interfaces, there is a THz-Raman™ solution for any application.