# Determining Layer Properties in 2D Materials

## Introduction

Few-layered materials have tunable optoelectronic characteristics that are largely governed by the interactions between the vertically stacked layers and are affected by the number and orientation of the layers. The "shear mode" vibrations corresponding to these interlayer interactions 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.

## Coherent Solutions

Coherent THz-Raman® systems extend the range of traditional Raman spectroscopy to the THz/low frequency Raman regime, enabling direct observation of lattice modes that correlate to material structure. 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, $MoSe_2$ with a distribution of two different relative orientations of the two layers was studied (Figure 1), using an Ondax TR-MICRO-532nm THz-Raman® system connected to a single-stage spectrometer with a spectral resolution of 1.5 $cm^{-1}$. Normalized THz-Raman® spectra of the two orientations of $MoSe_2$ are shown in Figure 2.

## THz-Raman Analysis

Both two-layer $MoSe_2$ samples show an out-of-plane bulk mode as a peak at 242 $cm^{-1}$ in the Raman spectrum. The shear modes appearing at ~18 $cm^{-1}$ (which are not present for single layer $MoSe_2$) can be further differentiated according to their orientation: the opposing two-layer $MoSe_2$ case has a shear mode peak at 18.9 $cm^{-1}$, however for the concentric sample 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® can provide direct information about both the number and orientation of the layers in 2D materials, enabling a fast, non-destructive, "in-situ" and cost-effective alternative to slower techniques that require more expensive, offline analysis.

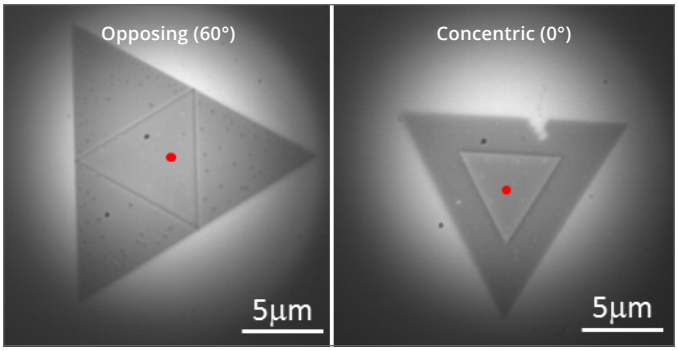


Figure 1. Optical Micrographs (100x) of 2-layer $MoSe_2$ substrates with concentric (right image) and opposing (left image) layer orientations. Red dot indicates the approximate location of the Raman measurement (see Figure 2).*

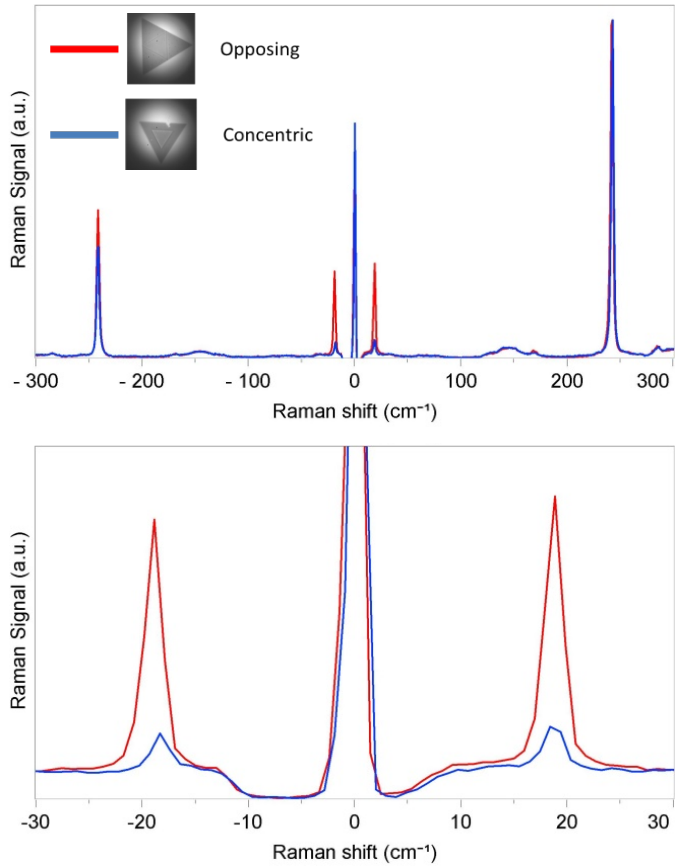


Figure 2. Normalized THz-Raman® spectra of two-layer $MoSe_2$ materials showing the corresponding shift and change in magnitude of the peak corresponding to the bulk mode at 242 $cm^{-1}$ (top) and the shear mode peak at 18 $cm^{-1}$ (bottom).

## Application Field

Nanomaterials characterization, real-time non-destructive structural analysis, low-frequency THz-Raman spectroscopy.

## Contact

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* 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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