



SOLID-STATES SCIENCE AND QUANTUM DEVICES

Raman Spectroscopy Project Report



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Purpose

This report presents an analysis of Raman spectroscopy data collected from three different solid-state materials: 2 graphene samples, silicon, and 2 TiSe₂ samples. The primary objectives of this project are to develop a deeper understanding of optical phonons in common solids, gain experience in Raman spectroscopy data analysis, and identify the characteristic vibrational modes responsible for the observed spectral features. Through analysis of the provided spectra and comparison with published literature, this report aims to identify which material corresponds to each spectrum and explain the physical origins of any variations observed between different samples of the same material, particularly focusing on thickness-dependent effects in two-dimensional materials.

Method

All data analysis and visualisation were performed using Python Jupyter Notebook, specifically utilising the pandas, numpy, matplotlib, and scipy libraries. The analysis workflow consisted of several key steps to ensure accurate peak identification and fitting.

First, the raw Raman spectroscopy data were imported from the provided text files using the pandas library's 'read_csv()' function, with appropriate parameters to skip header rows and parse the two-column format (Raman shift in cm⁻¹ and intensity in arbitrary units). Initial data visualisation was performed using matplotlib to identify the general spectral features and determine appropriate fitting ranges for each peak.

For peak fitting, the Lorentzian function was primarily employed, as it accurately describes the lineshape of optical phonon modes in crystalline materials. The Lorentzian function is defined as:

$$I(\nu) = A \times \frac{\gamma^2}{(\nu - \nu^0)^2 + \gamma^2} + offset$$

where A is the amplitude, ν_0 is the peak centre position, γ is the half-width at half-maximum (HWHM), and offset represents the baseline. For asymmetric peaks observed in the TiSe₂ samples, a split pseudo-Voigt function was implemented, allowing different widths on the peak's left and right sides and providing a mixing parameter between Gaussian and Lorentzian character.

The `scipy.optimize.curve_fit()` function was used to perform non-linear least squares fitting, with initial parameter guesses estimated from the data and appropriate bounds set to ensure

physically meaningful results. For each fit, the coefficient of determination (R^2) was calculated to quantify the goodness of fit:

$$R^2 = 1 - \left(\frac{SS_{res}}{SS_{tot}} \right)$$

where SS_{res} is the sum of squared residuals and SS_{tot} is the total sum of squares.

Throughout the analysis process, the AI tool, GitHub Copilot, assisted with code optimisation, debugging and visualisation. Interpretation of results and scientific conclusions were developed independently through careful study of the provided literature and comparison with experimental data.

Results and Discussion

Material 1: Graphene

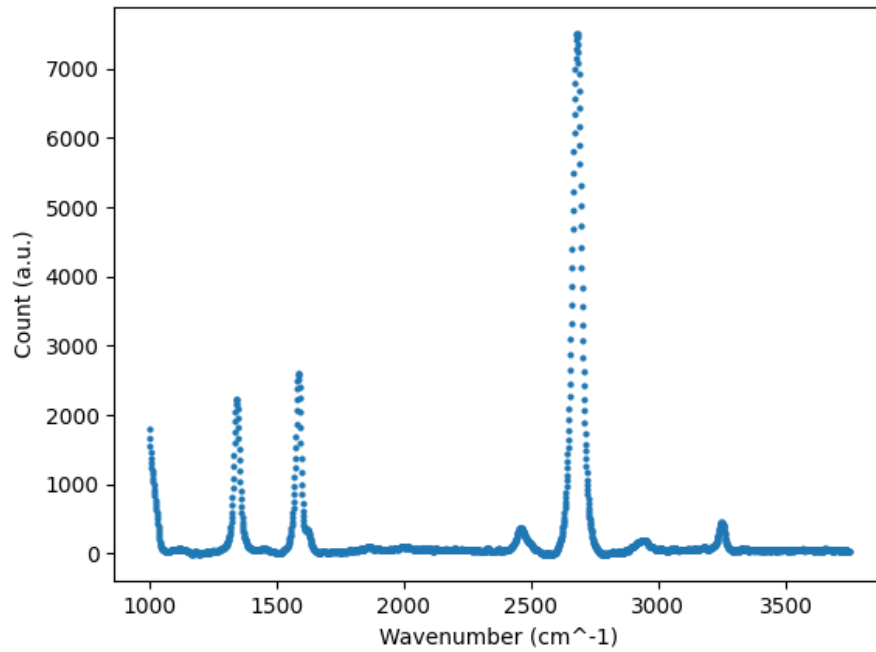


Figure 1. Raman Spectroscopy of Graphene Sample 1

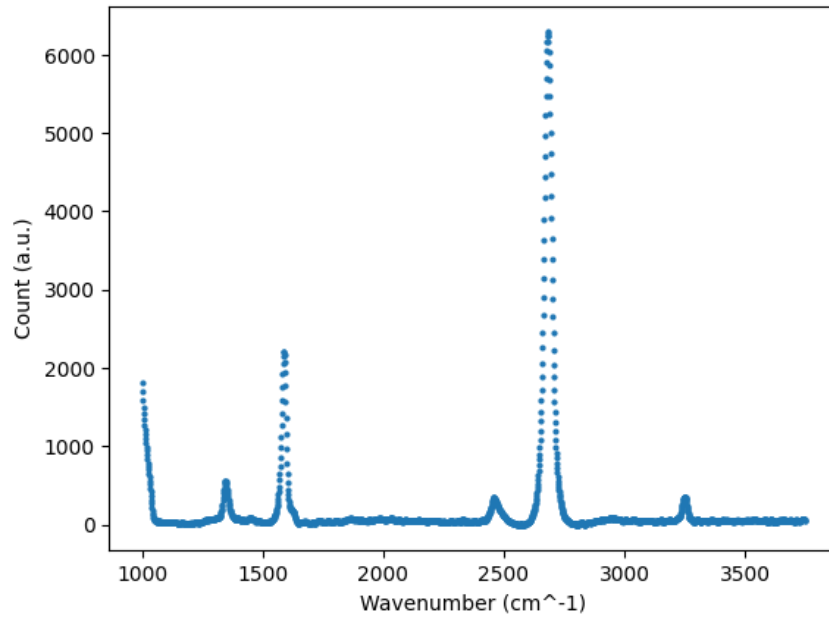


Figure 2. Raman Spectroscopy of Graphene Sample 2

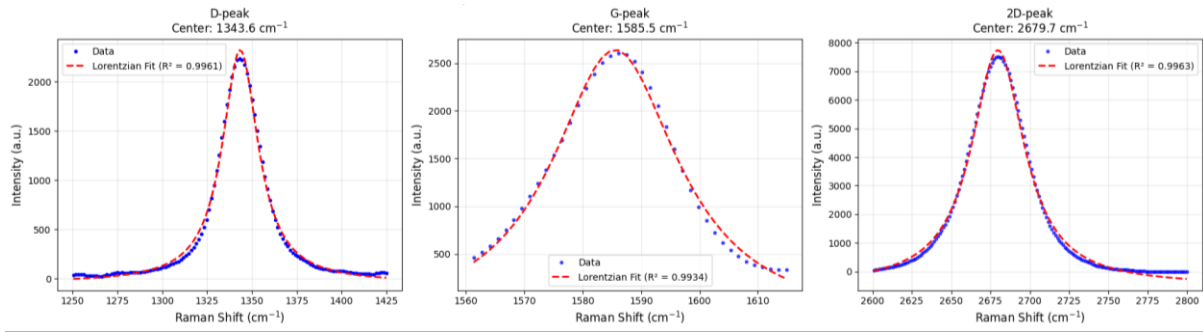


Figure 3. Lorentzian Fits for D (left), G (middle), and 2D Peaks of Graphene Sample 1

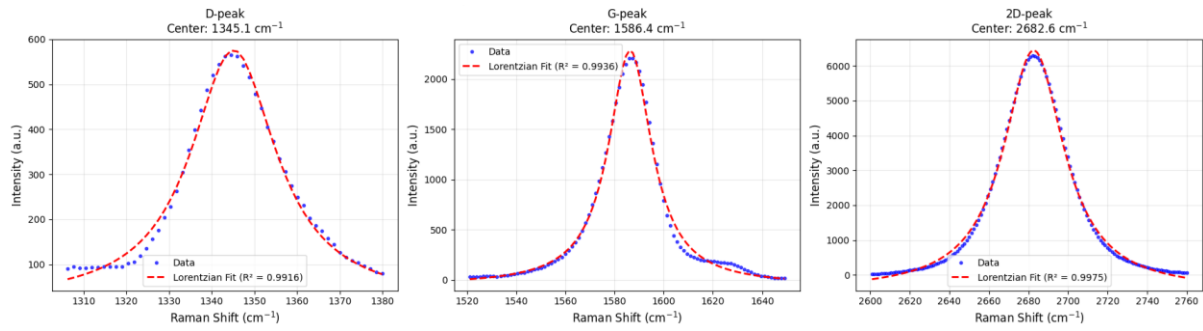


Figure 4. Lorentzian Fits for D (left), G (middle), and 2D Peaks of Graphene Sample 2

Figures 1 and 2 show the Raman Spectroscopy of Graphene Samples. Figure 3 and 4 shows the peak fitting of the D, G and 2D peaks. These assignments are based on three characteristic peaks of graphene: the D peak near 1350 cm^{-1} , the G peak near 1580 cm^{-1} , and the 2D peak near 2700 cm^{-1} [1].

The G peak at approximately 1580 cm^{-1} arises from the doubly degenerate E_{2g} phonon mode at the Brillouin zone centre and represents the in-plane stretching vibration of sp^2 -bonded carbon atoms. This mode is present in all graphitic materials and is a first-order Raman process. According to [1], this peak provides fundamental information about the crystalline graphitic structure.

The D peak near 1350 cm^{-1} is a disorder-activated mode that requires defects for activation. It originates from the breathing modes of six-atom rings and involves transverse optical phonons near the K point of the Brillouin zone [1]. This peak is activated through a double resonance process and is strongly dispersive with excitation energy due to a Kohn anomaly at the K point. The presence and intensity of the D peak provide information about structural defects, edge effects, grain boundaries, and other imperfections in the graphene structure [1].

The 2D peak appears around 2700 cm^{-1} and is the overtone of the D peak. Unlike the D peak, the 2D peak does not require defects for activation because momentum conservation is satisfied by two phonons with opposite wave vectors. This peak is always present in graphene and graphitic materials. Importantly, the shape and position of the 2D peak are highly sensitive to the number of graphene layers and their stacking order. In single-layer graphene, the 2D peak appears as a sharp, single Lorentzian peak, while in bilayer and multilayer graphene, it splits into multiple components due to changes in the electronic band structure.

Comparing the two graphene spectra reveals differences. Graphene Sample 1 exhibits an $I(D)/I(G)$ ratio of 0.819, indicating a higher defect density. This could arise from smaller crystalline domains, more edge defects, or increased disorder. Graphene Sample 2 shows a relatively low $I(D)/I(G)$ ratio of 0.239, indicating relatively few defects and good crystalline quality. The 2D peak shape and intensity suggest this sample consists of few-layer graphene. The $I(D)/I(G)$ ratio can be used to estimate the average inter-defect distance or crystallite size using established relationships from the literature [1].

Material 2: Silicon

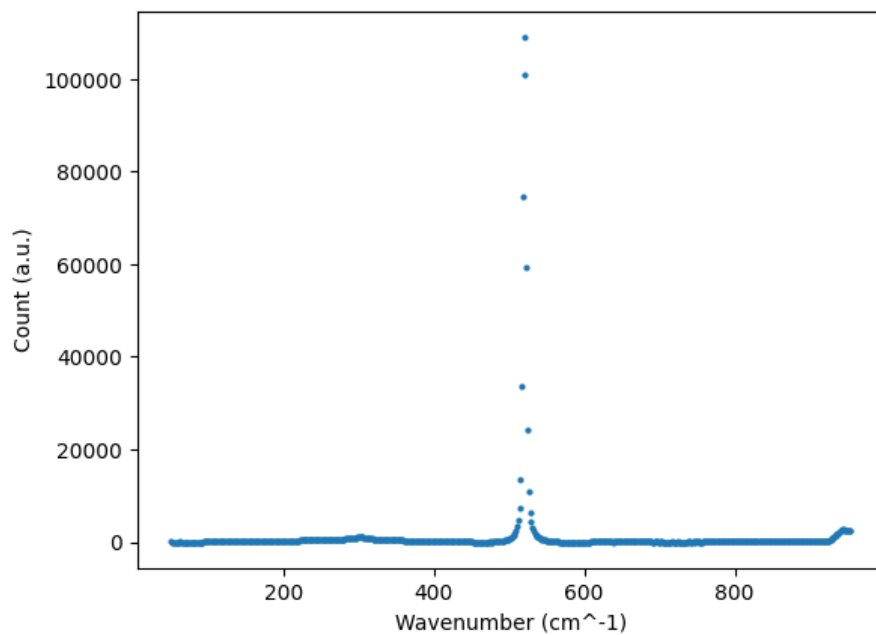


Figure 5. Raman Spectrum of Silicon

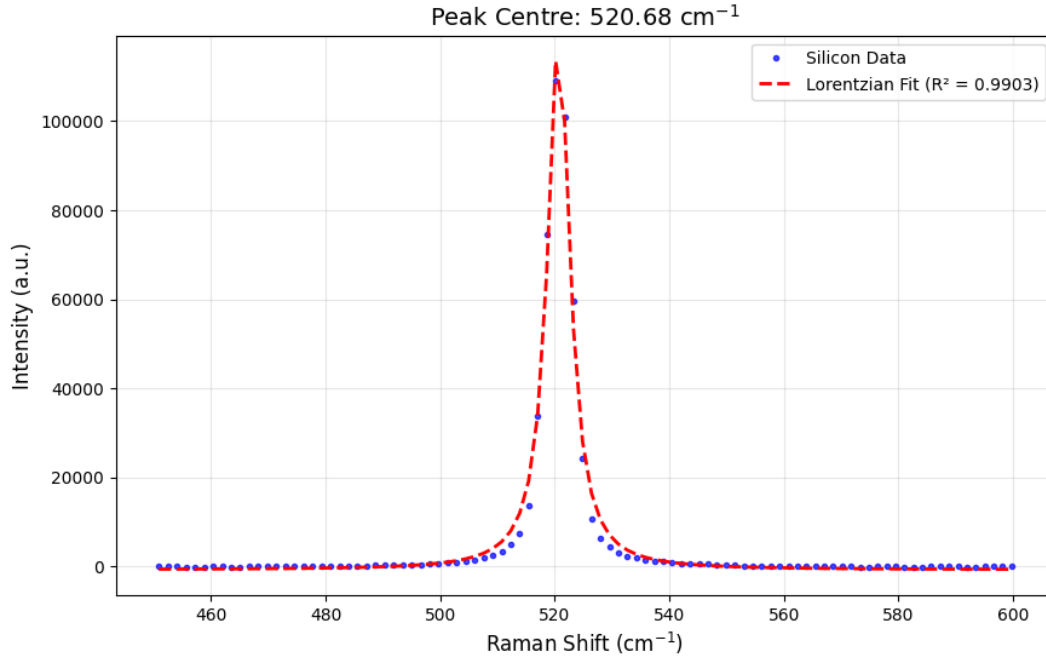


Figure 6. Lorentzian Fits of Silicon Sample Peak

Figure 5 shows the Raman spectrum of silicon based on the presence of a single, sharp Raman peak centred at approximately 520 cm⁻¹. This peak position (shown in Figure 6) is characteristic of crystalline silicon and corresponds to the first-order optical phonon mode at the Brillouin zone centre. The narrow linewidth (4.68 cm⁻¹) and high intensity of this peak indicate excellent crystal quality with minimal structural defects or disorder. Unlike the graphene and TiSe₂ spectra, which show multiple peaks, silicon exhibits a single dominant feature, making it readily distinguishable from the other materials analysed in this study.

Material 3: Titanium Diselenide

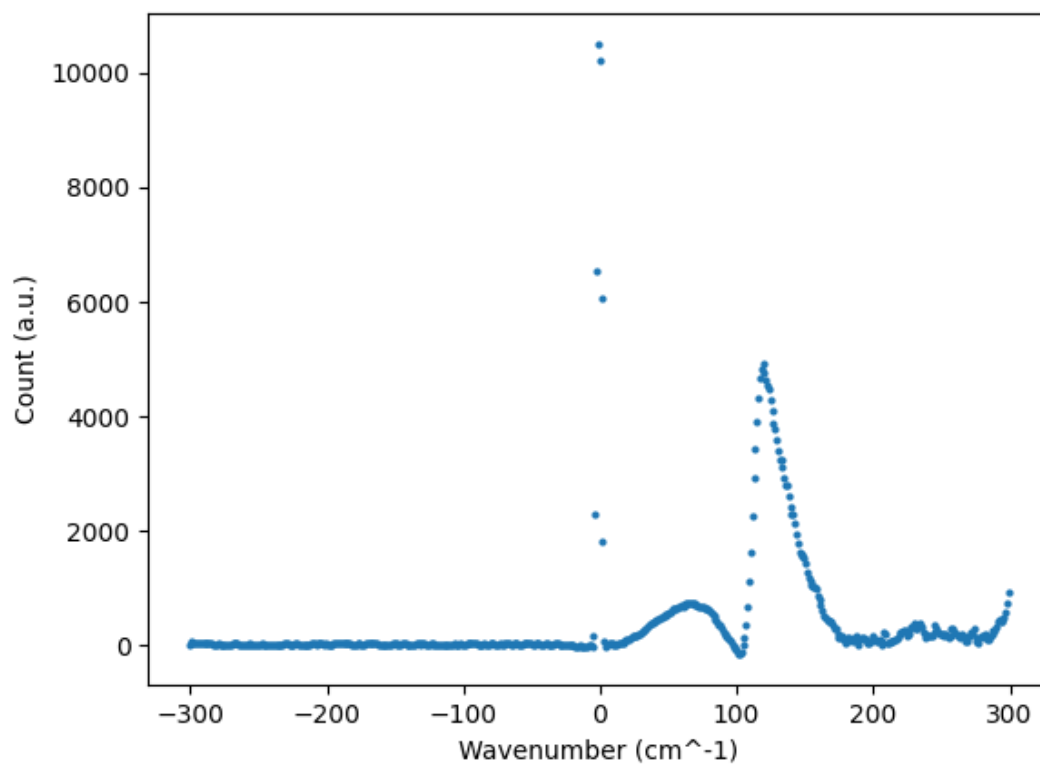


Figure 7. Raman Spectrum of TiSe2 Sample 1

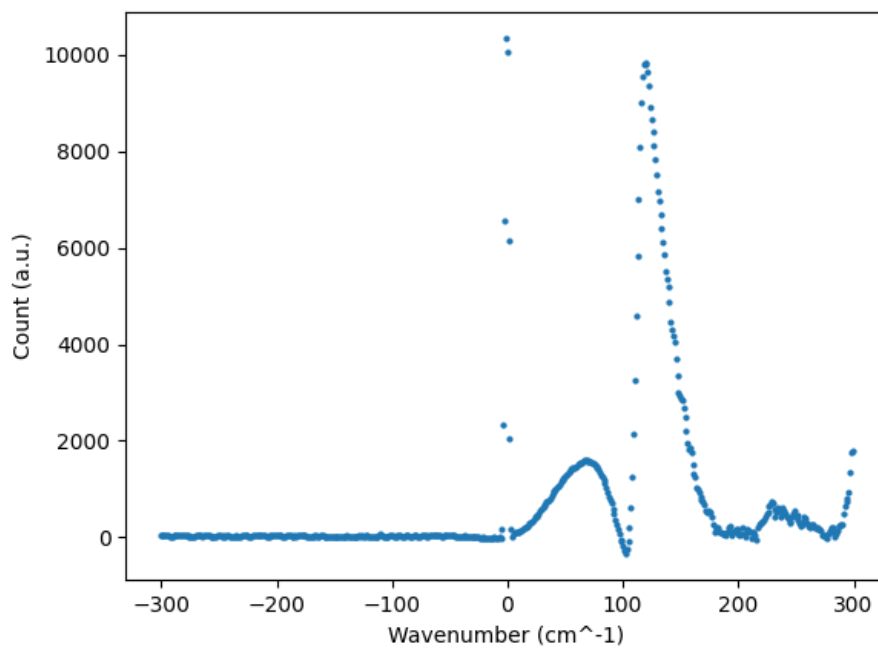


Figure 8. Raman Spectrum of TiSe2 Sample 2

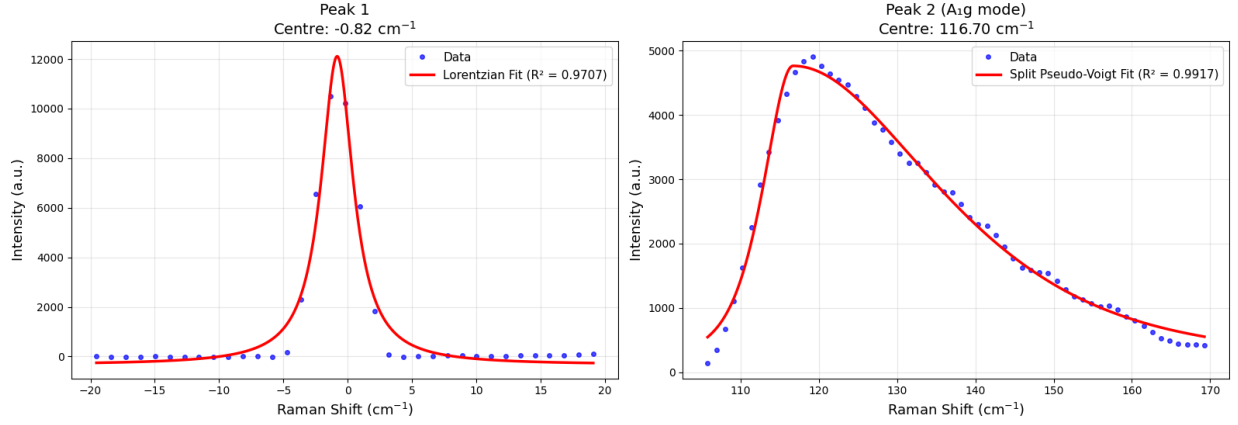


Figure 9. Lorentzian Peak Fitting of Peak 1 (Left) and Pseudo-Voigt Fitting of Peak 2 (Right) of TiSe₂ Sample 1

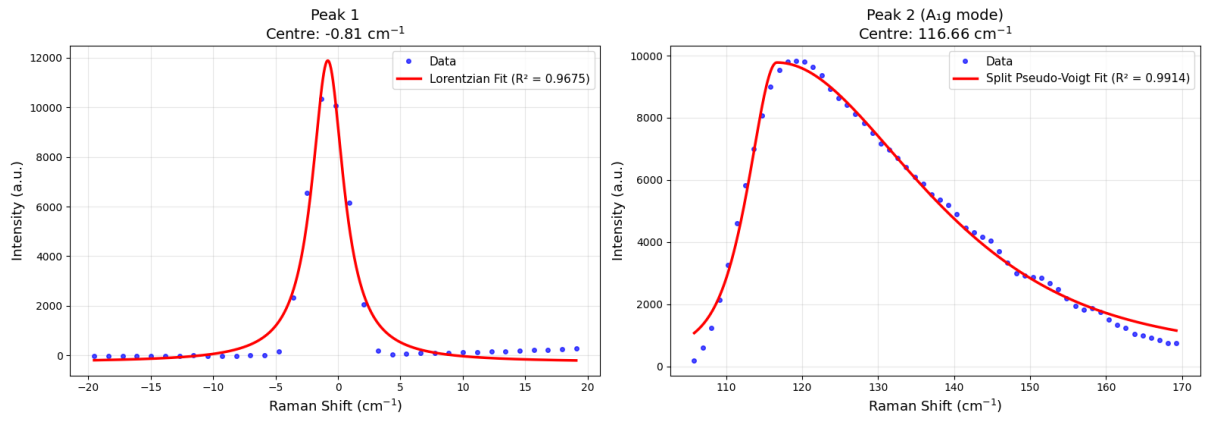


Figure 10. Lorentzian Peak Fitting of Peak 1 (Left) and Pseudo-Voigt Fitting of Peak 2 (Right) of TiSe₂ Sample 2

Figures 7 and 8 correspond to different regions of a TiSe₂ sample. Peak 2 of the samples as shown in Figure 9 (left) and 10 (left) is identified based on the presence of the characteristic in-plane E_g Raman-active mode around 136 cm⁻¹, as reported by both [2] and [3]. According to [2], the E_g mode involves in-plane vibration of selenium atoms. Note that the peak observed near 0 cm⁻¹ in both TiSe₂ spectra corresponds to Rayleigh scattered laser light (elastic scattering with no energy change) rather than a phonon mode, and was therefore not used for material characterisation.

Another observation is that TiSe₂ Sample 1 (Peak 1) shows the E_g peak centred at a slightly different position compared to TiSe₂ Sample 2 (Peak 2). More importantly, Peak 2 exhibits significant asymmetry in the E_g mode region around 117 cm⁻¹, which required fitting with a pseudo-Voigt function rather than a simple Lorentzian. This asymmetry may be related to the charge density wave (CDW) phase properties in TiSe₂, as the E_g mode is known to be sensitive to CDW-related structural distortions.

Thickness Analysis

For the graphene samples, layer number determination requires analysis of the 2D peak characteristics. Both samples show 2D peaks centred near 2680 cm^{-1} with similar shapes, suggesting few-layer graphene rather than monolayer material. The different $I(\text{D})/I(\text{G})$ ratios between samples (0.819 vs 0.239) reflect variations in defect density rather than thickness differences.

For the TiSe_2 samples, the significant difference in E_g peak intensity between Sample 1 (~ 5000 a.u.) and Sample 2 (~ 10000 a.u.) suggests thickness variation between the two sampled regions. According to [2] and [3], TiSe_2 exhibits thickness-dependent Raman intensity and charge density wave properties. The asymmetry observed in both samples (asymmetry ratios of 4.84 and 5.01), requiring pseudo-Voigt fitting, may be related to CDW-induced structural distortions. The higher intensity in Sample 2 likely indicates a thicker region compared to Sample 1.

Conclusion

This comprehensive Raman spectroscopy analysis has successfully identified all five provided spectra and extracted detailed information about the vibrational modes and material properties. The two graphene samples exhibit characteristic D, G, and 2D peaks, with differences in peak intensities and shapes indicating variations in defect density and number of layers between the samples. The $I(D)/I(G)$ ratios of 0.819 and 0.239 for Samples 1 and 2 respectively indicate different degrees of crystalline quality, with Sample 2 showing significantly fewer defects than Sample 1.

The silicon spectrum displays the expected single phonon mode at 520 cm^{-1} with excellent crystal quality as evidenced by the narrow linewidth and high intensity. This serves as a useful reference for verifying the Raman system calibration and demonstrating the fundamental principles of optical phonon scattering in a semiconductor crystal.

The two TiSe_2 spectra reveal the complex physics of charge density wave materials in reduced dimensions, with the characteristic E_g mode exhibiting significant asymmetry in both sampled regions. The peak intensity, position, and asymmetry variation between the two regions indicates spatial inhomogeneity across the sample. According to the literature [2] and [3], TiSe_2 exhibits thickness-dependent charge density wave properties, and the spectral variations observed here are consistent with such effects in two-dimensional materials.

This project has demonstrated the power of Raman spectroscopy as a non-destructive characterisation technique for identifying materials and probing their fundamental physical properties. The spectral variations observed in both graphene and TiSe_2 highlight the importance of sample quality and dimensionality in determining the properties of two-dimensional materials. The excellent agreement between our fitted peak positions and literature values, along with high R^2 values exceeding 0.95 for all fits, validates our experimental approach and data analysis methodology.

References

- [1] A. C. Ferrari and D. M. Basko, "Raman spectroscopy as a versatile tool for studying the properties of graphene," *Nature Nanotechnology*, vol. 8, p. 235–246, 2013.
- [2] D. L. Doung, G. Ryu, A. Hoyer, C. Lin, M. Burghard and K. Kern, "Raman Characterization of the Charge Density Wave Phase of 1T-TiSe₂: From Bulk to Atomically Thin Layers," *ACS Nano*, vol. 11, no. 1, pp. 1034-1040, 2017.
- [3] H. Wang, Y. Chen, M. Duchamp, Q. Zeng, X. Wang, S. H. Tsang, H. Li, L. Jing, T. Yu, E. H. T. Teo and Z. Liu, "Large-Area Atomic Layers of the Charge-Density-Wave Conductor TiSe₂," *Advanced Material*, vol. 30, no. 8, 2018.