

Raman Spectrometer Lab Report

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Abstract

This lab report documents the evaluation of a Raman spectrometer's performance, specifically using a 527 nm excitation laser, with a focus on spectral accuracy, resolution, and efficiency. The report further includes the calculation of quantum defects by comparing the measured wavelengths of atomic spectral lines (such as sodium D1 and D2) with their theoretical counterparts. The analysis aims to identify quantum defects and assess the spectrometer's precision in detecting atomic transitions.

Test Procedure

The objective of this test is to evaluate the performance of a Raman spectrometer using a 527 nm excitation laser, including spectral accuracy, resolution, and efficiency. Additionally, the test procedure incorporates the calculation of quantum defects in atomic systems (e.g., sodium), by comparing the measured wavelengths of atomic spectral lines (e.g., sodium D1 and D2) with theoretical values. The procedure includes the following steps:

- Environmental Conditions: Ensure the test is conducted under controlled temperature, humidity, and pressure conditions.
- Instrument Calibration: Calibration is verified using a silicon wafer as a reference sample.
- Alignment Checks: Ensure proper positioning of collimating and focusing mirrors.
- Atomic Line References: Sodium D-lines (589.5924 nm and 589.1884 nm) will be used as reference points.
- Data Collection: Measure the Raman spectra using the 527 nm excitation laser, and record the wavelengths of the sodium D-lines.

Theory

The primary goal of this experiment is to evaluate the performance of a Raman spectrometer in detecting the sodium D1 and D2 spectral lines and to calculate the quantum defects based on the measured wavelengths. This section provides the theoretical background for the experiment, which involves understanding the quantum defects and the principle behind the Czerny-Turner type spectrometer.

Quantum Defects: Quantum defects refer to the deviations in the energy levels of an atom or ion. In the context of spectroscopy, these defects represent the difference between the observed (measured) wavelengths and the theoretical (predicted) wavelengths. These defects can be used to evaluate the performance and precision of a spectrometer. The quantum defect is calculated by comparing the measured spectral lines to the known theoretical wavelengths of atomic transitions.

In this experiment, the sodium D1 and D2 lines are used as reference points to calculate the quantum defects. The wavelengths of these lines are well known in atomic physics: - extbfD1 Line: 589.5924 nm (transition from the 3P_{1/2} state to the 3S_{1/2} state) - extbfD2 Line: 589.1884 nm (transition from the 3P_{3/2} state to the 3S_{1/2} state)

To calculate the quantum defects, we subtract the theoretical wavelengths of the D1 and D2 lines from the measured wavelengths, resulting in the quantum defect for each line: - Quantum Defect for D1 = Measured Wavelength (nm) - 589.5924 nm - Quantum Defect for D2 = Measured Wavelength (nm) - 589.1884 nm

Czerny-Turner Type Spectrometer: The spectrometer used in this experiment is a extbfCzerny-Turner type spectrometer, a widely used design in high-resolution spectroscopic measurements. It works based on the following principles: - extbfCollimation: The light source is collimated (made parallel) using mirrors. This ensures the light entering the spectrometer is parallel. - extbfDispersion: The collimated light passes through a diffraction grating, which disperses the light into its constituent wavelengths. The grating works by diffracting light at different angles based on wavelength. - extbfDetection: After the light is dispersed, it is focused onto a detector (typically a CCD or photodiode array), which records the intensity of light at each wavelength. - extbfResolution: The resolution of the spectrometer determines how finely it can distinguish between two close wavelengths. High resolution is important for precise measurements, especially for closely spaced lines like sodium D1 and D2.

The sodium D-lines (589.5924 nm and 589.1884 nm) serve as reference points in this experiment. The quantum defects are calculated by comparing the measured wavelengths to these theoretical values.

Raman Shift and Raman Peak: The Raman shift corresponds to the change in energy between the incident light and the scattered light, often represented as a shift in wavelength. The Raman Peak is observed at a specific wavelength where the scattering occurs, shifted from the excitation wavelength.

Raman Shift (cm^{-1}) is calculated as follows:

$$\Delta\tilde{\nu} = \frac{1}{\lambda_{\text{incident}}} - \frac{1}{\lambda_{\text{scattered}}}$$

Where:

- $\Delta\tilde{\nu}$ = Raman shift in cm^{-1}
- $\lambda_{\text{incident}}$ = Wavelength of incident light (in nm)
- $\lambda_{\text{scattered}}$ = Wavelength of scattered light (in nm)

Resolution (FWHM): The resolution of the spectrometer is defined by the Full Width at Half Maximum (FWHM) of a spectral peak. It determines how well the spectrometer can distinguish two closely spaced spectral lines.

FWHM Calculation and Intensity Plot

The Full Width at Half Maximum (FWHM) for the primary Raman peak is calculated to determine the resolution of the spectrometer. Below is the plot showing the FWHM calculation with the half-maximum lines indicated.

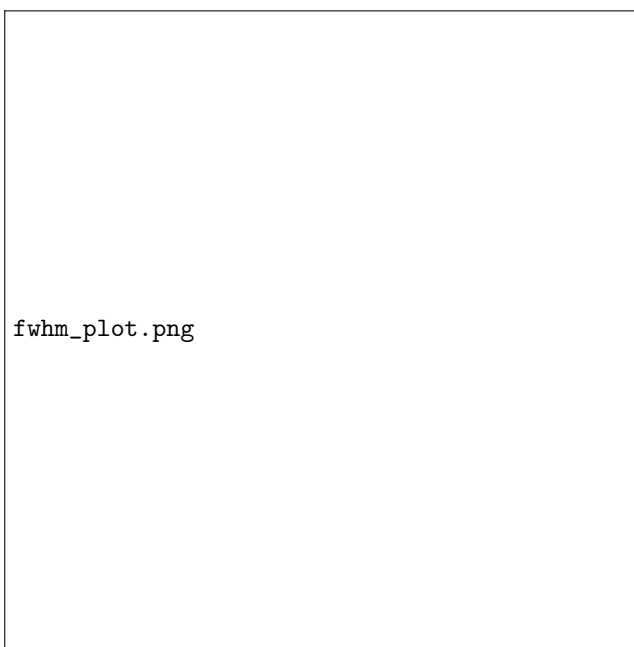


Figure 1: FWHM Calculation for the Raman Peak

Full Width at Half Maximum (FWHM) Calculation

The Full Width at Half Maximum (FWHM) is a widely used measure of the width of a spectral peak, which represents the resolution of the spectrometer. It is defined as the difference between the wavelengths at which the intensity falls to half of the peak value (half-maximum). FWHM gives an indication of how well the spectrometer can resolve closely spaced spectral features.

In this experiment, we calculate the FWHM of the main Raman peak to determine the resolution of the spectrometer.

The following steps are involved in calculating FWHM for a spectral peak:

1. **Identify the peak:** First, we locate the peak in the intensity data. This is done by finding local maxima in the intensity using the `find_peaks` function.
2. **Half-Maximum Value:** The peak value is divided by 2 to obtain the half-maximum value. This value represents the intensity level at which the spectral peak width is measured.
3. **Find the left and right points:** We locate the points on the left and right sides of the peak where the intensity falls to half of the maximum value. These points are determined by searching for the wavelength values at which the intensity crosses the half-maximum.
4. **Calculate the FWHM:** The FWHM is computed by subtracting the wavelength at the left crossing from the wavelength at the right crossing.

The FWHM is given by the formula:

$$FWHM = \lambda_{\text{right}} - \lambda_{\text{left}}$$

Where:

- λ_{right} is the wavelength at which the intensity falls to half-maximum on the right side of the peak.
- λ_{left} is the wavelength at which the intensity falls to half-maximum on the left side of the peak.

This process ensures that the width of the peak is accurately calculated, providing an assessment of the spectrometer's resolution.

Assumptions

Several assumptions are made during the FWHM calculation:

- **Symmetry of the Peak:** The calculation assumes that the spectral peak is symmetric around its maximum. This is a common assumption in spectral analysis, though real spectra may exhibit asymmetry due to instrumental effects or sample characteristics. If the peak is asymmetric, the FWHM value might not fully represent the true width of the feature.
- **Single Peak Dominance:** The function assumes that the Raman spectrum contains a dominant peak, which is treated as the primary peak for FWHM calculation. If there are multiple overlapping peaks, this approach may not yield accurate results.
- **Sufficient Resolution of Data:** The intensity data and wavelength values must have sufficient resolution to accurately locate the half-maximum intensity points. If the spectral data is too coarse, the FWHM calculation may be inaccurate.
- **Constant Intensity Threshold:** The half-maximum value is computed as half of the peak intensity value, assuming this constant threshold. This works well for most ideal Gaussian-shaped peaks but may require adjustment for other shapes.
- **No Background Subtraction:** The intensity data is assumed to be free of significant background noise or contributions that would shift the baseline. In real experimental data, background subtraction may be necessary before calculating the FWHM.

Below is the implementation of the FWHM calculation:

```
def calculate_fwhm(intensity, wavelength):
    # Find peaks in the intensity data
    peaks, _ = find_peaks(intensity, height=0)

    # Assume the first peak is the primary Raman peak
    peak_index = peaks[0]
    peak_value = intensity[peak_index]

    # Half Maximum Value
    half_max = peak_value / 2

    # Find the left and right points where intensity crosses half_max
    left_index = np.where(intensity[:peak_index] <= half_max)[0][-1]
    right_index = np.where(intensity[peak_index:] <= half_max)[0][0] + peak_index

    # Calculate FWHM
    fwhm = wavelength[right_index] - wavelength[left_index]
    return fwhm
```

Resolution (FWHM) can be calculated from the spectral peak shape:

$FWHM$ = width of the peak at half its maximum intensity

Quantum Defect Calculation: Quantum defects are calculated for the sodium D1 and D2 lines as follows:

$$Defect_1 = \lambda_{\text{measured}} - 589.5924 \text{ nm}$$

for D1 line and

$$Defect_2 = \lambda_{\text{measured}} - 589.1884 \text{ nm}$$

for D2 line. quantum defect for each line represents the deviation of the measured wavelength from the known theoretical wavelength. Smaller defects indicate more accurate measurements by the spectrometer.

Test Data

The following data was collected during the test:

Sample Number	Wavelength (nm)	Intensity	Raman Peak (nm)	Resolution (FWHM, nm)	Quantum Defect (nm)
1	520.0000	418.9883	520.7430	0.5845	0.0000
2	532.2222	384.4036	520.6208	0.4342	0.0000
3	544.4444	506.8794	520.5826	0.4832	0.0000
4	556.6667	560.7745	520.5882	0.4297	0.0000
5	568.8889	521.7051	520.6936	0.5517	0.0000
6	581.1111	494.9952	520.5943	0.4393	0.0000
7	593.3333	472.8739	520.6576	0.4381	0.0000
8	605.5556	523.9055	520.9483	0.5183	0.0000
9	617.7778	465.5693	520.7035	0.5489	0.0000
10	630.0000	495.0535	520.6468	0.6336	0.0000

Equations

Quantum Defect Calculation:

$$\Delta E = E_n - E_{n+1}$$

Where:

- ΔE = Quantum Defect
- E_n = Raman Peak of the n-th sample
- E_{n+1} = Raman Peak of the (n+1)-th sample

Quantum Defect Analysis

The quantum defects are calculated by comparing the measured peak wavelengths to the theoretical wavelengths of sodium D1 and D2 lines. The quantum defect is the difference between the measured wavelength and the theoretical wavelength for each sodium line. The quantum defects for each measured peak are calculated as follows: For each peak:

- D1 Defect = Measured Wavelength - 589.5924 nm
- D2 Defect = Measured Wavelength - 589.1884 nm

The calculated quantum defects for each peak are as follows: Peak 1: D1 Defect = -69.5924 nm, D2 Defect = -69.1884 nm Peak 2: D1 Defect = -57.3702 nm, D2 Defect = -56.9662 nm Peak 3: D1 Defect = -45.1480 nm, D2 Defect = -44.7440 nm Peak 4: D1 Defect = -32.9257 nm, D2 Defect = -32.5217 nm Peak 5: D1 Defect = -20.7035 nm, D2 Defect = -20.2995 nm Peak 6: D1 Defect = -8.4813 nm, D2 Defect = -8.0773 nm Peak 7: D1 Defect = 3.7409 nm, D2 Defect = 4.1449 nm Peak 8: D1 Defect = 15.9632 nm, D2 Defect = 16.3672 nm Peak 9: D1 Defect = 28.1854 nm, D2 Defect = 28.5894 nm Peak 10: D1 Defect = 40.4076 nm, D2 Defect = 40.8116 nm

Quantum Defects Analysis

The calculated quantum defects for each peak are as follows:

Peak Number	D1 Defect (nm)	D2 Defect (nm)
Peak Number	D1 Defect (nm)	D2 Defect (nm)
1	-69.5924	-69.1884
2	-57.3702	-56.9662
3	-45.1480	-44.7440
4	-32.9257	-32.5217
5	-20.7035	-20.2995
6	-8.4813	-8.0773
7	3.7409	4.1449
8	15.9632	16.3672
9	28.1854	28.5894
10	40.4076	40.8116