PROJECT 3
DETERMINING PRIME PEAK RATIO FOR CONTROLLING TYPE OF GRAPHENE PRODUCED

Stephanie Toole, University of Kansas
Dept. of Physics and Astronomy
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Abstract

Graphene is a popular 2D material for condensed matter physics. The graphene can be monolayer, bilayer, or multilayer. The graphene can be characterized using Raman spectroscopy. This paper looks at the peaks produced in this spectroscopy and focuses in on two peaks, G peak and 2D peak. This paper finds that the likelihood of finding monolayer graphene is highest when the peak ratio is near 2.2 based on the function.

I. INTRODUCTION

Raman spectroscopy can be used to characterize graphene. It is an analytical technique that utilizes the inelastic scattering of light to investigate molecular structure and composition in a non-destructive manner.This method can give an idea of if monolayer, bilayer, or multilayer graphene is most present. Raman spectroscopy is a valuable tool for graphene characterization, providing insights into the number of layers, structural defects, and doping levels by analyzing the vibrational modes and intensity ratios of the Raman peaks. This is done by comparing two peaks on the Raman outcomes. The difference in value between these peaks is how to characterized in this method.

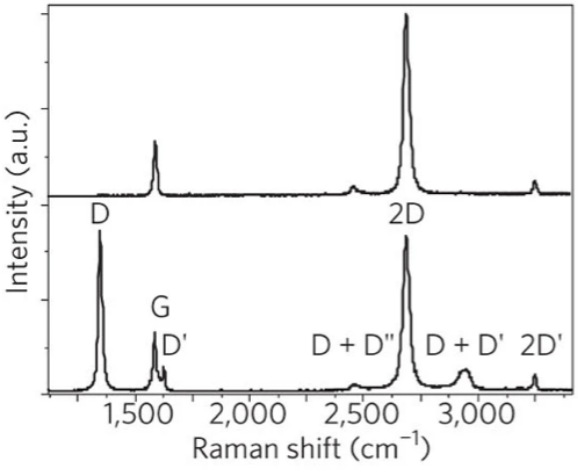

Figure 1: Raman spectroscopy of graphene example plot of G peak and 2D peaks. Top row is pristine graphene and bottom row has defects. [1]

The parameter represents the difference in the peaks. We want to determine the likelihood of finding monolayer graphene at a certain parameter, or difference between the peaks. The experiment will allow us to determine the ideal difference in peaks for consistent monolayer graphene and what kind of confidence interval that can be based upon.

II. ALGORITHM ANALYSIS

The question being answered is what value of peak ratio will give us the highest likelihood of producing monolayer graphene. The input program is a Python code that simulates an experiment. The simulation uses a normal distribution to create a random variable. [2] The code creates a variable with a mean of zero and the standard deviation is decided by the parameter.

The simulation then defines a likelihood function to find the probability of the data given a specified parameter value.[3][4] It uses the formula for the normal probability density function, taking the sum of the squared deviations of the data from the expected value divided by the estimated variance, and normalizes by a constant term to make the integral of the function over all possible parameter values equal to 1. [5]

The program defines a true value for the parameter of choice and sets the amount of measurements taken in the simulated experiment. The outcomes of the experiment are saved to a text file. [6]

The program that analyzes the output of the simulated experiment can produce calculations and a plot to more clearly understand the data. [7] This analysis code reads the text file and calculates the likelihood function for various values of the parameter. The plot shows the likelihood plotted as a function of the parameter value. It also estimates the maximum likelihood parameter value as well as the confidence interval. [8] The simulated data and parameter value are run through the likelihood function. First, the standard deviation is calculated. Then, the program calculates the likelihood via the formal for a normal distribution with mean zero and standard deviation as the parameter. [9] The function scales by a factor dependent on how many data points are collected. The maximum likelihood is also calculated and plotted with a vertical dashed line. [10] It prints the estimated parameter value and the confidence interval using print.

III. OUTPUT INTERPRETATION

The simulated experiment is done to better predict the difference in peaks that will result in monolayer graphene.

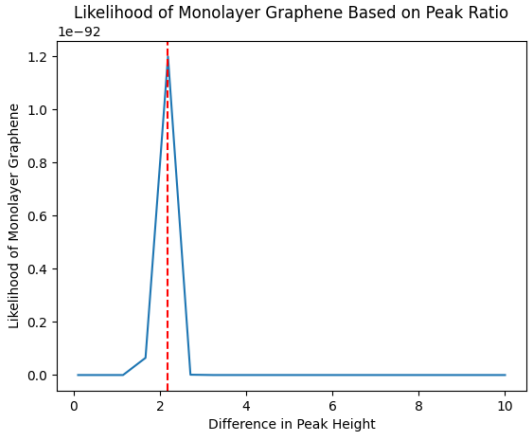

Figure 2: Likelihood function for finding monolayer graphene. For our sample it lies at around 2.3 to 2.5

By setting the value and a confidence interval, we can then, using real data, more easily rule out non monolayer data. Allowing us to focus in on a particular peak ratio that has highest likelihood of containing a monolayer area.

IV.CONCLUSION

In conclusion, we have found that we should aim for a difference in peaks that is greater than 2 but less than 2.5. Further research will be able to support or refute this early claim we are making of best parameters.

V. REFERENCES

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[5] https://analyticsindiamag.com/maximum-likelihood-estimation-python-guide/

[6] https://python.quantecon.org/mle.html

[7] https://www.geeksforgeeks.org/numpy-linspace-python/

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