

Final Report

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Abstract

In this work, grazing incidence X-ray diffraction (GIXRD) is utilized to investigate the depth profile of dopants in silicon. By systematically varying the X-ray incidence angle, one can precisely control the depth penetrated into doped silicon samples. This approach enables a non-destructive analysis of how dopant concentration evolves with depth. The findings provide crucial insights into the distribution and behavior of dopants, which is essential for optimizing semiconductor device performance and fabrication processes.

1 Background

Solids can be divided into two broad types: crystalline, and amorphous. Crystalline solids have repeating structure that is predictable, and is consistent throughout the entire solid. Amorphous solids have no repeating structures, and have no preferred orientation.

X-Ray diffraction (XRD) utilizes x-rays to non-destructively probe the inner atomic layers of materials. In this work it is used to probe different depths of doped silicon to see dopant levels as a function of depth. As the x-ray interacts with the sample it will reflect, refract, and diffract. Diffraction is the process of note, and the only one that will be investigated for this work.

When XRD is used on crystalline solids a diffraction pattern will emerge. The spacing between the atoms acts as the slit size that allows for the diffraction interference pattern, in accordance with Bragg's Law ($2d \sin \theta = n\lambda$). There also exist different spacings between atoms that are not nearest neighbors. Each of these different spacings are relegated into planes that act like a diffraction grating, existing for every possible repeating spacing within the atom. All of these in superposition produce a graph that shows sharp peaks correlating directly to the atomic plane's spacing (shown in figure 1).

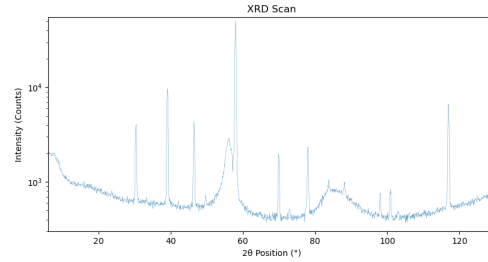


Figure 1: Diffractogram of pure crystalline solid

Amorphous solids under the x-ray beam behave in a similar manner. The difference being because every atom is arranged randomly, there are an infinite number of planes with their own spacing. As shown in figure 2, this correlates to a moderately low angle hump (called an amorphous hump) with all spacings that would correlate to higher angled peaks being nonexistent because of deconstructive interference[6, 1, 7].

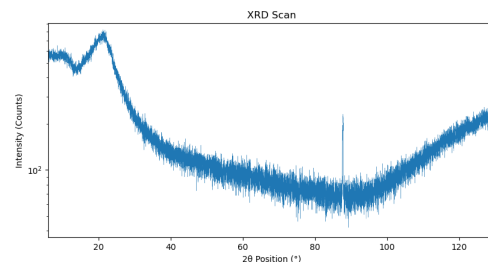


Figure 2: Diffractogram of pure amorphous solid

The materials analyzed in this work are silicon doped with phosphorous, silicon doped with boron, and pure silicon. The first two materials will be best thought of as a gradient from pure phosphorous or boron to pure silicon from top to bottom. Silicon is a crystalline material, while phosphorous and boron are amorphous. This means that the diffractogram will be a superposition of an amorphous diffractogram on a crystalline diffractogram. The silicon sample was only used to verify that the amorphous hump was present on the diffractograms.

The XRD process used to incrementally probe deeper depths is called grazing incidence x-ray diffraction (GIXRD, also called glancing incidence x-ray diffraction). Using this method the XRD will hold the incident beam at a fixed angle (called omega (ω)), while the diffracted beam side moves from a starting angle to an end angle. The detector is used in a 0D mode that simply counts all the x-rays that interact with it. The angle the counts correspond to is the angle the incident beam is added to the current diffracted beam angle all multiplied by 2: $2(\omega + \theta)$. After the scan finishes a new scan is started with a different incident angle to probe a different depth.

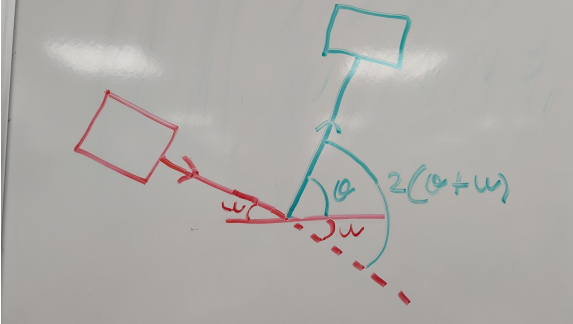


Figure 3: Diagram of XRD using GIXRD

The different incident angles probe different depths due to the different path lengths they provide the x-rays as they interact with the samples. This is due to the exponential attenuation of intensity as the beam travels given by this equation: $I(y) = I_0 e^{-\alpha y}$ with $\alpha = 2\omega n_I / c$ [4, 3]. With the complex index of refraction (n_I) strongly dependent on wavelength. The x-ray source is copper, producing K_α , and K_β in most abundance. Since one wavelength provides the most uniformity on the diffractogram, the incident beam optics include a filter to limit the unnecessary wavelength. K_α is what is most common, so the K_β gets mostly filtered out by a nickel filter. This results in a x-ray beam that has a wavelength of 1.54Å (uniformity in the wavelength is also neces-

sary for Bragg's law).

2 Methods

Three different methods for determining relative percentages of the dopant in the substrate are used. The methods are: 1. Take the ratio of the max peak intensity, 2. Fit the peaks to a Gaussian curve, and find the integrated area, 3. Perform a summation to find the numerical integral. These methods are predicated on certain assumptions. The mixture of the probed depth is uniform, which is a known simplification of how the diffused dopants actually spread (an analysis to correct this has been tried, but better data is needed for it to be effective). The intensity of the x-ray is also assumed to have attenuated by 90%, and all relevant data comes from that. The last assumption is that the sample is put in its preferred orientation for the silicon structure to be aligned with the x-ray beam. The index of refraction is the same as bulk samples[2].

Method 1: Ratio

With this method the program takes the max intensity of the amorphous hump, and the max intensity of the most intense crystalline peak, and takes the ratio of them. This ratio is then the relative percentages of the dopant and substrate[5].

Method 2: Curve Fitting

This method takes the position and intensity values as the x and y inputs of scipy's curve_fit function. It then outputs the best fit for amplitude, mean, standard deviation, and a background value. The function then gets integrated, and the ratio of the areas are taken.

Method 3: Summation

This is an integral method as in method 2, but instead of fitting the data to a curve the data is integrated using discrete methods. The dx is the same for all points, so it is ignored with the foresight that it will be divided out. The sum is of all the intensity values for the peak or hump. A ratio is then taken from these sums.

3 Results

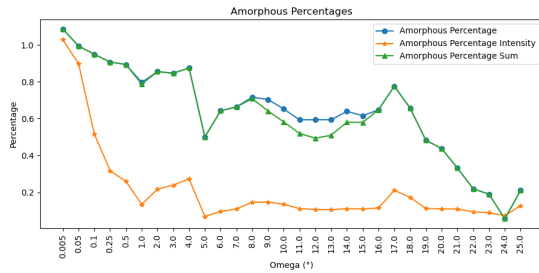


Figure 4: Percent amorphous at selected omegas

Figure 4 provides a concise overview of how the dopant and substrate mixture change with omega. All three methods show the amorphous percent decreases with depth, which is to be expected. They also show that the 0.005 omega is greater than 1 for the amorphous. This is due to the crystalline peak being nonexistent, but the program is still trying to see a peak. The curve fitting and summation method provide excellent agreement with each other, while the ratio method alludes to an exponential.

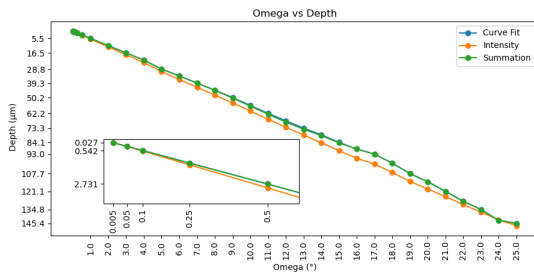


Figure 5: Depth vs omega for the three methods

Figure 5 shows the depth that correlates with the three methods. The methods have a close agreement, with the curve fit and summation method being right on top of each other. They all show a mostly linear relationship, which is to be expected since the indices of refraction are very similar for the dopant and substrate. Nevertheless, it is interesting that the methods more closely agree at lower and high omegas, but not the middle omegas.

4 Conclusion

Using GIXRD to determine relative composition of samples led to three analysis methods. Two of the methods utilized integration, and their results are closer aligned. One method used peak intensity ratios, and provides results that noticeably differ.

All three methods provide reasonable agreement as to the depth that each omega probed. Using GIXRD to see relative mixture amount dependent on depth has been shown to be useful, keeping in mind the limitations given by the assumptions.

5 Future Work

Performing this analysis on a known sample would be able to provide greater validity to the results of this analysis. Creating an analysis to correct for the real diffusion process by not assuming uniform layers. This would produce the greatest impact on the real world application of these results.

6 Notable Things Learned

- How to use GIXRD
- XRD sample preparation
- Leveraging dictionaries and dataframes for effective data analysis
- Write data to an Excel file for less error prone data storage
- Real world error handling in python

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7 Appendix A:

```
1 import matplotlib.pyplot as plt # Used for plotting
2 import numpy as np # Used for arrays, and some math functions
3 import pandas as pd # Used for reading and writing files
4 import os # Used for file handling
5 from scipy.optimize import curve_fit # Used for fitting functions to data
6 from scipy.stats import chi2 # Used for chi squared probability
   calculations
7 import traceback # Used for error handling
8 import sys # Used for error handling
9 import re # Used to extract omega from file names
10 import sympy as sp # Used for uncertainty calculations
11 np.set_printoptions(threshold=np.inf) # Forces numpy to print everything
   in an array. This is useful for exporting everything to a file
12 """
13 This script processes X-ray diffraction (XRD) data to fit peaks, calculate
   areas, and analyze sample depth.
14 It reads scan data from CSV files, fits Gaussian functions to the peaks,
   calculates the area under the peaks,
15 and determines the mixture of amorphous and crystalline phases. It also
   calculates the sample depth based on the peak areas.
16 It includes functions to read data, fit peaks, calculate areas, and
   analyze sample depth. It then exports the data to excel.
17
18 Mark Smith
19 """
20
21 def XRD_Data_Dictionary(path_name: str): # Gets position and intensity
   from file to a dictionary
22     """
23     Reads XRD data from a specified path and returns a dictionary with the
   data.
24
25     Parameters:
26         path_name (str): The path to the directory containing the XRD data
   files.
27
28     Returns:
29         dict: A dictionary where keys are file names, and values are
   position and intensity.
30     """
31     xrd_data = {} # Initialize an empty dictionary to store the data
32
33     os.chdir(path_name) # Change the current working directory to the
   specified path
34
35     # Inputs to get from the user (or to hardcode in options)
36     omega_in_file_name = 'y' # input('Are the omega values in the file
   names followed by a w? (y/n): ').strip().lower() # This allows for
   automatic omega extraction (highly recommended)
37     normalize_choice = 'n' # input("Do you want to normalize the intensity
   data? (y/n): ").strip().lower() # Ask the user if they want to
   normalize the intensity data
38     smooth = 'n' # input("Do you want to smooth the data? (y/n): ").strip
   ().lower() # Ask the user if they want to smooth the data
39     if smooth == 'y':
40         how_smooth = 25 # int(input("How many points do you want to smooth
   over? (e.g., 25): ")) # Ask the user how many points to
   smooth over
41
```

```

42     for file in os.listdir(path_name): # Iterate through each file in the
43         directory
44         if file.endswith('.csv'): # Process only CSV files
45             try:
46                 scan = pd.read_csv(file, index_col=0) # Read the CSV file
47                 into a DataFrame
48
49                 intensity = scan['Intensity [Counts]'].to_numpy() # Get
50                 the intensity data from the CSV file
51                 position = scan['Pos. [degree_symbol2theta]'].to_numpy()
52                 # Get the position data from the CSV file
53
54                 # Smooth data
55                 if smooth == 'y':
56                     i = 0
57                     intensity_smooth = []
58                     position_smooth = []
59                     while i < len(intensity)-how_smooth:
60                         intensity_sum = 0
61                         position_sum = 0
62                         for j in range(how_smooth):
63                             intensity_sum += intensity[i+j]
64                             position_sum += position[i+j]
65                         intensity_smooth.append(intensity_sum/how_smooth)
66                         position_smooth.append(position_sum/how_smooth)
67                         i += how_smooth
68                 else:
69                     intensity_smooth = intensity
70                     position_smooth = position
71
72                 if omega_in_file_name == 'y':
73                     # Extract omega using regex (matches numbers with
74                     optional decimal before 'w')
75                     match = re.search(r'([0-9.]+)w', file)
76                     if match:
77                         omega = float(match.group(1))
78                     else:
79                         print(f"Could not extract omega from filename: {
80                             file}")
81                         continue # Skip this file if omega can't be
82                         extracted
83                 else:
84                     omega = float(input(f'Input the omega for this file {
85                             file}: '))
86
87                 if normalize_choice == 'y':
88                     intensity = intensity/max(intensity) # Normalize the
89                     intensity data to the maximum value
90
91                 xrd_data[file] = {'omega': omega, 'Position': np.array(
92                     position_smooth), 'Intensity': np.array(
93                     intensity_smooth)} #, 'Time Step': position_smooth[1]-
94                     position_smooth[0]} # Store the data in the
95                     dictionary
96
97             except Exception as e: # Skips non scan files
98                 print(f"Error processing file {file}: {e}")
99                 pass
100
101     # Sort the dictionary by omega in descending order
102     sorted_data = dict(sorted(xrd_data.items(), key=lambda item: item[1]['
103         omega'], reverse=True))

```

```

90     print('\n')
91     return sorted_data
92
93 def Length_Peak(data: dict): # Just gets the peak ranges
94     """
95     Prompts the user to input the amorphous and crystalline ranges for
96     each file in
97     the data dictionary.
98
99     Parameters:
100         data (dict): A dictionary containing XRD data with file names as
101         keys and
102         position/intensity as values.
103
104     Returns:
105         dict: The updated dictionary with amorphous and crystalline ranges
106         added for each file.
107     """
108     manual_input = 'no' # input("Do you want to manually input the ranges?
109     (yes/no): ").strip().lower() # Ask the user if they want to
110     manually input the ranges
111
112     if manual_input == 'no':
113         peak_range_file = 'Peak_Ranges.txt' # input("Enter the file name
114         containing the peak ranges (e.g., 'peak_ranges.txt'): ")
115         peak_ranges = pd.read_csv(peak_range_file) # Read the peak ranges
116         from the specified file
117
118     for file_name in data.keys():
119
120         if manual_input == 'yes':
121             print(f"Processing file: {file_name}")
122             amorphous_range = input("Enter the amorphous range (e.g.,
123             20-30): ")
124             amorphous_range = [float(x) for x in amorphous_range.split('-')]
125             # Convert the input range to a list of floats
126
127             crystalline_range = input("Enter the crystalline range (e.g.,
128             30-40): ")
129             crystalline_range = [float(x) for x in crystalline_range.split(
130             '-')] # Convert the input range to a list of floats
131
132             print('\n')
133
134         else:
135             omega = data[file_name]['omega'] # Get the omega value from
136             the data dictionary
137             file_index = peak_ranges.index[peak_ranges['Omega'] == omega]
138             # Find the index of the file in the peak ranges DataFrame
139
140             amorphous_range = [float(x) for x in peak_ranges.loc[
141             file_index, 'Amorphous Range'].values[0].split('-')] #
142             Get the amorphous range from the DataFrame
143             crystalline_range = [float(x) for x in peak_ranges.loc[
144             file_index, 'Crystalline Range'].values[0].split('-')] #
145             Get the crystalline range from the DataFrame
146
147             data[file_name]['amorphous_range'] = amorphous_range
148             data[file_name]['crystalline_range'] = crystalline_range
149
150     return data

```

```

135 def Gaussian_function(current_x_value: float, amplitude: float, mean:
float, standard_deviation: float, background: float = 0): # Function
to fit to
136 """
137 Calculates the Gaussian function value for a given x value.
138
139 Parameters:
140     current_x_value (float): The x value at which to evaluate the
Gaussian function.
141
142     amplitude (float): The amplitude of the Gaussian peak.
143
144     mean (float): The mean (center) of the Gaussian peak.
145
146     standard_deviation (float): The standard deviation of the Gaussian
peak.
147
148     background (float): The background value to be added to the
Gaussian function.
149
150 Returns:
151     float: The value of the Gaussian function at the given x value.
152 """
153
154 func = amplitude*np.exp(-.5*((current_x_value-mean)/standard_deviation
)**2)/(standard_deviation*np.sqrt(2*np.pi))+ background #
Calculate the Gaussian function value
155
156 return func
157
158 def Peak_fit(data: dict, background: bool = True): # Fit the peaks to a
Gaussian function
159 """
160 Fits the peaks in the XRD data based on the provided ranges.
161
162 Parameters:
163     data (dict): A dictionary containing XRD data with file names as
keys and
164     position/intensity as values, including amorphous and
crystalline ranges.
165
166 Returns:
167     dict: An updated dictionary with fitted peak areas for each file.
168 """
169
170 for file_name, file_data in list(data.items()): # Iterate through each
file in the data dictionary using key and value
171     try:
172         # Unpack the values from the file data
173         position = file_data['Position']
174         intensity = file_data['Intensity']
175         amorphous_range_start_user, amorphous_range_end_user =
file_data['amorphous_range']
176         crystalline_range_start_user, crystalline_range_end_user =
file_data['crystalline_range']
177
178         # Pull out the actual data for the amorphous and crystalline
peaks
179         amorphous_mask = ((position >= amorphous_range_start_user) & (
position <= amorphous_range_end_user) & ~((position >
crystalline_range_start_user) & (position <
crystalline_range_end_user)))

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```

180     crystalline_mask = ((position >= crystalline_range_start_user)
181                         & (position <= crystalline_range_end_user))
182
183     x_values_amorphous = position[amorphous_mask]
184     y_values_amorphous = intensity[amorphous_mask]
185
186     x_values_crystalline = position[crystalline_mask]
187     y_values_crystalline = intensity[crystalline_mask]
188
189     # Subtract background when needed
190     if background == False:
191         y_values_amorphous = y_values_amorphous - data[file_name][
192             'amorphous_fit_background'] # Get the intensity values
193             for the amorphous range
194         y_values_crystalline = y_values_crystalline - data[
195             file_name]['crystalline_fit_background'] # Get the
196             intensity values for the crystalline range
197
198     # Get guesses for the Gaussian parameters
199     guess_background = min(intensity) # Guess the background for
200     the peaks
201
202     guess_amplitude_amorphous = y_values_amorphous.max() # Guess
203     the amplitude for the amorphous peak
204     guess_mean_amorphous = x_values_amorphous.mean() # Guess the
205     mean for the amorphous peak
206     guess_std_amorphous = x_values_amorphous.std()/2 # Guess the
207     standard deviation for the amorphous peak
208     guess_amorphous = [guess_amplitude_amorphous,
209                       guess_mean_amorphous, guess_std_amorphous,
210                       guess_background] # Create a list of guesses for the
211     amorphous peak
212
213     guess_amplitude_crystalline = y_values_crystalline.max() #
214     Guess the amplitude for the crystalline peak
215     guess_mean_crystalline = x_values_crystalline.mean() # Guess
216     the mean for the crystalline peak
217     guess_std_crystalline = x_values_crystalline.std()/2
218     guess_crystalline = [guess_amplitude_crystalline,
219                         guess_mean_crystalline, guess_std_crystalline,
220                         guess_background]
221
222     if background == False:
223         guess_amorphous = guess_amorphous[:-1] # Remove the
224         background guess for the amorphous peak
225         guess_crystalline = guess_crystalline[:-1] # Remove the
226         background guess for the crystalline peak
227
228     # Fit the Gaussian function to the data
229     fit_amorphous, error_amorphous = curve_fit(Gaussian_function,
230         x_values_amorphous, y_values_amorphous, p0=guess_amorphous)
231     uncert_amorphous = np.sqrt(np.diag(error_amorphous))
232
233     fit_crystalline, error_crystalline = curve_fit(
234         Gaussian_function, x_values_crystalline,
235         y_values_crystalline, p0=guess_crystalline)
236     uncert_crystalline = np.sqrt(np.diag(error_crystalline))
237
238     # Check the fit of the fit (chi-squared test)
239     nu_amorphous = len(x_values_amorphous)-3
240     chi_squared_amorphous = np.sum(((y_values_amorphous -
241         Gaussian_function(x_values_amorphous, *fit_amorphous))**2

```

```

220         / y_values_amorphous))
221     p_value_amorphous = chi2.sf(chi_squared_amorphous,
222                                nu_amorphous)
223
224     nu_crystalline = len(x_values_crystalline)-3
225     chi_squared_crystalline = np.sum(((y_values_crystalline -
226         Gaussian_function(x_values_crystalline, *fit_crystalline))
227         **2 / y_values_crystalline))
228     p_value_crystalline = chi2.sf(chi_squared_crystalline,
229                                   nu_crystalline)
230
231     # Store the fitted parameters and uncertainties in the data
232     dictionary
233     data[file_name]['amorphous_fit_amplitude'] = fit_amorphous[0]
234     data[file_name]['amorphous_fit_amplitude_uncertainty'] =
235         uncert_amorphous[0]
236     data[file_name]['amorphous_fit_mean'] = fit_amorphous[1]
237     data[file_name]['amorphous_fit_mean_uncertainty'] =
238         uncert_amorphous[1]
239     data[file_name]['amorphous_fit_std_dev'] = fit_amorphous[2]
240     data[file_name]['amorphous_fit_std_dev_uncertainty'] =
241         uncert_amorphous[2]
242     if background == True:
243         data[file_name]['amorphous_fit_background'] =
244             fit_amorphous[3]
245         data[file_name]['amorphous_fit_background_uncertainty'] =
246             uncert_amorphous[3]
247         data[file_name]['chi_squared_amorphous'] =
248             chi_squared_amorphous
249         data[file_name]['amorphous_nu'] = nu_amorphous
250         data[file_name]['chi_squared_amorphous_p'] =
251             p_value_amorphous
252         data[file_name]['amorphous_fit_amorphous_x_range_used'] =
253             x_values_amorphous
254         data[file_name]['amorphous_fit_amorphous_y_range_used'] =
255             y_values_amorphous
256
257     data[file_name]['crystalline_fit_amplitude'] = fit_crystalline
258         [0]
259     data[file_name]['crystalline_fit_amplitude_uncertainty'] =
260         uncert_crystalline[0]
261     data[file_name]['crystalline_fit_mean'] = fit_crystalline[1]
262     data[file_name]['crystalline_fit_mean_uncertainty'] =
263         uncert_crystalline[1]
264     data[file_name]['crystalline_fit_std_dev'] = fit_crystalline
265         [2]
266     data[file_name]['crystalline_fit_std_dev_uncertainty'] =
267         uncert_crystalline[2]
268     if background == True:
269         data[file_name]['crystalline_fit_background'] =
270             fit_crystalline[3]
271         data[file_name]['crystalline_fit_background_uncertainty'] =
272             uncert_crystalline[3]
273         data[file_name]['chi_squared_crystalline'] =
274             chi_squared_crystalline
275         data[file_name]['crystalline_nu'] = nu_crystalline
276         data[file_name]['chi_squared_crystalline_p'] =
277             p_value_crystalline
278         data[file_name]['crystalline_fit_crystalline_x_range_used'] =
279             x_values_crystalline
280         data[file_name]['crystalline_fit_crystalline_y_range_used'] =
281             y_values_crystalline

```

```

256         # Store max values for the peaks
257         data[file_name]['max_amorphous'] = max(y_values_amorphous) #
258         Store the maximum value of the amorphous peak
259         data[file_name]['max_crystalline'] = max(y_values_crystalline)
260         # Store the maximum value of the crystalline peak
261
262     except RuntimeError as e: # This error will happen when a fit
263         cannot be calculated
264         print(f"{file_name} was not able to be fitted")
265         print(e)
266
267     # Determine what caused the error
268     my_script = os.path.basename(__file__)
269     exc_type, exc_value, exc_tb = sys.exc_info()
270     tb = traceback.extract_tb(exc_tb)
271     for frame in reversed(tb):
272         if os.path.basename(frame.filename) == my_script:
273
274             if 'amorphous' in frame.line:
275                 print("The amorphous range caused the error")
276             elif 'crystalline' in frame.line:
277                 print("The crystalline range caused the error")
278             else:
279                 print("Unforeseen error occurred on line ", frame.
280                     lineno)
281                 # print(f"Error occurred on line {frame.lineno}: {
282                     frame.line}") # This will show the line where
283                     the error happened
284
285             break
286
287     data.pop(file_name, None) # Get rid of the file for analysis
288
289     show_plot = input("Would you like to see the plot to see
290                       potential issues? (y/n): ").strip().lower()
291     if show_plot == 'y':
292         plt.title(file_name)
293         plt.plot(position, intensity)
294         plt.plot(x_values_amorphous, y_values_amorphous, 'ko')
295         plt.plot(x_values_crystalline, y_values_crystalline, 'bo')
296         plt.yscale('log')
297         plt.show()
298
299     print('\n') # Helps distinguish the next print group
300
301     return data
302
303 def Peak_Area_Calculation(data: dict):
304     """
305     Calculates the area under the fitted peaks for each file in the data
306     dictionary.
307
308     Parameters:
309         data (dict): A dictionary containing XRD data with fitted peak
310                     parameters.
311
312     Returns:
313         dict: An updated dictionary with calculated peak areas for each
314              file.
315     """

```

```

308     for file_name, file_data in data.items():
309         # Calculate the area under the amorphous peak
310         amplitude_amorphous = file_data['amorphous_fit_amplitude']
311         mean_amorphous = file_data['amorphous_fit_mean']
312         std_dev_amorphous = file_data['amorphous_fit_std_dev']
313         background_amorphous = file_data['amorphous_fit_background']
314         x_values_amorphous = file_data['
            amorphous_fit_amorphous_x_range_used']
315         # area_amorphous = np.trapz(Gaussian_function(x_values_amorphous,
            amplitude_amorphous, mean_amorphous, std_dev_amorphous,
            background_amorphous), x=x_values_amorphous) # Calculate the
            area under the amorphous peak
316         area_amorphous = np.trapz(Gaussian_function(x_values_amorphous,
            amplitude_amorphous, mean_amorphous, std_dev_amorphous), x=
            x_values_amorphous) # Calculate the area under the amorphous
            peak
317
318         # Calculate the area under the crystalline peak
319         amplitude_crystalline = file_data['crystalline_fit_amplitude']
320         mean_crystalline = file_data['crystalline_fit_mean']
321         std_dev_crystalline = file_data['crystalline_fit_std_dev']
322         background_crystalline = file_data['crystalline_fit_background']
323         x_values_crystalline = file_data['
            crystalline_fit_crystalline_x_range_used']
324         # area_crystalline = np.trapz(Gaussian_function(
            x_values_crystalline, amplitude_crystalline, mean_crystalline,
            std_dev_crystalline, background_crystalline), x=
            x_values_crystalline) # Calculate the area under the
            crystalline peak
325         area_crystalline = np.trapz(Gaussian_function(x_values_crystalline
            , amplitude_crystalline, mean_crystalline, std_dev_crystalline
            ), x=x_values_crystalline) # Calculate the area under the
            crystalline peak
326
327         amorphous_intensity_sum = sum(file_data['
            amorphous_fit_amorphous_y_range_used']) # Sum the intensity
            values for the amorphous peak
328         crystalline_intensity_sum = sum(file_data['
            crystalline_fit_crystalline_y_range_used']) # Sum the
            intensity values for the crystalline peak
329         # area_amorphous = amorphous_intensity_sum/(
            amorphous_intensity_sum+crystalline_intensity_sum)
330         # area_crystalline = crystalline_intensity_sum/(
            amorphous_intensity_sum+crystalline_intensity_sum)
331
332         # Store the areas in the data dictionary
333         data[file_name]['amorphous_area'] = area_amorphous
334         # data[file_name]['amorphous_area_rate'] = area_amorphous/data[
            file_name]['Time Step']
335         data[file_name]['crystalline_area'] = area_crystalline
336         data[file_name]['amorphous_area_sum'] = amorphous_intensity_sum
337         data[file_name]['crystalline_area_sum'] =
            crystalline_intensity_sum
338
339     return data
340
341 def Peak_Mixture_Calculation(data: dict): # Calculates the mixture
    fraction from amorphous and crystalline areas
342     """
343     Calculates the mixture of amorphous and crystalline areas for each
    file in the data dictionary.
344

```

```

345     Parameters:
346         data (dict): A dictionary containing XRD data with calculated peak
347                     areas.
348
349     Returns:
350         dict: An updated dictionary with calculated peak mixtures for each
351              file.
352     """
353
354     for file_name, file_data in data.items():
355         # Unpack needed values from data
356         area_amorphous = file_data['amorphous_area']
357         area_crystalline = file_data['crystalline_area']
358         area_amorphous_sum = file_data['amorphous_area_sum']
359         area_crystalline_sum = file_data['crystalline_area_sum']
360
361         amorphous_percentage = area_amorphous / (area_amorphous +
362                                                  area_crystalline) # Calculate the amorphous percentage
363         crystalline_percentage = area_crystalline / (area_amorphous +
364                                                    area_crystalline) # Calculate the crystalline percentage
365
366         data[file_name]['amorphous_percentage'] = amorphous_percentage
367         data[file_name]['crystalline_percentage'] = crystalline_percentage
368         data[file_name]['amorphous_percentage_intensity'] = file_data['
369             max_amorphous'] / (file_data['max_amorphous'] + file_data['
370             max_crystalline']) # Calculate the amorphous percentage based
371                               on intensity
372         data[file_name]['crystalline_percentage_intensity'] = file_data['
373             max_crystalline'] / (file_data['max_amorphous'] + file_data['
374             max_crystalline'])
375         data[file_name]['amorphous_percentage_sum'] = area_amorphous_sum/(
376             area_amorphous_sum+area_crystalline_sum)
377         data[file_name]['crystalline_percentage_sum'] =
378             area_crystalline_sum/(area_amorphous_sum+area_crystalline_sum)
379
380     return data
381
382 def Sample_Depth_Analysis(data: dict):
383     """
384     Analyzes the sample depth based on the calculated peak areas.
385
386     Parameters:
387         data (dict): A dictionary containing XRD data with calculated peak
388                     mixtures.
389
390     Returns:
391         dict: An updated dictionary with sample depth analysis results for
392              each file.
393     """
394
395     def skin_depth(alpha: float): # Skin depth calculation (only used in
396                                   this function)
397         """
398         Calculate the skin depth for a given attenuation coefficient.
399
400         Parameters:
401             alpha (float): Attenuation coefficient in m-1.
402
403         Returns:
404             float: Skin depth in meters.
405         """
406         return 1 / alpha # Skin depth in meters

```

```

393 def real_depth(skin_depth: float, omega: float): # Real depth
394     calculation (only used in this function)
395     """
396     Calculate the real depth for a given attenuation coefficient and
397     angle.
398     This calculates the depth at which 90% of the signal is attenuated
399     .
400
401     Parameters:
402         skin_depth (float): Skin depth of mixture.
403         omega (float): Angle in degrees.
404
405     Returns:
406         float: Real depth in micrometers.
407     """
408     return 5 * skin_depth * np.sin(np.radians(omega)) * 1e6 # Convert
409                     to micrometers
410
411 def attenuation_coefficient(ni: complex): # Attenuation coefficient
412     calculation (only used in this function)
413     """
414     Calculate the attenuation coefficient for a given material.
415
416     Parameters:
417         ni (complex): Complex refractive index of the material.
418
419     Returns:
420         float: Attenuation coefficient in m-1.
421     """
422     lambda = 1.5406e-10 # Cu Kalpha radiation wavelength in meters
423     return 4 * np.pi * -ni.imag / lambda # Attenuation coefficient in
424     m-1
425
426 material = input("Enter the chemical formula of the material (e.g., 'P'
427                 ' for Phosphorus, 'B' for Boron. Case sensitive): ").strip() #
428                 Ask the user for the material type
429
430 for file_name, file_data in data.items():
431     # Unpack needed values from data
432     omega = file_data['omega']
433     amorphous_percentage = file_data['amorphous_percentage']
434     crystalline_percentage = file_data['crystalline_percentage']
435
436     amorphous_percentage_intensity = file_data['
437         amorphous_percentage_intensity']
438     crystalline_percentage_intensity = file_data['
439         crystalline_percentage_intensity']
440
441     amorphous_percentage_sum = file_data['amorphous_percentage_sum']
442     crystalline_percentage_sum = file_data['crystalline_percentage_sum
443         ']
444
445     # website for index of refraction https://henke.lbl.gov/
446     optical_constants/getdb2.html
447     # Get indices of refraction based on the file name
448     if material == 'P':
449         n = 1-6.96137067E-06-1.98567363E-07J # Phosphorus index of
450         refraction
451     elif material == 'B':
452         n = 1-6.94444225E-06-5.98799899E-09J # Boron index of
453         refraction

```

```

441         else:
442             print("Please update code to include the correct indices of
443                   refraction for your material.")
444             raise ValueError("Material index of refraction unknown.")
445
446     Sin = 1-7.57442876E-06-1.72761077E-07J
447
448     # Calculate the effective index of refraction based on the mixture
449     effective_n = (amorphous_percentage * n + crystalline_percentage *
450                   Sin)
451     effective_n_intensity = (amorphous_percentage_intensity * n +
452                             crystalline_percentage_intensity * Sin) # Effective index of
453                             refraction based on intensity
454     effective_n_sum = (amorphous_percentage_sum * n +
455                       crystalline_percentage_sum * Sin) # Effective index of
456                       refraction based on area sum
457
458     # Calculate the attenuation coefficients
459     effective_alpha = attenuation_coefficient(effective_n) #
460                     Attenuation coefficient in m-1
461     effective_alpha_intensity = attenuation_coefficient(
462         effective_n_intensity) # Attenuation coefficient based on
463         intensity
464     effective_alpha_sum = attenuation_coefficient(effective_n_sum) #
465                     Attenuation coefficient based on area sum
466
467     # Calculate skin depth and real depth
468     skin = skin_depth(effective_alpha)
469     skin_intensity = skin_depth(effective_alpha_intensity) # Skin
470                     depth based on intensity
471     skin_sum = skin_depth(effective_alpha_sum) # Skin depth based on
472                     area sum
473
474     effective_depth = real_depth(skin, omega)
475     effective_depth_intensity = real_depth(skin_intensity, omega) #
476                     Real depth based on intensity
477     effective_depth_sum = real_depth(skin_sum, omega) # Real depth
478                     based on area sum
479
480     data[file_name]['effective_depth'] = effective_depth
481     data[file_name]['effective_depth_intensity'] =
482         effective_depth_intensity
483     data[file_name]['effective_depth_sum'] = effective_depth_sum
484
485     return data
486
487 def Store_Data(data: dict, path_name: str):
488     """
489     Stores the processed data into a excel file.
490
491     Parameters:
492         data (dict): A dictionary containing processed XRD data.
493         path_name (str): The path where the excel file will be saved.
494     """
495     try:
496         df = pd.DataFrame.from_dict(data, orient='index') # Convert the
497                     dictionary to a DataFrame
498         df = df.sort_values(by='omega', ascending=True) # Sort by Omega
499                     from smallest to largest
500         df.to_excel(os.path.join(path_name, 'Processed_XRD_Data.xlsx')) #
501                     Save the DataFrame to a excel file

```

```

485     except PermissionError as e:
486         print(f"Permission denied: {e}. Please check if the file is open,
487               and close it.")
488         input("Press Enter to try saving again after closing the file.")
489         df.to_excel(os.path.join(path_name, 'Processed_XRD_Data.xlsx')) #
490             Save the DataFrame to a excel file
491
492 def bar_graph_depths(path_name: str, area: str = ''):
493     """
494     Create a bar graph of the depths calculated for each mixture.
495     Parameters:
496         path_name (str): The path to the directory containing the
497             processed XRD data file.
498         area (str): A string to append to the area labels in the graph (
499             default is empty).
500     """
501     df = pd.read_excel(path_name + '//Processed_XRD_Data.xlsx')
502     x = np.arange(len(df['omega']))
503     plt.bar(x, df['crystalline_percentage'+ area] + df['
504             amorphous_percentage'+ area], label="Si")
505     plt.bar(x, df['amorphous_percentage'+ area], label="P")
506     plt.xlabel('Omega (degree_symbol) and Depth (mum)')
507     plt.ylabel('Mix')
508     plt.title('Depths for Mixtures'+ area)
509     plt.xticks(ticks=x, labels=[f"{df['omega'][i]}omega-{df['
510             effective_depth'+ area][i]:.2f}mum"for i in range(len(df['omega']))
511             ]], rotation=90)
512     plt.legend()
513     plt.tight_layout()
514     plt.show()
515
516 def uncertainties(data: dict):
517     """
518     Calculate uncertainties for the fitted parameters and peak areas in
519     the XRD data.
520     This function uses symbolic mathematics to derive the uncertainty
521     equations for the parameters.
522     Parameters:
523         data (dict): A dictionary containing XRD data with fitted
524             parameters and peak areas.
525     Returns:
526         dict: An updated dictionary with calculated uncertainties for each
527             file.
528     """
529     # Step up equations for calculations
530     # Make symbolic variables
531     amplitude, current_x_value, mean, standard_deviation, background,
532     part_1, part_2 = sp.symbols('A x mu std b p1 p2')
533     d_amplitude, d_current_x_value, d_mean, d_standard_deviation,
534     d_background, d_part_1, d_part_2 = sp.symbols('d_A d_x d_mu d_std
535             d_b d_p1 d_p2')
536
537     # Make symbolic equations
538     gaussian_symbolic = amplitude*sp.exp(-.5*((current_x_value-mean)/
539             standard_deviation)**2)/(standard_deviation*sp.sqrt(2*sp.pi))+
540             background
541     percentage_symbolic = part_1 / (part_1+part_2)
542
543     # Make uncertainty equations

```



```

530 uncertainty_gaussian_symbolic = sp.sqrt((sp.diff(gaussian_symbolic,
    amplitude)*d_amplitude)**2+(sp.diff(gaussian_symbolic,
    current_x_value)*d_current_x_value)**2+(sp.diff(gaussian_symbolic,
    mean)*d_mean)**2+(sp.diff(gaussian_symbolic, standard_deviation)*
    d_standard_deviation)**2+(sp.diff(gaussian_symbolic, background)*
    d_background)**2)
531 uncertainty_percentage_symbolic = sp.sqrt((sp.diff(percentage_symbolic
    , part_1)*d_part_1)**2+(sp.diff(percentage_symbolic, part_2)*
    d_part_2)**2)
532
533 # Unpack data
534 for file_name, file_data in data.items():
535
536     # # Unpack amorphous
537     amplitude_amorphous = file_data['amorphous_fit_amplitude']
538     amplitude_amorphous_uncertainty = file_data['
        amorphous_fit_amplitude_uncertainty']
539     mean_amorphous = file_data['amorphous_fit_mean']
540     mean_amorphous_uncertainty = file_data['
        amorphous_fit_mean_uncertainty']
541     std_dev_amorphous = file_data['amorphous_fit_std_dev']
542     std_dev_amorphous_uncertainty = file_data['
        amorphous_fit_std_dev_uncertainty']
543     background_amorphous = file_data['amorphous_fit_background']
544     background_amorphous_uncertainty = file_data['
        amorphous_fit_background_uncertainty']
545
546     # # Unpack Crystalline
547     amplitude_crystalline = file_data['crystalline_fit_amplitude']
548     amplitude_crystalline_uncertainty = file_data['
        crystalline_fit_amplitude_uncertainty']
549     mean_crystalline = file_data['crystalline_fit_mean']
550     mean_crystalline_uncertainty = file_data['
        crystalline_fit_mean_uncertainty']
551     std_dev_crystalline = file_data['crystalline_fit_std_dev']
552     std_dev_crystalline_uncertainty = file_data['
        crystalline_fit_std_dev_uncertainty']
553     background_crystalline = file_data['crystalline_fit_background']
554     background_crystalline_uncertainty = file_data['
        crystalline_fit_background_uncertainty']
555
556     # # Unpack things that are shared
557     amorphous_area = file_data['amorphous_area']
558     crystalline_area = file_data['crystalline_area']
559     amorphous_area_sum = file_data['amorphous_area_sum']
560     crystalline_area_sum = file_data['crystalline_area_sum']
561     max_amorphous = file_data['max_amorphous']
562     max_crystalline = file_data['max_crystalline']
563
564     # Gets the uncertainty at each point for the Gaussian fit
565     amorphous_uncertainty_dictionary = {amplitude: amplitude_amorphous
        , mean: mean_amorphous, standard_deviation: std_dev_amorphous,
        background: background_amorphous, d_amplitude:
        amplitude_amorphous_uncertainty, d_mean:
        mean_amorphous_uncertainty, d_standard_deviation:
        std_dev_amorphous_uncertainty, d_background:
        background_amorphous_uncertainty}
566     amorphous_fit_uncertainty = uncertainty_gaussian_symbolic.evalf(
        subs = amorphous_uncertainty_dictionary)
567
568     crystalline_uncertainty_dictionary = {amplitude:
        amplitude_crystalline, mean: mean_crystalline,

```

```

        standard_deviation: std_dev_crystalline, background:
        background_crystalline, d_amplitude:
        amplitude_crystalline_uncertainty, d_mean:
        mean_crystalline_uncertainty, d_standard_deviation:
        std_dev_crystalline_uncertainty, d_background:
        background_crystalline_uncertainty}
569 crystalline_fit_uncertainty = uncertainty_gaussian_symbolic.evalf(
        subs = crystalline_uncertainty_dictionary)

570
571 # Get numerical uncertainty for Gaussian fit
572 amorphous_area_list = []
573 crystalline_area_list = []
574
575 for i in range(1000):
576     amorphous_amplitude = amplitude_amorphous +
        amplitude_amorphous_uncertainty * np.random.randn()
577     amorphous_mean = mean_amorphous + mean_amorphous_uncertainty *
        np.random.randn()
578     amorphous_std_dev = std_dev_amorphous +
        std_dev_amorphous_uncertainty * np.random.randn()
579
580     crystalline_amplitude = amplitude_crystalline +
        amplitude_crystalline_uncertainty * np.random.randn()
581     crystalline_mean = mean_crystalline +
        mean_crystalline_uncertainty * np.random.randn()
582     crystalline_std_dev = std_dev_crystalline +
        std_dev_crystalline_uncertainty * np.random.randn()
583
584     amorphous_area_list.append(np.trapz(Gaussian_function(
        file_data['amorphous_fit_amorphous_x_range_used'],
        amorphous_amplitude, amorphous_mean, amorphous_std_dev), x
        =file_data['amorphous_fit_amorphous_x_range_used'])) #
        Calculate the area under the amorphous peak
585     crystalline_area_list.append(np.trapz(Gaussian_function(
        file_data['crystalline_fit_crystalline_x_range_used'],
        crystalline_amplitude, crystalline_mean,
        crystalline_std_dev), x=file_data['
        crystalline_fit_crystalline_x_range_used'])) # Calculate
        the area under the crystalline peak
586
587     amorphous_area_uncertainty = np.std(amorphous_area_list) #
        Calculate the standard deviation of the amorphous area
588     crystalline_area_uncertainty = np.std(crystalline_area_list) #
        Calculate the standard deviation of the crystalline area
589
590 # Uncertainty for the percentages
591     amorphous_percent_uncertainty = uncertainty_percentage_symbolic.
        evalf(subs = {part_1: amorphous_area, part_2: crystalline_area
        , d_part_1: amorphous_area_uncertainty, d_part_2:
        crystalline_area_uncertainty})
592     crystalline_percent_uncertainty = uncertainty_percentage_symbolic.
        evalf(subs = {part_2: amorphous_area, part_1: crystalline_area
        , d_part_2: amorphous_area_uncertainty, d_part_1:
        crystalline_area_uncertainty})
593
594     amorphous_area_sum_uncertainty = uncertainty_percentage_symbolic.
        evalf(subs = {part_1: amorphous_area_sum, part_2:
        crystalline_area_sum, d_part_1: np.sqrt(amorphous_area_sum),
        d_part_2: np.sqrt(crystalline_area_sum)})
595     crystalline_area_sum_uncertainty = uncertainty_percentage_symbolic.
        evalf(subs = {part_2: amorphous_area_sum, part_1:
        crystalline_area_sum, d_part_2: np.sqrt(amorphous_area_sum),

```

```

        d_part_1: np.sqrt(crystalline_area_sum)})

596
597     max_amorphous_uncertainty = uncertainty_percentage_symbolic.evalf(
        subs = {part_1: max_amorphous, part_2: max_crystalline,
        d_part_1: np.sqrt(max_amorphous), d_part_2: np.sqrt(
        max_crystalline)})
598     max_crystalline_uncertainty = uncertainty_percentage_symbolic.
        evalf(subs = {part_2: max_amorphous, part_1: max_crystalline,
        d_part_2: np.sqrt(max_amorphous), d_part_1: np.sqrt(
        max_crystalline)})

599
600     # Store the uncertainties in the data dictionary
601     data[file_name]['amorphous_percent_uncertainty'] = float(
        amorphous_percent_uncertainty)
602     data[file_name]['amorphous_fractional_uncertainty'] = float(
        amorphous_percent_uncertainty / data[file_name]['
        amorphous_percentage'])
603     data[file_name]['crystalline_percent_uncertainty'] = float(
        crystalline_percent_uncertainty)
604     data[file_name]['crystalline_fractional_uncertainty'] = float(
        crystalline_percent_uncertainty / data[file_name]['
        crystalline_percentage'])

605
606     data[file_name]['amorphous_percent_sum_uncertainty'] = float(
        amorphous_area_sum_uncertainty)
607     data[file_name]['amorphous_percent_sum_fractional_uncertainty'] =
        float(amorphous_area_sum_uncertainty / data[file_name]['
        amorphous_percentage_sum'])
608     data[file_name]['crystalline_percent_sum_uncertainty'] = float(
        crystalline_area_sum_uncertainty)
609     data[file_name]['crystalline_percent_sum_fractional_uncertainty']
        = float(crystalline_area_sum_uncertainty / data[file_name]['
        crystalline_percentage_sum'])

610
611     data[file_name]['amorphous_percent_intensity_uncertainty'] = float
        (max_amorphous_uncertainty)
612     data[file_name]['
        amorphous_percent_intensity_fractional_uncertainty'] = float(
        max_amorphous_uncertainty / data[file_name]['
        amorphous_percentage_intensity'])
613     data[file_name]['crystalline_percent_intensity_uncertainty'] =
        float(max_crystalline_uncertainty)
614     data[file_name]['
        crystalline_percent_intensity_fractional_uncertainty'] = float
        (max_crystalline_uncertainty / data[file_name]['
        crystalline_percentage_intensity'])

615
616     return data
617
618 def Peak_Area_Fitting(data_path: str):
619     """
620     Main function to perform peak area fitting on XRD data.
621
622     Parameters:
623         data_path (str): The path to the directory containing the XRD data
        files.
624     """
625
626     data_raw = XRD_Data_Dictionary(data_path) # Create a dictionary with
        the XRD data
627     data_ranges = Length_Peak(data_raw) # Get the ranges for each file,
        only function that requires user input

```

```

628     data_fit_parameters = Peak_fit(data_ranges) # Fit the peaks to a
        Gaussian function
629     data_fit_parameters_no_background = Peak_fit(data_ranges, background =
        False) # Fit the peaks to a Gaussian function, subtracting the
        background
630     data_peak_areas = Peak_Area_Calculation(
        data_fit_parameters_no_background) # Calculate the area under the
        peaks
631     data_mixture = Peak_Mixture_Calculation(data_peak_areas) # Calculate
        the mixture of amorphous and crystalline areas
632     data_depth = Sample_Depth_Analysis(data_mixture) # Analyze the sample
        depth based on the calculated peak areas
633     data_uncertainties = uncertainties(data_depth)
634     Store_Data(data_uncertainties, data_path) # Store the processed data
        into a excel file
635
636     return data_depth # Return the processed data for further use or
        analysis
637
638 def Plot_Peak_Fit(data: dict):
639     """
640     Plots the fitted peaks for a given file.
641
642     Parameters:
643         data (dict): A dictionary containing XRD data with fitted peak
        parameters.
644     """
645
646     num_files = len(data)
647     grid_size = int(np.ceil(np.sqrt(num_files))) # e.g., 3 for 9 files
648
649     fig, axes = plt.subplots(grid_size, grid_size, figsize=(5*grid_size,
        4*grid_size))
650     fig.suptitle("Fitted Peaks for All Files", fontsize=16)
651     axes = axes.flatten() # Flatten to 1D for easy indexing
652
653     for idx, (file_name, file_data) in enumerate(data.items()):
654         ax = axes[idx]
655
656         # Unpack the values from the file data
657         position = file_data['Position']
658         intensity = file_data['Intensity']
659
660         # Plot the original data
661         ax.plot(position, intensity, label='Original Data', color='blue')
662
663         # Plot the amorphous fit
664         x_values_amorphous = file_data['
        amorphous_fit_amorphous_x_range_used']
665         y_values_amorphous = Gaussian_function(
666             x_values_amorphous,
667             file_data['amorphous_fit_amplitude'],
668             file_data['amorphous_fit_mean'],
669             file_data['amorphous_fit_std_dev'],
670             background = file_data['amorphous_fit_background']
671         )
672         ax.plot(x_values_amorphous, y_values_amorphous, label='Amorphous
        Fit', color='orange')
673
674         # Plot the crystalline fit
675         x_values_crystalline = file_data['
        crystalline_fit_crystalline_x_range_used']

```

```

676     y_values_crystalline = Gaussian_function(
677         x_values_crystalline,
678         file_data['crystalline_fit_amplitude'],
679         file_data['crystalline_fit_mean'],
680         file_data['crystalline_fit_std_dev'],
681         background = file_data['crystalline_fit_background']
682     )
683     ax.plot(x_values_crystalline, y_values_crystalline, label='
        Crystalline Fit', color='green')
684
685     # Place omega value inside the plot area, upper right
686     ax.text(
687         0.98, 0.98,
688         # x, y position in axes fraction
689         # (0=left/bottom, 1=right/top)
690         file_data['omega'], # Text to display
691         transform=ax.transAxes, # Use axes coordinates
692         ha='right', va='top', # Align text to the right and top
693         fontsize=12 #
694         # bbox=dict(facecolor='white', alpha=0.7, edgecolor='none') #
695         # Optional: background for readability
696     )
697
698     # ax.set_xlabel('Position [degree_symbol2theta]')
699     # ax.set_ylabel('Intensity [Counts]')
700     # ax.set_title(f'Peak Fit for {file_name}')
701     # ax.legend()
702     ax.set_yscale('log')
703
704     # Turn off tick marks
705     ax.set_xticks([])
706     ax.set_yticks([])
707     ax.tick_params(axis='both', which='both', bottom=False, top=False,
708         left=False, right=False, labelbottom=False, labelleft=False)
709
710     # Hide any unused subplots
711     for j in range(idx + 1, len(axes)):
712         fig.delaxes(axes[j])
713
714     plt.tight_layout(pad=4) # Adjust spacing between subplots
715     plt.show()
716
717 def Line_Graph(data: dict):
718     """
719     Creates a line graph of the amorphous and crystalline percentages for
720     each file.
721
722     Parameters:
723         data (dict): A dictionary containing XRD data with calculated peak
724         mixtures.
725     """
726
727     amorphous_percentages = [file_data['amorphous_percentage'] for
728         file_data in data.values()]
729     amorphous_percentages_uncertainty = [file_data['
730         amorphous_percent_uncertainty'] for file_data in data.values()]
731     crystalline_percentages = [file_data['crystalline_percentage'] for
732         file_data in data.values()]
733     crystalline_percentages_uncertainty = [file_data['
734         crystalline_percent_uncertainty'] for file_data in data.values()]
735     amorphous_percentages_intensity = [file_data['
736         amorphous_percentage_intensity'] for file_data in data.values()]

```

```

726     amorphous_percentages_intensity_uncertainty = [file_data['
           amorphous_percent_intensity_uncertainty'] for file_data in data.
           values()]
727     crystalline_percentages_intensity = [file_data['
           crystalline_percentage_intensity'] for file_data in data.values()]
728     crystalline_percentages_intensity_uncertainty = [file_data['
           crystalline_percent_intensity_uncertainty'] for file_data in data.
           values()]
729     amorphous_percentages_sum = [file_data['amorphous_percentage_sum'] for
           file_data in data.values()]
730     amorphous_percentages_sum_uncertainty = [file_data['
           amorphous_percent_sum_uncertainty'] for file_data in data.values()
           ]
731     crystalline_percentages_sum = [file_data['crystalline_percentage_sum']
           for file_data in data.values()]
732     crystalline_percentages_sum_uncertainty = [file_data['
           crystalline_percent_sum_uncertainty'] for file_data in data.values
           ()]
733     omegas = [file_data['omega'] for file_data in data.values()]
734
735     x_axis = np.arange(len(omegas))
736
737     plt.plot(x_axis, amorphous_percentages, label='Amorphous Percentage',
           marker='o')
738     plt.plot(x_axis, crystalline_percentages, label='Crystalline
           Percentage', marker='o')
739     plt.plot(x_axis, amorphous_percentages_intensity, label='Amorphous
           Percentage Intensity', marker='*')
740     plt.plot(x_axis, crystalline_percentages_intensity, label='Crystalline
           Percentage Intensity', marker='*')
741     plt.plot(x_axis, amorphous_percentages_sum, label='Amorphous
           Percentage Sum', marker='^')
742     plt.plot(x_axis, crystalline_percentages_sum, label='Crystalline
           Percentage Sum', marker='^')
743
744     plt.xlabel('Omega (omega)')
745     plt.ylabel('Percentage')
746     plt.title('Amorphous and Crystalline Percentages')
747     plt.xticks(x_axis, [f"{omega}omega" for omega in omegas], rotation=90)
748     plt.legend()
749     # plt.grid(True)
750     plt.tight_layout()
751     plt.show()
752
753     plt.errorbar(x_axis, amorphous_percentages, yerr=
           amorphous_percentages_uncertainty, label='Amorphous Percentage',
           marker='o', capsize=3)
754     plt.errorbar(x_axis, crystalline_percentages, yerr=
           crystalline_percentages_uncertainty, label='Crystalline Percentage
           ', marker='o', capsize=3)
755     plt.errorbar(x_axis, amorphous_percentages_intensity, yerr=
           amorphous_percentages_intensity_uncertainty, label='Amorphous
           Percentage Intensity', marker='*', capsize=3)
756     plt.errorbar(x_axis, crystalline_percentages_intensity, yerr=
           crystalline_percentages_intensity_uncertainty, label='Crystalline
           Percentage Intensity', marker='*', capsize=3)
757     plt.errorbar(x_axis, amorphous_percentages_sum, yerr=
           amorphous_percentages_sum_uncertainty, label='Amorphous Percentage
           Sum', marker='^', capsize=3)
758     plt.errorbar(x_axis, crystalline_percentages_sum, yerr=
           crystalline_percentages_sum_uncertainty, label='Crystalline
           Percentage Sum', marker='^', capsize=3)

```

```

759     plt.xlabel('Omega (omega)')
760     plt.ylabel('Percentage')
761     plt.title('Amorphous and Crystalline Percentages')
762     plt.xticks(x_axis, [f"{omega}omega" for omega in omegas], rotation=90)
763     plt.legend()
764     # plt.grid(True)
765     plt.tight_layout()
766     plt.show()
767
768
769 if __name__ == "__main__":
770
771     material = input("p, p01, or dt: ")
772
773     path_name = f'E://Full//{material} csv' # input("Enter the path to the
774                                             XRD data folder: ").strip() # Get the path to the XRD data files
775                                             from the user
776
777     try:
778         data = Peak_Area_Fitting(path_name) # Call the main function with
779                                             the path to the XRD data files
780
781         Line_Graph(data) # Create a line graph of the amorphous and
782                           crystalline percentages
783
784         Plot_Peak_Fit(data) # Plot the fitted peaks for each file
785
786         bar_graph_depths(path_name, area = '_intensity') # Create a bar
787                                                           graph of the depths calculated for each mixture
788         bar_graph_depths(path_name, area = '_sum') # Create a bar graph of
789                                                       the depths calculated for each mixture
790         bar_graph_depths(path_name) # Create a bar graph of the depths
791                                       calculated for each mixture
792
793     except FileNotFoundError as e:
794         print(e)

```