06-681: Data Science in Chemical Engineering

LEIS Peak fitting

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Outline

1

Introduction to LEIS – Data format

Motivation and scope of the project

2

Peak fitting procedure

Finding peaks and means of gaussian function

3

Jupyter notebook overview

Interactive graph

LEIS experiment

Characterization technique used for surface analysis.

Used to find elemental identity and relative position of atoms in a surface lattice.

We get Outputs for different KE

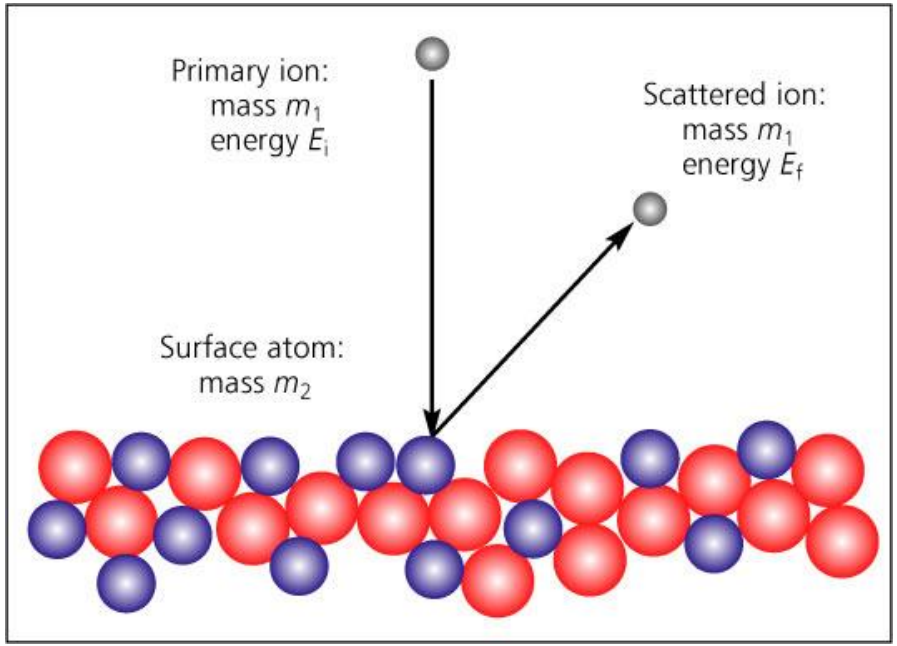
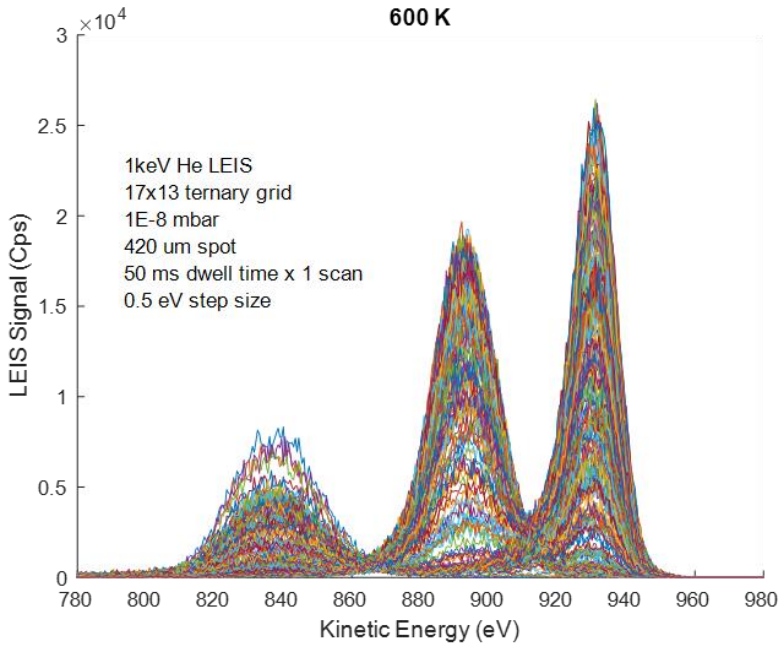


Figure take from: Brongersma, Hidde H., et al. "Analysis of the Outer Surface of Platinum-Gold Catalysts by Low-Energy Ion Scattering." Platinum Metals Review 54.2 (2010): 81-87.

Sample LEIS spectra

- 13 x 13 grid source
- 481 KE energies in eV from each grid point
- Multiple excel files
- 3 dominant peaks
- Software fitting takes 4-5 hours – cannot export results in efficient manner



Scope of project

Data handling

Currently multiple excel files are created with no way to keep track of progress

Need for data organization

Peak Fitting

Current peak fitting software is slow

Need for faster and customizable peak fitting

Export to Interactive graph

Allow user to have interactive nature with the exported results.

Data format and Peak fitting

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1															
2	Axis	Energy	Elements=	481											
3	Axis	Angle	Elements=	1											
4	Axis	X	Elements=	1											
5	Axis	Y	Elements=	13											
6															
7	C:\Zhitao\PdNiAu\20190607 PdNiAu#2\20190615 400K 150ms 440um LEIS\Manual Source\Area Scan #004\Scan 860eV.VGD														
8															
9															
10	X(X)	11999.5	µm												
11															
12	Angle(Ø)	27.5	°		<----------Y Values ---------->										
13															
14		Y (Y)\µm	0	999.937	1999.87	2999.81	3999.75	4999.69	5999.62	6999.56	7999.5	8999.43	9999.37	10999.3	11999.2
15	Kinetic Energy (E)														
16	eV		Counts / s	Counts / s	Counts / s	Counts / s	Counts / s	Counts / s	Counts / s	Counts / s	Counts / s	Counts / s	Counts / s	Counts / s	Counts / s
17	740		77.8373	9.0368	44.0111	20.204	127.109	74.2479	82.1058	116.285	115.28	138.433	89.0662	114.398	52.8269
18	740.5		32.0089	24.9141	37.3587	60.9155	90.386	80.6958	120.751	152.227	192.676	177.628	122.239	73.7316	52.9077
19	741		31.8559	37.8785	48.4627	35.6571	57.3413	69.4564	119.894	144.097	208.679	134.511	45.5291	46.3165	92.8351
20	741.5		20.4772	18.7088	64.1576	55.1791	42.4272	84.901	84.1871	112.244	145.901	145.086	65.8053	84.6241	75.463
21	742		31.2381	22.5665	34.3892	39.7407	56.3964	62.1717	113.857	146.568	152.429	122.955	50.8673	78.943	56.0834
22	742.5		56.4703	39.4879	33.6231	26.7034	63.5338	51.4513	128.935	186.618	134.71	116.689	96.2451	93.1334	71.2861
23	743		39.0902	45.1102	19.368	33.5031	50.9135	83.4442	121.252	174.463	155.668	116.101	111.291	72.4107	63.6648
24	743.5		57.9788	36.1287	43.7607	18.4893	73.2662	69.3894	78.7747	134.773	184.167	168.873	50.8309	84.7854	85.9623
25	744		65.529	45.3797	34.9211	22.4875	73.9303	75.6084	137.276	186.295	154.563	127.051	82.9265	40.4477	82.137
26	744.5		31.848	36.9223	41.1981	23.0642	56.1122	55.2189	119.049	125.517	131.547	116.8	94.9545	66.536	138.069
27	745		25.6571	55.8685	71.4498	53.2723	40.2624	83.0438	95.0725	116.635	156.961	165.044	148.18	160.576	97.3876
28	745.5		45.6238	46.1692	61.3486	57.9476	72.5889	81.9373	46.5643	98.5036	130.159	165.345	98.0798	76.2613	82.2651
29	746		44.1211	69.0977	13.7893	34.401	44.3688	114.215	85.0874	88.2443	143.789	99.5356	77.1406	83.6593	50.1529
30	746.5		37.3614	63.6185	37.4333	45.7581	24.5915	85.9301	123.645	143.129	152.016	176.709	59.492	75.2669	108.195
31	747		56.1425	24.9602	40.5771	47.7152	30.4228	65.8383	124.548	123.901	142.703	124.374	57.4062	73.2585	103.115

0 1 2 3 4 5 6 7 8 9 10 11 12

<-------X values------->

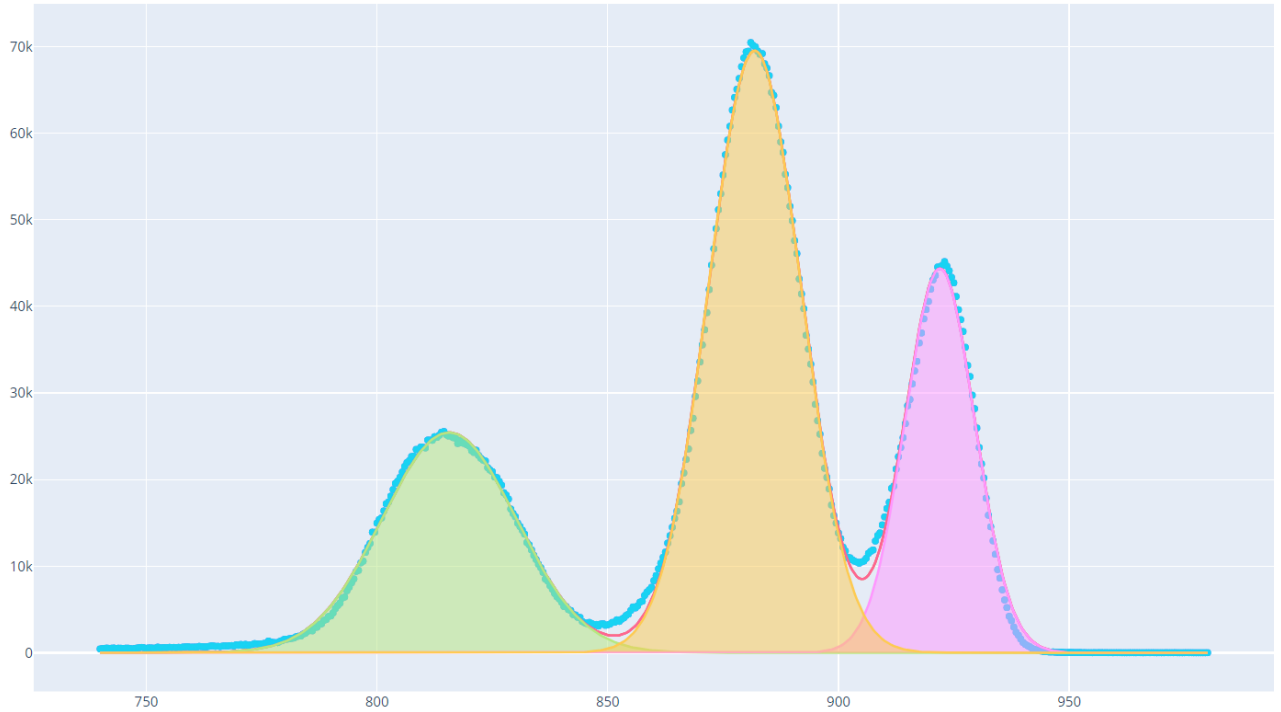
13 X and 13 Y

Using pandas read_excel to load data into numpy array

Gaussian function

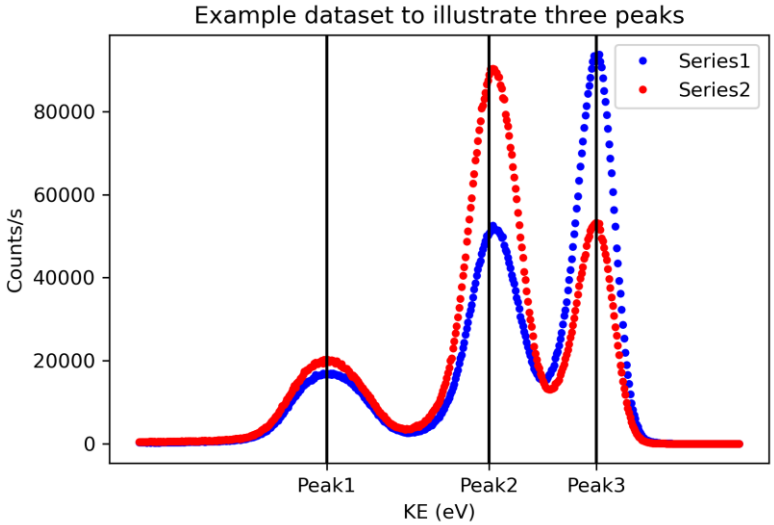
Amplitude
Center
Spread

Fit peaks to get center of peaks



Peaks positions

The three peaks occur at almost same mean everytime
This is used a first estimate for fit



Peak fitting algorithm

Step 1: Find number of peaks

Using `scipy.signal.peaks` find the number of peaks and their estimate

Step 2: Fit for specified number of peaks

Using best estimates, fit that many peaks using Ordinary least square

Step 3: Add fitted data to a data file

For each data point, write the following to a dictionary:

1. Number of peaks
2. y_fit
3. y1, y2, y3 as applicable
4. μ_1, μ_2, μ_3 as applicable

Using plotly for interactive graph

Plotly steps

1

Create marker grid

13 x 13 marker points each representing X and Y points

2

Callback function

When marker clicked, do following

- Change color of marker
- Plot that index spectra
- Update legend with fit data

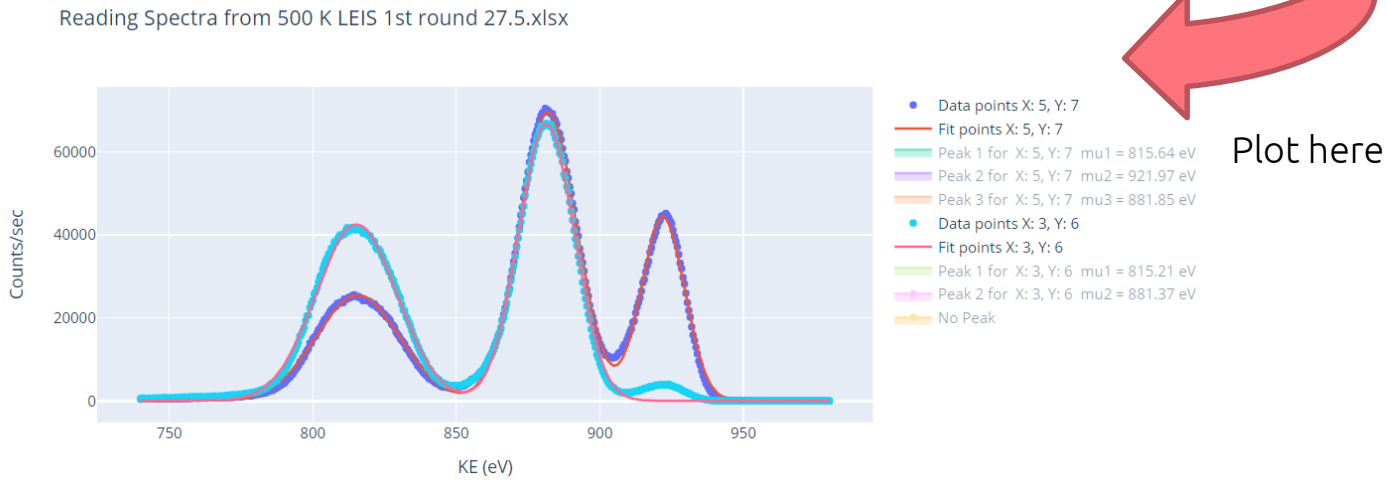
3

FigureWidget

Update and collect fitted data

Click here

Plot here



Thanks!

Any questions?

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