Mean Filter Method in Finding and Identifying Peaks for PIGE and PIXE and Elements Signal Sensitivity Analysis under 2.4-5.1 MeV Proton

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2019 NSF/REU Program

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Abstract

In this article, we analyze the PIGE and PIXE data under different proton beam energy: 2.4MeV, 3.4MeV, 4.2MeV, 5.1MeV of elements with Z=9, 11-17, 19-23, 25-30, 35, 37, 40-42, 44-45, 47, 49-50, 53, 55-56. We introduce the mean filter method to smooth raw data, determine background, find peaks, integral and normalize the peak areas. Then we obtain tables of γ-ray and X-ray signal sensitivity of different isotopes under four different proton beam energy. And we made lists of elements for γ-ray and X-ray peaks.

1 Introduction

Particle induced prompt γ-ray emission (PIGE) is a good way to analyze the elements in samples according to the special γ-ray of elements and isotopes. However, sometimes it is hard to identify peaks from spectrum because there might be a lot of background noises and peaks and to find and identify every peak manually is a time-consuming and boring work. Moreover, for some elements, they might need enough proton energy to induce to emit γ-ray. And the signal sensitivity is quite different under different proton energy. Knowing the sensitivity of elements can help us better select material when running sample test and analyzing peaks. Thus, we need to find a good method to erase background and use computer to find and identify peaks automatically, and make a table of elements and isotopes with their special peaks and signal sensitivity.

In 1980s, Kiss[1] (1984) and Räisänen[2,3] (1982, 1987) have tested some elements γ-ray peaks under low energy (2.4 MeV) and high energy (7 MeV) and made tables of target γ-ray yield. But there is no data in medium energy. So we run our samples at 2.4-5.1 MeV proton beams. Sometimes PIGE can't give the right peaks either we want to reconfirm our identification, so we can use X-ray data (PIXE) to support it. And there is no data about X-ray emission on these elements with their signal sensitivity. Therefore in our experiment, we also collect the X-ray data under the four energy and analyze their peaks and sensitivity.

2 Experimental Arrangement

In our experiment, we use the alpha toss and 9SDH 5MeV St.Andre accelerator at University of Notre Dame (see Fig.1) to generate high energy proton beams of 2.4 MeV, 3.4 MeV, 4.2 MeV and 5.1 MeV by adjusting the power supply. The whole accelerator system runs in high vacuum about 10^{-7} psi, to reduce the energy loss of proton beam when colliding with particles in air. And we also use magnetic quadrupole to focus the proton beam.

We grind the samples into powder and put them into small bags, which is around 5mm$\times$ 5mm in length and width, and about 2mm thick. Then we use tapes to

Figure 1: Alpha toss and 9SDH St.Andre accelerator in Notre Dame. The box in the left is the alpha toss generated from H or He. And the big blue tank holds a 6MeV accelerator.

stick the bags to our iron frame and fix them to target wheel (see Fig.2), which has a hole in center to let the beam go through target sample. We run samples in air and three minutes for each. In our experiment, we use samples Ag_2S, BaOH, $CaCO_3$, Co_3P_2, CsCl, $CuCl_2$, Dy, NaF, $FeCl_3$, In, KBr, KI, $MgCO_3$, $MgSO_4$, $Mn(OAc)_2$, Mo, N_2NiO_4, $NaHCO_3$, Nd_2O_3, Pt, RbCl, Rh, RuO_2, SiO_2, Sm_2O_3, Ti, ZnS.

Figure 2: Target wheel and γ-ray detector. One wheel can be mounted sixty samples. The γ-ray detector is at the right of the target wheel and the X-ray detector is behind the wheel at top right in this figure.

3 Measurement and Data Analysis

We plot the counts received from the detector under different γ-ray energy. The raw data of Ag_2S sample at 3.4 MeV proton beam is shown in Fig.3. The γ-ray energy ranges from around 50keV through 2500 keV. From the figure we can see that there are several dominant peaks and it seems easy to determine the energy of the peaks and then identify them by looking up online γ - ray chart of nuclides.

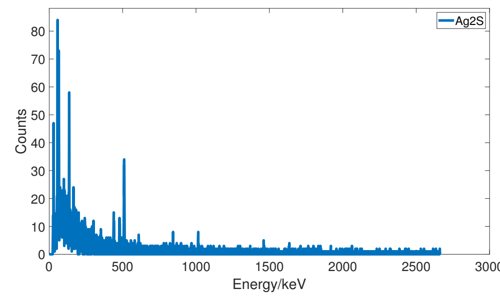

Figure 3: γ-ray raw spectrum of Ag2S with 3.4MeV proton.There are clear dominant peaks as well as a lot of background noise in this figure.

However, there are a lot of peaks are generated from background reactions, for example, 511 keV is from positronium annihilation. And if we zoom in the spectrum, as shown in Fig.4, we can see that there are a lot of background noises and even for the peaks, there are a lot of fluctuations. And also, the background noise counts are different under different energy, for instance, the background noise is higher in low energy (less than 500kV) than in high energy (more than 1000 keV). That is because our γ-ray detector sensitivity is different under different energy. It is much more sensitive in low energy than in high energy. So what we need to do first is to smooth the spectrum and find the background then subtract it from real peaks.

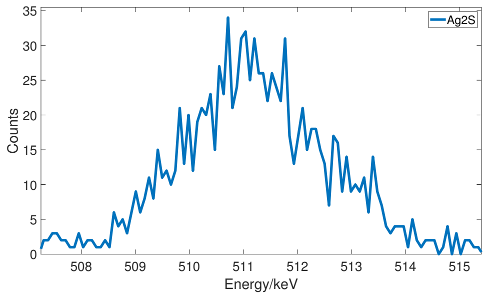

Figure 4: γ-ray raw spectrum of Ag_2S at 3.4MeV proton beam, zoom in around 511 keV (positronium annihilation).

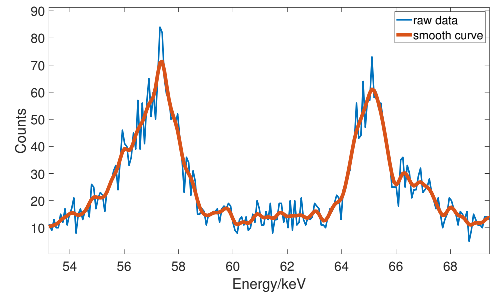

Figure 5: Mean filter smooth curve (in thick red line) and the raw data (in thin blue line), zoom in around 54-68keV

3.1 Smooth Spectrum

We use Mean Filter Method to smooth the spectrum. For some data point, we calculate the average of three front and three back points and take this average value as the value of the selected point. We do this for all points except for a few points at the beginning and the end of the data set because there is no front either back points for them to take average. After doing this, we obtain a new set of data. And we repeat the procedure for the new data for 10 times. Then we get a satisfied smooth curve of raw data. As shown in Fig.5, the blue thin line is raw data and the red thick curve is the smooth curve after using Mean Filter Method. The smooth curve lower the peak height to some extent, but this does't affect too much on our calculation, and it will be discussed later at the end of the article. In general, the smooth curve well represents the peaks shape and position, and it reduce the fluctuations of raw data. It also shows us a clear line of background, which can help us to find the background.

3.2 Determine Background

From Fig.5, we can see that most of the background noises fluctuations have been reduced. But there are still some fluctuations in the smooth curve. So we utilize these fluctuations to determine the background value under different energy.

To determine the background, we first find all the minimal points of the smooth curve. However, if two peaks overlap, there would be a minimal point between two peaks but it is much higher than background. So we design a filter to eliminate those minimal points on the peaks. To do so, we compare the point with its adjacent points. Specifically, for any point, we calculate the average of two front and two back points separately. Then we compare the point value with the front average and the back average. If it is larger than both of the half of the front average and the back average, then the point is regarded as invalid and eliminated. After determining all the valid minimal points, we still use Mean Filter Method to smooth these minimal points and then use the smooth curve as the background.

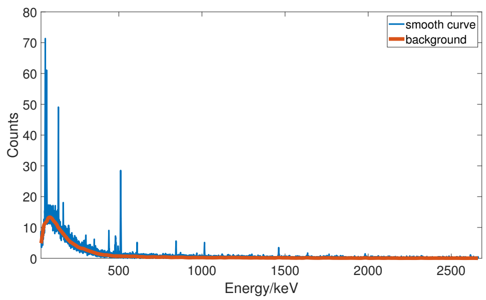

Figure 6: Smooth spectrum (thin blue line) and background (thick red line) of Ag_2S at 3.4 MeV proton beam.

In Fig.6, the thick red line shows the background we determined, and the thin blue line is the smooth spectrum. It clearly shows us the strong background at low energy and weak background at high energy.

3.3 Find Peaks and Integral Areas

Once we have determined the background, we can subtract it and then find real peaks. After subtracting the background, although there is still some noises fluctuations, they are all around zeros and the positive and negative number are roughly equal, which verifies that we determine the right background.

To find the peaks, we first find all the maximal points, and then set thresholds to eliminate fake peaks, including peaks that overlap too much, and small peaks. We find that the residual background noises fluctuations are related to the value of the background, i.e., higher background usually has higher noises fluctuations. So we set different thresholds according to different background values. Generally, we set the threshold as twice of the local background noises fluc-

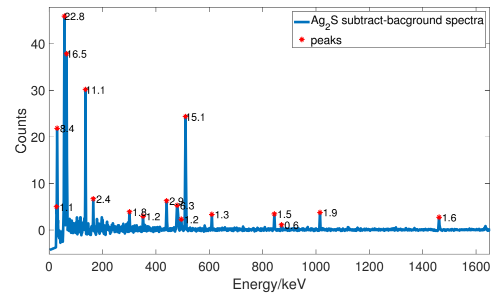

Figure 7: Subtract-background spectrum and peaks with normalized area. The blue line is the smooth curve of raw spectrum in which the background has been subtracted. The red asterisks show the position of peaks we find in Ag_2S sample at 3.4 MeV proton beam. And the numbers near asterisks show the normalized area of every peak.

tuations amplitudes. If the maximal point is lower than the threshold, then it is regarded as a small or fake peak and eliminated. As for overlapped peaks, we set a overlapped rate as 0.75. For every adjacent peaks, we first find the lowest points between the two peaks. And then compare the minimal value with the lowest peak height. If the minimal value is higher than the overlapped rate multiplies the lowest peak height, the two peaks are viewed as undistinguishable and we eliminate the lower one and reserve the higher one. Then compare the reserved peak with next peak.

After locating the real peaks, we continue to locate the peak bases of every peak. For each peak, we first find two locations (left and right around the peak) of the points with half height of the maximal peak height. Then calculating the distance between the half-height points and the summit of the peak. Then we multiply the distances with a factor of 1.7 to locate the peak base. That is because the Full Width at Half Maximum (FWHM) is about 2.4σ and the peak width is about 4.2σ. So the peak width is about 1.7 times FWHM. Then we use trapezoid method to integral the peak area from one peak base to another. And we also normalize the areas by the amount of charge of proton beam, i.e., divide the area by the currents and time when running the sample. The subtract-background spectrum and the peaks we found with normalized areas are shown in Fig.7.

3.4 X-ray Data Processing

X-ray data is easier to analyze because it doesn't have too much background noises. So we don't need to determine and subtract background. Other procedures are the same as dealing with γ-ray data. The X-ray spectrum of Ag_2S at 3.4 MeV proton beam is shown in Fig.8.

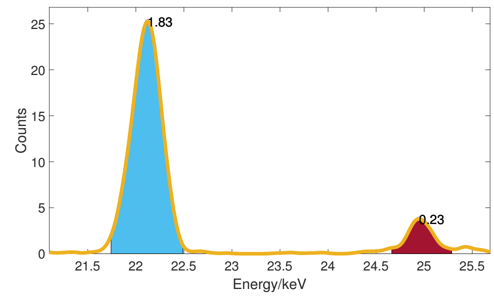

Figure 8: X-ray data processing result. The thick yellow line shows the smoothed curve of raw spectrum. The coloured areas is the peak areas we determined and the number near the peaks are normalized peak areas. The dominant two peaks are 22.1 keV and 24.9 keV, which are the K_α and K_β decay of silver.

4 Results

We run the program for all of our samples and we can obtain the table of γ-ray and X-ray lines for different elements and isotopes. And we also calculate the signal sensitivity of different elements based there amount in sample and the natural abundance of isotopes. This is helpful because if you get a peak, then you can look up our tables to determine the what the element is. And you can confirm your identification by using PIGE and PIXE data simultaneously. And you can select appropriate element if you want to do sample test according to our signal sensitivity table.

Table 1: Isotopes for γ-ray peaks

Energy(keV)	Isotope	Energy(keV)	Isotope
110	^{19}F	808	^{51}V
121.5	^{152}Sm	843	^{27}Al
122	^{57}Fe	847	^{56}Fe
126	^{55}Mn	858.5	^{55}Mn
127	^{101}Ru	889	^{45}Sc
130	^{150}Nd	889	^{46}Ti

159	^{47}Ti	926.5	^{45}Sc
170	^{27}Al	928.5	^{51}V
172	^{127}I	931	^{55}Mn
182.5	^{79}Br	962	^{45}Sc
190	^{81}Br	962	^{63}Cu
197	^{19}F	974.5	^{45}Sc
203	^{127}I	975	^{25}Mg
217	^{79}Br	980.5	^{41}K
231.5	^{85}Rb	983.5	^{48}Ti
255	^{113}In	1014	^{27}Al
276	^{81}Br	1024	^{113}In
302	^{133}Cs	1049	^{45}Sc
302	^{148}Nd	1093	^{47}Ti
306	^{79}Br	1120.5	^{45}Sc
311	^{109}Ag	1131	^{113}In
320	^{51}V	1149	^{51}V
324	^{107}Ag	1157	^{44}Ca
334	^{150}Sm	1165	^{51}V
338	^{59}Co	1220	^{35}Cl
358	^{104}Ru	1228	^{87}Rb
364	^{45}Sc	1235	^{19}F
370.5	^{48}Ca	1237	^{45}Sc
383	^{133}Cs	1263.5	^{59}Co
390	^{25}Mg	1274	^{29}Si
411	^{55}Mn	1294	^{41}K
415	^{109}Ag	1300	^{114}Sn
423	^{107}Ag	1312	^{48}Ti
431.5	^{45}Sc	1327	^{63}Cu
440	^{23}Na	1333	^{60}Ni
454	^{146}Nd	1368	^{27}Al
475	^{102}Ru	1369	^{24}Mg
484.5	^{87}Rb	1380	^{25}Mg
520.5	^{48}Ca	1408	^{55}Mn
523	^{79}Br	1410	^{37}Cl
530.5	^{45}Sc	1438	^{48}Ti
539.5	^{100}Ru	1454	^{58}Ni
543	^{45}Sc	1480	^{51}V
550	^{148}Sm	1525	^{42}Ca
585	^{25}Mg	1609	^{51}V
617	^{79}Br	1611	^{37}Cl
628.5	^{127}I	1634	^{23}Na
632	^{133}Cs	1643	^{37}Cl
638	^{113}In	1663	^{45}Sc
670	^{63}Cu	1728	^{37}Cl
691	^{45}Sc	1763	^{35}Cl
696.5	^{144}Nd	1779	^{28}Si
700	^{119}Sn	1809	^{26}Mg
720.5	^{45}Sc	1813	^{51}V
749	^{51}V	1943	^{41}K
780	^{48}Ca	2028	^{29,30}Si
804	^{55}Mn	2128	^{37}Cl

Table 2: Isotopes for γ-ray peaks

Element	Signal Sensitivity (MeV)			
	E_p=2.4	3.4	4.2	5.1

^{107}Ag	0	0	0	223
^{109}Ag	0	0	14	274
^{27}Al	0	193	9494	47600
^{79}Br	0	65	858	5663
^{81}Br	0	41	599	4754
^{42}Ca	0	0	0	5748
^{44}Ca	0	0	1339	7699
^{48}Ca	0	1688	25650	112388
^{35}Cl	0	0	293	2298
^{37}Cl	0	0	0	2686
^{133}Cs	0	4	21	58
^{63}Cu	0	0	61	941
^{19}F	135	37626	265322	684468
^{56}Fe	0	0	291	3210
^{57}Fe	0	0	0	4958
^{127}I	0	0	0	69
^{113}In	0	0	0	3316
^{41}K	0	0	695	10043
^{24}Mg	0	140	2223	13178
^{25}Mg	0	3388	20827	60306
^{26}Mg	0	0	5042	14064
^{55}Mn	0	794	9852	60556
^{58}Ni	0	0	0	249
^{60}Ni	0	0	0	237
^{23}Na	0	184	3012	50070
^{144}Nd	0	0	0	48
^{146}Nd	0	7	79	225
^{148}Nd	0	88	473	1118
^{150}Nd	0	284	1063	2051
^{85}Rb	0	0	115	746
^{87}Rb	0	0	87	357
^{100}Ru	0	0	0	282
^{101}Ru	0	0	0	294
^{102}Ru	0	8	103	484
^{104}Ru	0	33	323	1250
^{45}Sc	0	238	2606	12396
^{28}Si	0	0	2066	7914
^{29}Si	0	49	4735	19182
^{30}Si	0	0	0	4467
^{148}Sm	0	0	0	176
^{150}Sm	0	30	279	1035
^{152}Sm	0	205	838	2386
^{154}Sm	0	45	144	515
^{114}Sn	0	0	11286	0
^{119}Sn	0	0	0	137
^{46}Ti	0	8	1637	8813
^{47}Ti	0	724	13589	47351
^{48}Ti	0	7	1339	7964
^{51}V	0	13	1322	9326

Table 3: X-ray peaks and signal sensitivity

Element	Energy	Signal Sensitivity(MeV)			
	(keV)	2.4	3.4	4.2	5.1
Ag	22.1	0	2	53	258
	24.9	0	0	8	41

Ba	4.5	0	2	4	6
	4.8	0	5	11	18
	32.2	0	1	4	12
	36.3	0	0	1	2
Br	11.9	7	728	2764	5966
	13.3	1	155	609	1353
Co	6.9	1	116	655	1319
	7.6	0	26	159	344
Cs	4.3	0	0	1	1
	4.6	0	1	3	5
	30.9	0	5	30	68
	34.9	0	1	5	10
Cu	8	2	450	2304	3840
	8.9	1	110	597	1024
Dy	6.5	0	4	53	243
	7.2	0	3	46	297
Fe	6.4	8	240	863	1603
	7	3	77	293	569
I	28.5	0	0	10	56
	32.3	0	0	1	8
Mn	5.9	14	1099	3754	0
	6.5	6	392	1374	47
Mo	17.5	33	678	1882	3810
	19.6	5	124	356	721
Ni	7.5	0	344	1723	3310
	8.3	0	88	448	875
Nd	5.2	1	10	24	29
	5.7	1	24	59	75
Pt	7.4	269	2599	1184	2266
	8.2	64	639	321	617
Rb	13.4	0	64	237	1516
	15	0	11	42	285
	13.4	2	349	1219	2171
	15	0	68	249	461
Rh	20.2	18	292	1142	2035
	22.7	3	46	184	334
Ru	19.2	0	57	382	0
	21.7	0	10	69	0

Table 3: (continued)

Element	Energy (keV)	Signal Sensitivity(MeV) 2.4	3.4	4.2	5.1
Sc	4.1	0	2	8	11
	4.4	0	3	9	14
Sm	5.6	2	39	90	160
	6.2	2	69	181	335
Sn	25.2	0	13	81	201
	28.5	0	2	13	34
Ta	8.1	3	78	186	609
	9.3	2	75	197	761
Ti	4.5	0	7	18	22
	4.9	0	6	15	19
V	5	0	19	96	134
	5.4	0	9	53	75
W	8.4	0	53	421	427
	9.7	0	39	421	651
Zr	15.7	1	59	295	644
	17.7	0	11	55	122
Zn	8.6	0	27	447	6
	9.6	0	6	100	0

5 Discussion

In our data analysis, we use the mean smooth curve to integral the areas. It is mentioned earlier that our curve will lower the peak summit, which may cause some uncertainty. We can do uncertainty analysis by using FWHM. And we plan to combine Föurier Transformation Filter Method to smooth the spectrum to overcome the shortcoming of Mean Filter Method.

6 Acknowledgement

During this summer, I have received much useful guidance and advice and I thank all those students and professor who took the time to help me. I greatly thank professor Graham Peaslee for giving me the project and for his patient guidance. I am grateful to John Wilkinson and Sean McGuinness who taught me a lot of nuclear physics. And I thank Emily McGill, Matt Roddy, Alec Gonzales and Nick Caterisano for their warm help.

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