Additional Notes and Suggestions for the X-Ray Fluorescence Lab

A. Marino, October 2017

1 Additional Information about Data Collection

The password for the computer attached to the setup is XRF2014.

To run the device start the Mini-X Controller by clicking on the "LaunchMiniXCntrl.exe". Click on the"Start Amptek MiniX" button on the top. To actually collect and analyze the data, click on the "DppMCA" icon. (You will need to leave both the MiniX and DppMCA programs running.) The DppMCA screeen should be blank, but if there is previous data in the panel, goto "Delete data and reset time". To connect to the spectrometer device, click on MCA→Connect. Then go back to the Mini-X controller and hit "HV on". Then back in the Dpp MCA program, click on MCA→Start Acqusition" . It will collect data for about 60 seconds and you will hear a beeping noise. Counts will also appear in the plot in DppMCA program. When the data acquisition ends you should manually hit "HV off" on the Mini-X Controller program.

To calibrate, in the DppMCA, go to "Calibrate". For a given peak, find the channel number that corresponds to the location of the peak, and enter in the energy value in eV for that peak. Figures 1 might be helpful for identifying peaks.

To export the data from the DppMCA program to a file, go to "Copy Spectrum Data", then open the"Notepad" application within windows and paste the data there. This file might look strange on the screen in Notepad, but If you save the file and copy it over to another computer, you can just import it into Mathematica and it should interpret it properly with columns for the channel number and the counts. (You need to apply your calibration to convert it back to energy.)

2 Suggestions for Additional Investigations

Ultimately it would be nice not just identify the contents of a sample, but also to estimate the fractional composition. The yield of x-rays due to fluorescence will vary from material to material. The x-rays are also absorbed as an exponential function of the material that they pass through:

$$I = I_0 e^{-\mu_s \rho x} \tag{1}$$

where I_0 is the initial intensity, ρ is the density, μ_s is the mass absorption coefficient of the sample (which depends on the material and potentially the wavelength). The x-rays from the source are both absorbed by the sample exponentially (leading to a larger signal for a thicker sample) but then the emitted x-rays from the material also are attenuated on their way back

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Amptek K and L Emission Line Lookup Chart

XR-100CR / XR-100T-CdTe / GAMMA-8000 / X-123

X-Ray and Gamma Ray Detectors

Key to Energy Values in keV

$K_{\alpha 1}$ $K_{\beta 1}$
Au
79
$L_{\alpha 1}$ $L_{\beta 1}$

Group IA	IIA	IIIB	IVB	VB	VIB	VIIB	Group VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA
H 1																	He 2
0.052 Li 3	0.110 Be 4											0.185 B 5	0.282 C 6	0.392 N 7	0.526 O 8	0.677 F 9	0.851 Ne 10
1.04 1.07 Na 11	1.25 1.30 Mg 12											1.49 1.55 Al 13	1.74 1.83 Si 14	2.02 2.14 P 15	2.31 2.46 S 16	2.62 2.82 Cl 17	2.96 3.19 Ar 18
3.31 3.59 K 19	3.69 4.01 Ca 20 0.34	4.09 4.46 Sc 21 0.40	4.51 4.93 Ti 22 0.45 0.46	4.95 5.43 V 23 0.51 0.52	5.41 5.95 Cr 24 0.57 0.58	5.90 6.49 Mn 25 0.64 0.65	6.40 7.06 Fe 26 0.70 0.72	6.93 7.65 Co 27 0.78 0.79	7.48 8.26 Ni 28 0.85 0.87	8.05 8.90 Cu 29 0.93 0.95	8.64 9.57 Zn 30 1.01 1.03	9.25 10.26 Ga 31 1.10 1.12	9.89 10.98 Ge 32 1.19 1.21	10.54 11.73 As 33 1.28 1.32	11.22 12.50 Se 34 1.38 1.42	11.92 13.29 Br 35 1.48 1.53	12.65 14.11 Kr 36 1.59 1.64
13.39 14.96 Rb 37 1.69 1.75	14.16 15.83 Sr 38 1.81 1.87	14.96 16.74 Y 39 1.92 2.00	15.77 17.67 Zr 40 2.04 2.12	16.61 18.62 Nb 41 2.17 2.26	17.48 19.61 Mo 42 2.29 2.40	18.41 19.61 Tc 43 2.42 2.54	19.28 21.66 Ru 44 2.56 2.68	20.21 22.72 Rh 45 2.70 2.83	21.18 23.82 Pd 46 2.84 2.99	22.16 24.94 Ag 47 2.98 3.15	23.17 26.09 Cd 48 3.13 3.32	24.21 27.27 In 49 3.29 3.49	25.27 28.48 Sn 50 3.44 3.66	26.36 29.72 Sb 51 3.61 3.84	27.47 30.99 Te 52 3.77 4.03	28.61 32.29 I 53 3.94 4.22	29.80 33.64 Xe 54 4.11 4.42
30.97 34.98 Cs 55 4.29 4.62	32.19 36.38 Ba 56 4.47 4.83	57 - 71	55.76 63.21 Hf 72 7.90 9.02	57.52 65.21 Ta 73 8.15 9.34	59.31 67.23 W 74 8.40 9.67	61.13 69.30 Re 75 8.65 10.01	62.99 71.40 Os 76 8.91 10.35	64.89 73.55 Ir 77 9.19 10.71	66.82 75.74 Pt 78 9.44 11.07	68.79 77.97 Au 79 9.71 11.44	70.82 80.26 Hg 80 9.99 11.82	72.86 82.56 Tl 81 10.27 12.21	74.96 84.92 Pb 82 10.55 12.61	77.10 87.34 Bi 83 10.84 13.02	79.30 89.81 Po 84 11.13 13.44	81.53 92.32 At 85 11.42 13.87	83.80 94.88 Rn 86 11.72 14.32
86.12 97.48 Fr 87 12.03 14.77	88.46 100.14 Ra 88 12.34 15.23	90.89 102.85 Ac 89 12.65 15.71	93.33 105.59 Th 90 12.97 16.20	95.85 108.41 Pa 91 13.29 19.70	98.43 111.29 U 92 13.61 17.22	101.00 114.18 Np 93 13.95 17.74	103.65 117.15 Pu 94 14.28 18.28	106.35 120.16 Am 95 14.62 18.83	109.10 123.24 Cm 96 14.96 19.39	111.90 126.36 Bk 97 15.31 19.97	114.75 129.54 Cf 98 15.66 20.56	117.65 132.78 Es 99 16.02 21.17	120.60 136.08 Fm 100 16.38 21.79	Md 101	No 102	Lr 103	Actinides 89-103
Lanthanides 57-71		33.44 37.80 La 57 4.65 5.04	34.72 39.26 Ce 58 4.84 5.26	36.02 40.75 Pr 59 5.03 5.49	37.36 42.27 Nd 60 5.23 5.72	38.65 43.96 Pm 61 5.43 5.96	40.12 45.40 Sm 62 5.64 6.21	41.53 47.03 Eu 63 5.85 6.46	42.98 48.72 Gd 64 6.06 6.71	44.47 50.39 Tb 65 6.28 6.98	45.99 52.18 Dy 66 6.50 7.25	47.53 53.93 Ho 67 6.72 7.53	49.10 55.69 Er 68 6.95 7.81	50.73 57.58 Tm 69 7.18 8.10	52.36 59.35 Yb 70 7.41 8.40	54.06 61.28 Lu 71 7.65 8.71	

Actinium - Ac 89 (10.07)
Aluminum - Al 13 (2.70)
Americium - Am 95 (11.87)
Antimony - Sb 51 (6.62)
Argon - Ar 18 (0.001783)
Arsenic - As 33 (5.73)
Astatine - At 85
Barium - Ba 56 (3.5)
Berkelium - Bk 97
Beryllium - Be 4 (1.85)
Bismuth - Bi 83 (9.78)
Boron - B 5 (2.53)

Bromine - Br 35 (0.007139)
Cadmium - Cd 48 (8.65)
Calcium - Ca 20 (1.55)
Californium - Cf 98
Carbon - C 6 (2.25-G; 3.51-D)
Cerium - Ce 58 (6.90)
Cesium - Cs 55 (1.87)
Chlorine - Cl 17 (0.003220)
Chromium - Cr 24 (7.14)
Cobalt - Co 27 (8.71)
Copper - Cu 29 (8.96)
Curium - Cm 96

Dysprosium - Dy 66 (8.55)
Einsteinium - Es 99
Erbium - Er 68 (9.066)
Europium - Eu 63 (5.234)
Fermium - Fm 100
Fluorine - F 9 (0.00169)
Francium - Fr 87
Gadolinium - Gd 64 (7.90)
Gallium - Ga 31 (5.93)
Germanium - Ge 32 (5.46)
Gold - Au 79 (19.32)
Hafnium - Hf - 72 (13.3)

Helium - He 2 (0.0001785)
Holmium - Ho 67 (8.795)
Hydrogen - H 1 (0.0000899)
Indium - In 49 (7.28)
Iodine - I 53 (4.94)
Iridium - Ir 77 (22.42)
Iron - Fe 26 (7.88)
Krypton - Kr 36 (0.00368)
Lanthanum - La 57 (6.15)
Lawrencium - Lr 103
Lead - Pb 82 (11.34)
Lithium - Li 3 (0.534)

Lutetium - Lu 71 (9.84)
Magnesium - Mg 12 (1.74)
Manganese - Mn 25 (7.41)
Mendelevium - Md 101
Mercury - Hg 80 (13.55)
Molybdenum - Mo 42 (10.22)
Neodymium - Nd 60 (6.96)
Neon - Ne 10 (0.000900)
Neptunium - Np 93 (20.4)
Nickel - Ni 28 (8.88)
Niobium - Nb 41 (8.57)
Nitrogen - N 7 (0.001251)

Nobelium - No 102
Osmium - Os 76 (22.5)
Oxygen - O 8 (0.001429)
Palladium - Pd 46 (12.16)
Phosphorus - P 15 (1.83-Y 2.20-R)
Platinum - Pt 78 (21.45)
Plutonium - Pu 94 (19.8)
Polonium - Po 84 (9.27)
Potassium - K 19 (0.86)
Praseodymium - Pr 59 (6.48)
Promethium - Pm 61
Protactinium - Pa 91 (15.4)

Radium - Ra 88 (5.0)
Radon - Rn 86 (4.4)
Rhenium - Re 75 (21.0)
Rhodium - Rh 45 (12.44)
Rubidium - Rb 37 (1.53)
Ruthenium - Ru 44 (12.1)
Samarium - Sm 62 (7.75)
Scandium - Sc 21 (3.02)
Selenium - Se 34 (4.82)
Silicon - Si 14 (2.42)
Silver - Ag 47 (10.49)
Sodium - Na 11 (0.97)

Strontium - Sr 38 (2.56)
Sulphur - S 16 (1.92)
Tantalum - Ta 73 (16.6)
Technetium - Tc 43 (11.5)
Tellurium - Te 52 (6.25)
Terbium - Tb 65 (8.229)
Thallium - Tl 81 (11.86)
Thorium - Th 90 (11.3)
Thulium - Tm 69 (9.321)
Tin - Sn 50 (7.3)
Titanium - Ti 22 (4.5)
Tungsten - W 74 (19.3)

Uranium - U 92 (18.7)
Vanadium - V 23 (5.98)
Xenon - Xe 54 (0.00585)
Ytterbium - Yb 70 (6.965)
Yttrium - Y 39 (3.8)
Zinc - Zn 30 (7.1)
Zirconium - Zr 40 (6.4)

(density in g/cm^3 at NTP)

Figure 1: The L and K lines for all of the elements.

to the detector. So eventually the signal should plateau as some constant yield. In general for thick samples determining the fractional composition can be a very complicated iterative proceedure, but you can try to estimate it here for a simple sample.

- Using different thicknesses of copper (both different layers of foil and some of the larger pieces) investigate the yield vs thickness. Does it increase linearly with thickness, or does it saturate at some max value? Not that since copper oxidizes easily, you might want to polish the surface a bit (or soak it in white vinegar for a few minutes).

- You have been given a new and an old penny. Take measurements of the Lincoln face side of the pennies and determine the composition. What elements do you see? The surface has been filed off of the back side of both pennies. Measure the composition of this filed side too. Based on these studies, and your measurements in the previous step what can you say about how deep into the sample the x-rays are penetrating?

- Challenge: Identify the elements and their composition in a 100 yen coin. First determine what elements are present. Determine the expected yields from thin foils of the same metals. Using the thin foils as calibration, try determine the fractional abundances of the elements in the coin. Here you might want to export the data in Mathematica and do a fit for coin spectrum $= A_1 *$ element 1 spectrum $+ A_2 *$ element 2 spectrum $+ ...$, and then the fractional abundances are $A_1/(A_1 + A_2 + ...)$. To turn a calibration spectrum dataset into a "function", you might want to use the Interpolation function in Mathematica.