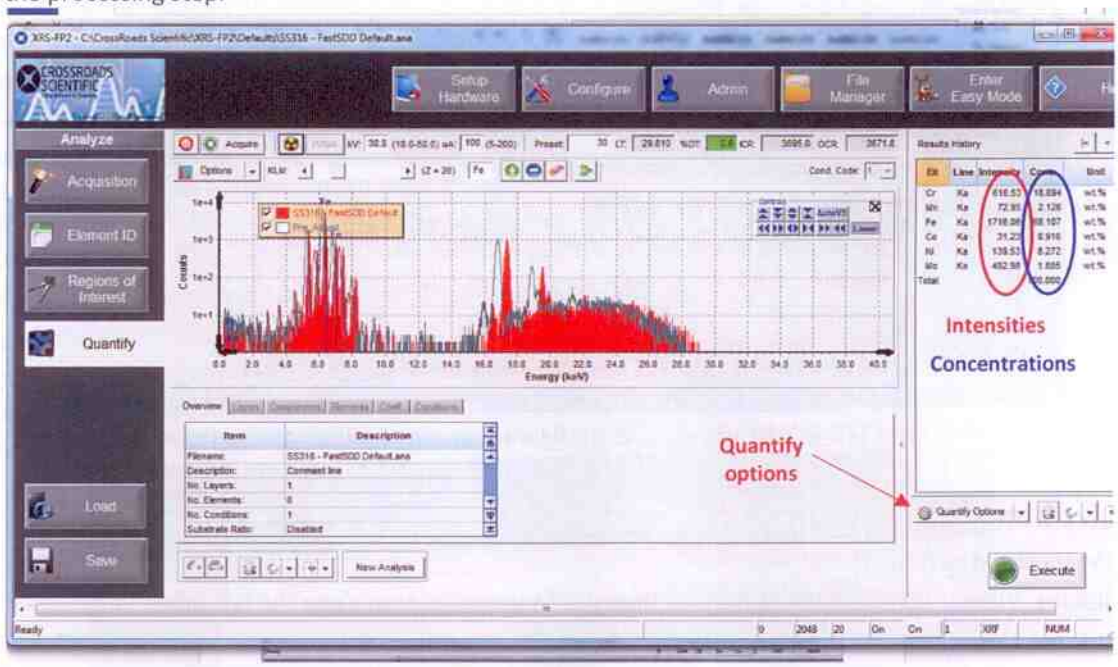
2. Select the "Quantify" button at the left side. If you now click the green "Execute" button, the software would go through all the processing steps quickly. In this demonstration, we will go step by step to observe what each is doing.
3. Select "Quantify Options", then "Smooth." Observe the result of smoothing in the spectrum window.
4. Select "Quantify Options", then "Escape Peaks." The software corrected for escape peaks; observe the result in the spectrum window. You can see both the corrected spectrum and the escape peak correction.
5. Select "Quantify Options", then "Sum." The software corrected for pileup by removing sum peaks; observe the result in the spectrum window. You can see both the corrected spectrum and the sum peak correction.
6. Select "Quantify Options", then "Background Fit", then "Background Subtract". Observe the result in the spectrum window. You can see both the photopeaks and the background that was removed.
7. Select "Quantify Options", then "Compton Peak". Nothing is visible in the window but values were calculated.
8. Select "Quantify Options", then "Deconvolute." It may take many seconds but is fitting the peaks as a sum of Gaussians.
9. The "Results table" will show intensities: the rate of X-rays observed in each photopeak. This is the output of the processing step.



10. Analyze Intensities

1. Now click "Quantify Options", then "Quantify.". Using the intensities, the software applies corrections for matrix effects and attenuations and applies calibration factors to determine concentrations. Since this is a "standardless" analysis, the calibration factors are computed from theory rather than measured.
2. The result is shown in the "Concentration" column. By default, these are in units of weight % and have been normalized to 100%.
3. Print the report, then save the file. Enter a name for the sample, e.g., "Steel.ANA." The .ANA is a CSV file (in ASCII) which can be read by Excel or Wordpad.

Congratulations! You have now set up the system and completed a standardless analysis.

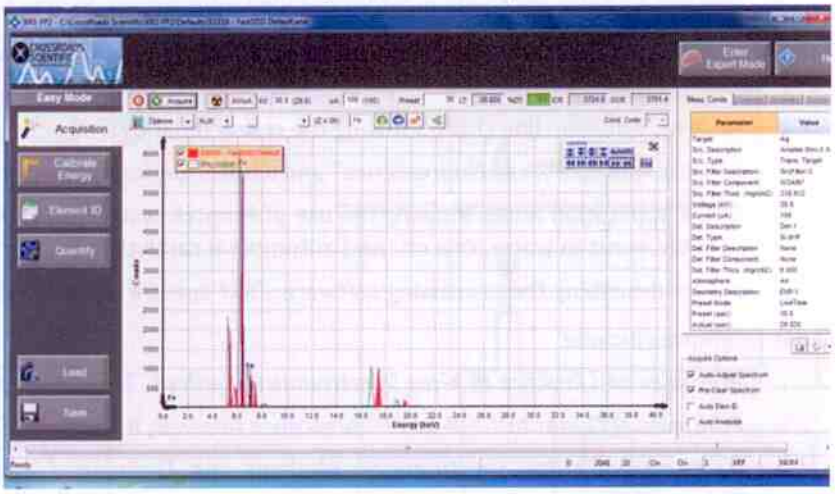
11. Next Steps

Now that you have carried out your first, standardless analysis of a metal alloy, what can you do now?

Easy Mode

So far, we have been using "Expert Mode", which is used to set up, configure, and calibrate the instrument. Once this has been completed, "Easy Mode" can be used for routine acquisition and analysis. To use "Easy Mode",

1. Select the "Home" button at upper left.
2. Select the "Enter Easy Mode" button at upper right.
3. The simplified screen shown to the right appears. To run an analysis, first use the "Load" button to recall the proper .ANA file, the one applicable to this instrument and sample.
4. Select the "Acquisition" button, then use the Mini-X icon and "Acquire" button to obtain a spectrum.



5. If needed, the "Calibrate Energy" button can be used to recalibrate the energy scale. Note that you will need to enter the energies of two peaks which are in your sample; this should be strong peaks (high concentration) and well separated in energy.
6. The "Element ID" button permits one to find if additional elements are present.
7. Select the "Quantify" button, then "Execute", to perform the analysis as above.
8. Save the resulting .ANA file.

Optimize the configuration

It is very important that the configuration of the system be optimized for each particular application. This includes

- Optimizing the excitation source: the HV bias, the filtering, and the current are all important. Many novice users do not fully understand the important of the X-ray tube parameters, bias and filtering, in obtaining high quality results; these are very important.
- Optimizing the X-123: the gain, the peaking time, number of channels, and thresholds are very important. There are many other parameters but these are the most vital.
- Optimizing the deconvolution parameters: the "Methods" tab gave access to many parameters which affect the accuracy and precision of the analysis results.

Calibrate the analysis parameters

This summary describes "standardless" analysis: the software uses simple models and nominal values to estimate the coefficients which relate the X-ray intensity to the concentrations. Much greater accuracy results are found by calibrating the analysis coefficients. These are calibrated from spectra measured using standards, reference materials of known compositions. Refer to the "Help" section of XRS-FP. The "Bulk Analysis" and "Standards Calibration" tutorials will be most helpful.

12. Learning More

The Installation CD contains a *Documentation* folder which includes user manuals, application notes, software installation guides, and a great deal of information describing the components in the Experimenter's Kit.

- The *DPPMCA* software's "Help" file includes detailed information on setting the parameters.
- The XRS-FP Software Guide provides detailed information on how to configure the analytical software.

For XRF novices, Amptek has a few application notes which may be helpful. These are all found on the "Links and PDFs" section of Amptek's web site.

- An X-ray emission line chart, showing the characteristic X-ray energies for each element
- A "Description of X-ray Fluorescence" and a note "Understanding characteristic X-rays"
- Three application notes showing the use of Amptek systems in EDXRF (one on RoHS/WEEE materials, one on light elements in water, one on used automotive catalytic converveters)
- A note describing the processing software, "XRF spectra and analysis software".

Other references include

- *Principles and Practice of X-ray Spectrometric Analysis*, 2nd Ed, E.P. Bertin, Plenum Press, (1975).
- *Principles of Quantitative X-Ray Fluorescence Analysis*, R. Tertian, F. Claisse, Heyden & Son Ltd., (1982).
- *Handbook of X-Ray Spectrometry: Methods and Techniques*, eds. R. van Grieken, A. Markowicz, Marcel Dekker, (1993).
- *Quantitative X-ray Spectrometry*, 2nd Edition, R. Jenkis, R. Gould, D. Gedcke, Marcel Dekker (1995)
- *Handbook of Practical X-ray Fluorescence Analysis*, eds. B. Beckhoff, B. Kanngiesser, et al, Springer (2006)
- http://xdb.lbl.gov/

13. Frequently Asked Questions

Can I just use the default calibrations and settings?

No! There has been no calibration at Amptek. You should expect no meaningful results if you use the configuration in the X-123 when it shipped or the calibration values in the default files.

Is this XRF Experimenter's Kit comparable to a turn-key XRF system?

No. This kit contains all of the critical hardware and software required to do energy dispersive X-ray fluorescence (EDXRF) but it is NOT a turn-key system. To get accurate results requires fabrication of radiation shielding and sample mount hardware, determining the optimum configuration of the hardware and software for your samples, and calibration. Obtaining quality results takes considerable effort.

A turn-key system is generally designed to handle a wide range of measurement applications. If a user has a specific application, particularly one that is challenging for turn-key systems, the Experiment's Kit lets the user optimize the entire system for that one application. It is a very powerful tool for specific and challenging measurement applications. But to obtain its advantages, the user must invest the time to fully optimize the hardware, the software, the calibration procedures, and so on.

A turn-key system is designed for an operator with minimal training. The operator turns on the system, takes a measurement, and the system gives the answer. The designers of the turn-key system have already optimized the configuration, calibrated the system, and evaluated its measurement uncertainty. The Experimenter's Kit requires a user to carry out these steps and to have the knowledge to carry them out.

Where do I turn if I am having a problem?

There is a "Troubleshooting Guide" in the documentation section of the Installation CD. You can refer to this or to the User Manuals for the various components.