X-ray photoelectron spectroscopy Energy Calibration

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Introduction

The X-ray photoelectron spectroscopy (XPS) lab currently outputs spectra as shown in fig 1. Due to errors the spectra need to be corrected and scaled in shift and scale. This is a slow process when done by hand. The aim of the scholarship was to write a program which could automatically calibrate spectra from the lab, allowing the spectra to be rapidly analysed.
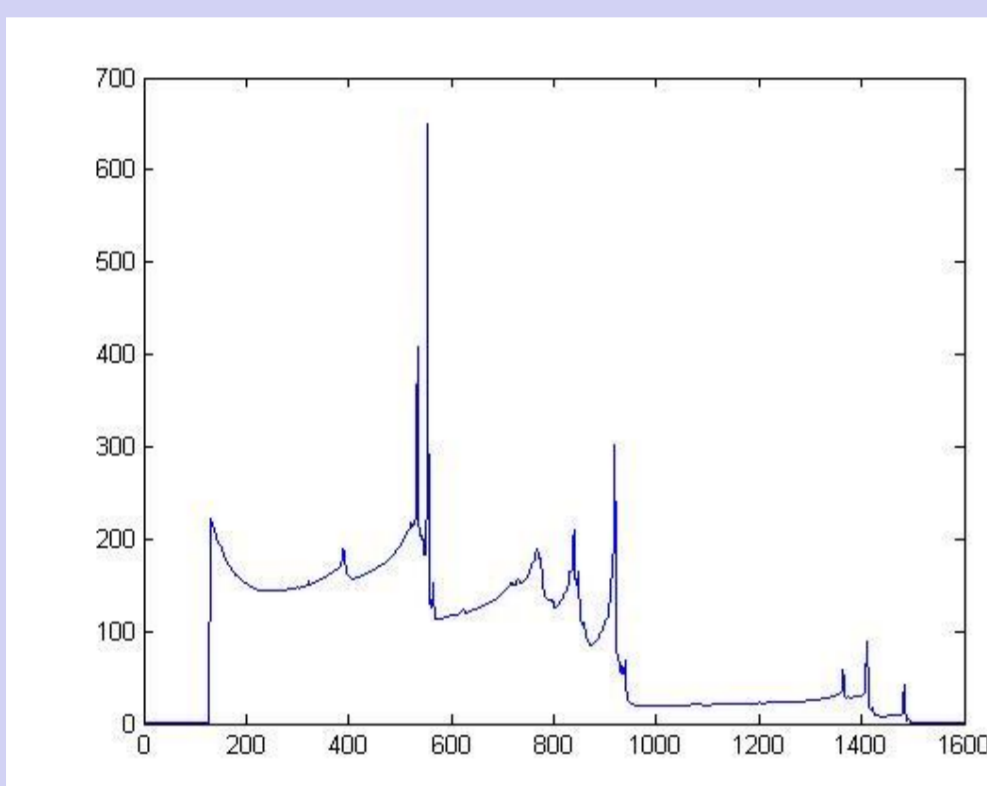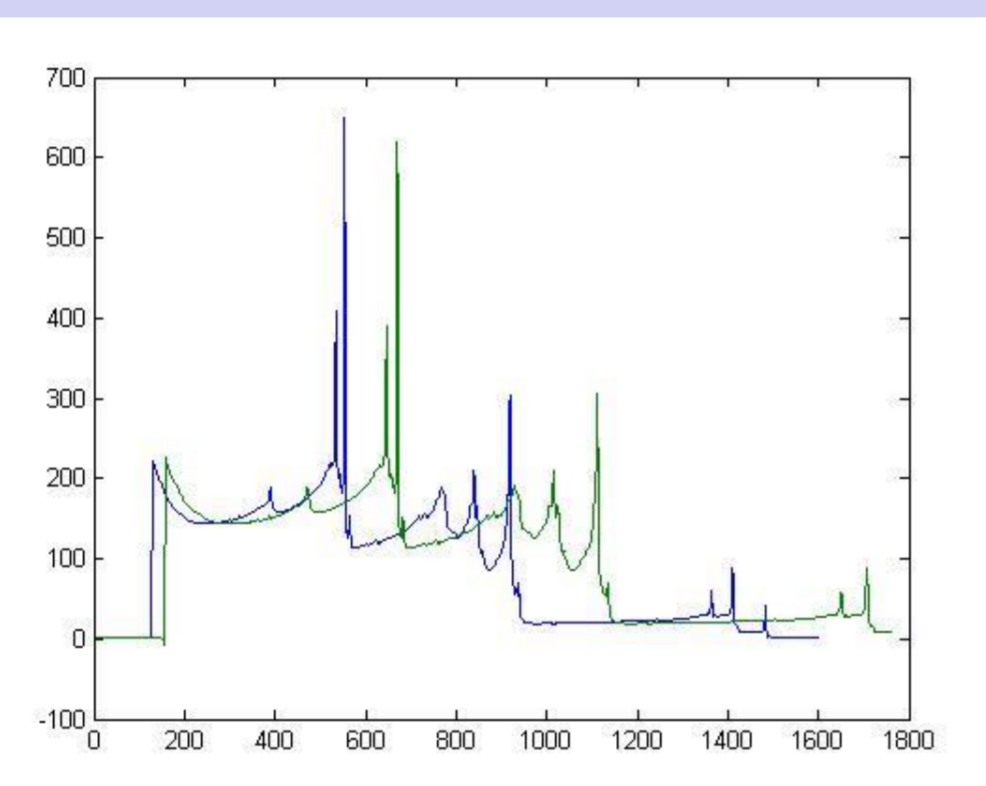

Fig 1-An XPS Spectra

Fig 2-an XPS reference data overlaid with XPS test spectra

First Steps

The first section was produced using the software "matlab" to write a code to compare the difference in the spectral peaks of copper, silver and gold with the same peaks from reference data from the National Physical Laboratory (NPL). Figure 2 shows an exaggerated difference between the reference data and 'test' data. By comparing the positions of these peaks, and by using a numerical solving method recommended by the international standards, it was possible to obtain two errors. These errors where the difference in scale and shift, equivalent to the M and C errors in a straight line formula.

$$y = mx + c$$

These errors were used to scale and shift the spectra of the a material being tested on in the lab. The idea was then to use these errors to then shift and scale a fourth test spectrum produced under the same conditions

To first test the program, the errors where added to the reference data and then the program was used to work out the errors which would be the same if the program was working correctly. Once the program was reliably returning the same errors as imputed, it could then be used against real test data.

Fig 3-The matlab code used to find and sum peak spectrum,

E-science

E-science is a program being developed at Newcastle University as a means of allowing scientists and engineers at different laboratories and universities to be networked. In addition to being able to communicate with each other, the software would allow people in the same project, or similar projects to share files at anytime. To effectively fulfil the aims of the scholarship it was necessary to upload to E-science the code which had been written and then develop it into a 'workflow' which everyone in the XPS project could access. The strength of this software allows someone in the XPS lab to upload raw test spectra and almost immediately receive a calibrated spectra back.

Workflows

The code to calibrate test spectra was spread across five different files which were all linked together. E-science uses a similar system but each section of code is formatted into a visual block. Blocks can be linked together in sequence without much experience of coding into a workflow. The workflow will then run from inputting test spectra to outputting answers.

Developing workflows

The project was now at a stage where it could be tested against real test spectra. The workflows in figure 4 were used to test against real test data. The first workflow imports test spectra for copper, sliver and gold and compares them to find the scale and shift errors. It then outputs the errors as images of the spectra similar to figures 1 and 2. The second workflow then inputs the errors along with the test spectra of any material being studied. This then scales and shifts the spectra to the correct positions and outputs the spectra both as an image and in numeric form. Two workflows were used to allow the operator to check the program following calculation of the scale and shift errors but before they were used to scale the spectra.
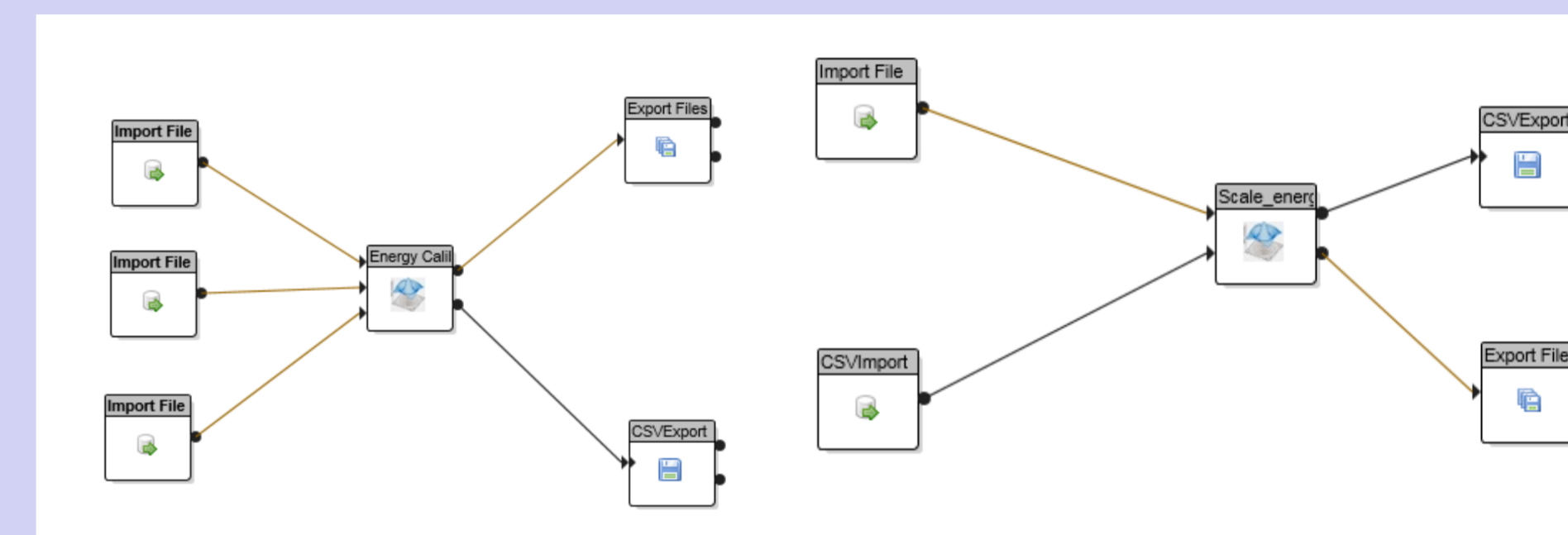

Fig 4 – the two workflows used in the energy calibration.

Conclusion

Overall the project was a success, allowing users in the lab to upload their spectra to e-science and quickly download a calibrated version. This has saved time and research can be done more quickly as each individual spectra doesn't have to be calibrated individually. In addition this work could be shared across e-science to other XPS labs to allow for similar calibration and even to be improved upon by other users.

In future the addition of another block would allow for calibration by directory, allowing the program to run over night calibrating anything from a day's worth to week's worth of test spectra.

References
-ISO 15472 2001, Page 17