D-parameters: Development of program to automate Sp2:Sp3 Carbon analysis of XPS image

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Supervised by: Prof P. Cumpson (Supervisor), Dr. A. Barlow (PhD Research), Dr. S. Woodman (eScience developer)

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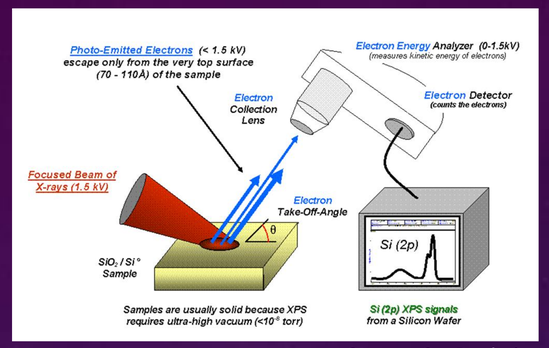
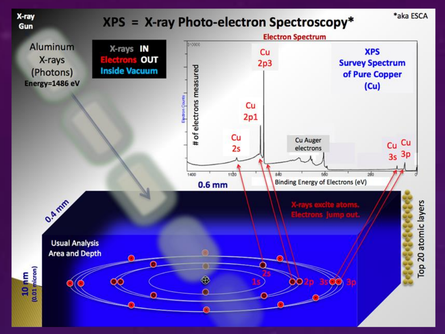


System2 - Bvchrist



XPS Physics - Bvchrist

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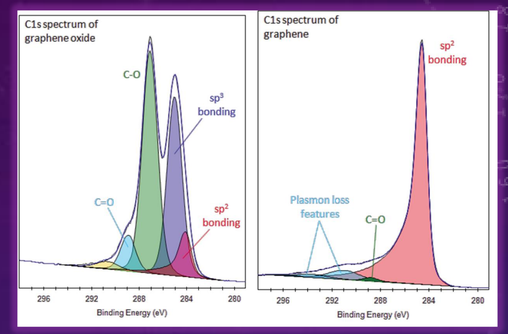

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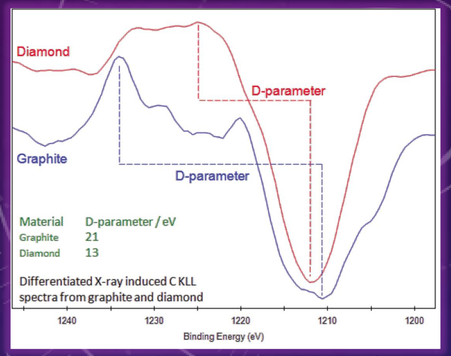

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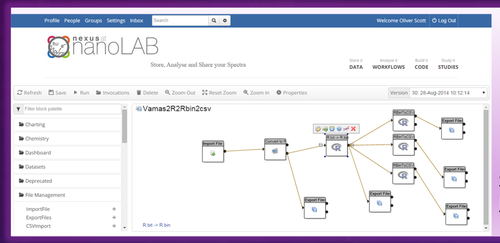
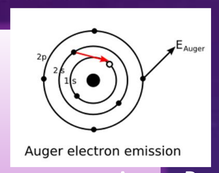
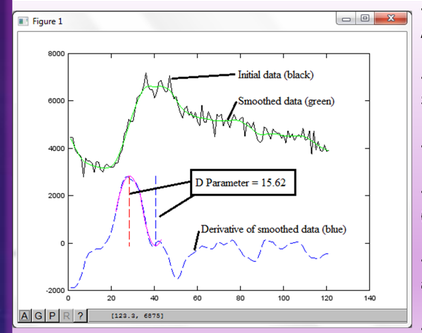


+ eScience – scientific research collaboration website developed at Newcastle – used to share work within team



Auger Process – A. Carlson



+ XPS frequently used to determine type (Sp2/3) of carbon in sample – this is done using Auger electrons

+ Difference between maximum and minimum differential of Auger spectrum represents Sp2/3 prevalence (called the 'D parameter')

+ Dr. Barlow had already developed program to extract D parameter from single spectrum

+ One capability is to create 'XPS image data' – a spectrum is created at each pixel (256x256 pixels!!)

+ Aim of this project was to create a MATLAB-type program to represent this data as an actual image

+ For one full image the program takes around 8 hours to complete!!

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Aims of project as a whole

During this summer a team of six undergraduates have worked with Professor Cumpson, Dr. Barlow and Dr. Sano in Newcastle's NEXUS (NEwcastle Xps User Service) facility and Dr. Hiden and Dr. Woodman in the Computer Science department who had developed an internet-based scientific research collaboration medium called eScience. The aim of this project as a whole was to construct an automated online processing and analysis service to be used by the Newcastle XPS NEXUS research facility. The other individual projects undertaken by the team included the calibration of the XPS machine, multivariate analysis of the data and the design of a sample rotation device for the machine itself.

Aims of this individual project

The project allocated to me was producing a code to automate the process of carbon analysis of the XPS results with minimal user input besides the data. This would improve the turnaround time for incoming samples and streamline the service. Therefore the first part of the project involved optimizing the raw code that Dr. Barlow had already written to be able to cope with different types of input data and spectra.

Depending on the completion of this code, the project had also a second part. As well as the regular mode of collecting data from one point on a sample for the whole energy range, the XPS machine is also capable of collecting data from a large area for one single energy value where each pixel of the resulting (256x256 pixel) 'data image' represents one energy value at one point on the sample. By taking 'data images' for a range of energy values of one area, one can build up spectrums for each pixel over a large area of a sample. The overall aim of this project was then to use the optimized code developed in the first half of the project, along with data from this operation mode, to produce an XPS image of the analysis of an area of the sample. However the resulting data file produced by such an operation can be very large, and the process of analysing these spectra therefore a task which required automation using eScience.

Theory behind the work

A carbon atom has two modes of bonding to itself – the 3 dimensional Sp3 bonding typified in Diamond and the flat hexagonal Sp2 bonding seen in Graphene. With carbon being such an important material in many areas, and especially with the current fascination with graphene and carbon nanotubes, a high proportion of the work undertaken at NEXUS is determining which of these types of carbon bonding is prevalent in a sample. Although the regular XPS spectral signatures of both bonds are so similar they are almost impossible to distinguish, it has been found that an analysis of the spectra around the Auger peak can yield an indicator of the proportion of the two types of carbon in the sample.

This indicator is a number called the D-parameter. The data image produced by the final code was to yield a D-parameter for each pixel of the area, effectively being then a picture of Sp2/3 carbon prevalence over an area of a sample.

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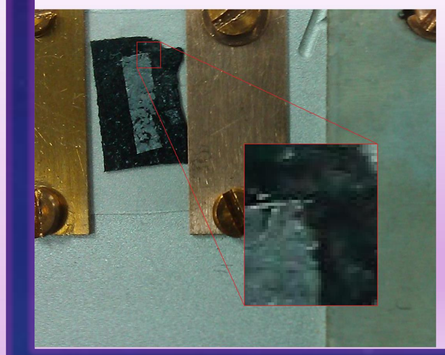
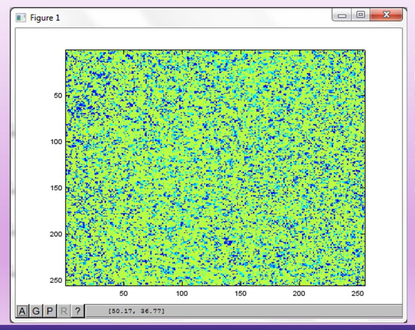
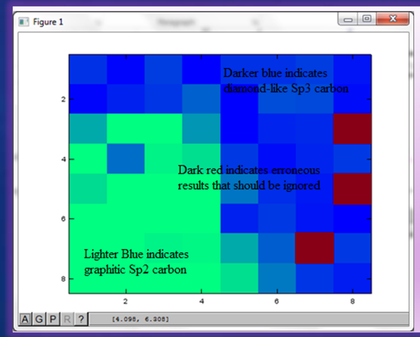
+ Using condensed data program creates accurate but simple representation





+ At full resolution data too indistinct and program unable to find D-parameter

+ Next stage for NEXUS to extend XPS capture to output more distinctive data



References

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Thermo Fisher Scientific Inc. (2013) "Carbon: Interpretation of XPS Spectra" Retrieved on August 10th 2014 from http://xpssimplified.com/elements/carbon.php