Guide to the posted videos

Guide to the 14 posted videos

The videos illustrate different potentials for quantitative XPS by spectral analysis involving both the peak and the background of inelastically scattered electrons as implemented in the QUASES software (www.quases.com).

It is recommended to view the videos in numerical order. If you own a software license, you may find the videos useful as tutorials and go through the steps on your own.

You are also recommended to **download and read the paper:**
S. Tougaard, ´Practical guide to the use of backgrounds in quantitative XPS´, J. Vac. Sci. Technol. A 39, 011201 (2021); https://doi.org/10.1116/6.0000661. It gives a general introduction to the problems met in traditional quantitative XPS and discusses ways to improve the reliability of quantitative XPS.

Further reading: Sven Tougaard, ´Energy loss in XPS: Fundamental processes and applications for quantification, non-destructive depth profiling and 3D imaging´ J. Electron Spectroscopy and Related Phen. 178, 128-153 (2010) (general theory). S. Tougaard. 'Accuracy of the Non-destructive Surface Nano-structure Quantification Technique based on Analysis of the XPS or AES Peakshape.' Surface Interface Analysis, 26, 249-269, 1998.

Sven Tougaard, March 26, 2021

1. Fe-oxide

This video illustrates the general procedure for spectral analysis: - noise reduction (optional), correction for analyzer transmission, isolating the individual peaks, finding the appropriate IMFP, doing the basic analysis. The analyzed example is a rather noisy survey spectrum of iron exposed to a maritime environment.

2. Au-Ni_1

Here is shown how one can find the distribution of island heights formed (small and tall islands and their height and relative surface coverage) when Au is deposited on Ni.

3. Au-Ni_2

With the same spectra as in *2. Au-Ni_1* this shows how a reference spectrum from pure Au is applied to determine the absolute coverage of the two types of Au islands formed on the Ni surface.

4. Ni-Au-Ni_1

Analysis of a Au layer buried at increasing depths in a Ni sample

5. Ni-Au-Ni_2

Using the same spectra as in *4. Ni-Au-Ni_1*, this Illustrates how to use the facilities for automated determination of the start and end depths for the layer. This is done by finding the structure with the smallest RMS deviation to the background in a wide energy region. It is also discussed how the displayed RMS deviation can be applied to find the uncertainty of the determined structure. Two algorithms for automation are implemented: the Simplex and the Powell methods. The use of these are illustrated and discussed.

6. Ni-Au-Ni_3

Using the same spectra again as in *4.Ni-Au-Ni_1*, this Illustrates that by using a reference spectrum from a pure Au foil, one can identify the formation of islands in the first sample and the absolute concentration of Au in the buried layers can be determined.

7. Ni-Au-Ni_4

Using again the same spectra as in *4. Ni-Au-Ni_1*, this Illustrates how one can make a rough correction for the influence of elastic electron scattering. The theory behind this method is described in the following video: *8. Understand the XPS intensity*.

8. Understand the XPS intensity

Goes through the factors that are responsible for the measured XPS intensity. This includes a simple practical way to approximately correct for elastic scattering effects. Another way to make this correction is to use instead of the IMFP, the "effective attenuation length (EAL), the "mean escape depth (MED)", or the "information depth (ID)". Which of these is to be applied depends on the particular situation studied. To avoid this complexity, this simplified analysis is done simply with the IMFP and the result is then corrected for elastic scattering by a correction factor CF which an be easily calculated (see below in the text description of video 9).

9. Practical procedure to correct for elastic electron scattering

In its present form this video is essentially the same as video 7. The correction is done with the CF factor as in video 8. As discussed in a section on elastic scattering in the paper https://doi.org/10.1116/6.0000661, there are two simple approximations to the CF factor of which one is slightly more accurate. Both CF values are easily calculated with the free QUASES-IMFP-TPP2M+CF software (download at www.quases.com). I hope to make a future version of this video to illustrate this.

10. Using_1 the external cross section facility

The video demonstrates a facility in the QUASES software to construct an improved cross section for analysis of a given sample. This is done by fitting to a small energy range below the peak energy. It is done interactively and as the example shows it is rather quick and easy to apply.

At the end of the video I downplay the general importance of this facility. I did this because I was reluctant to overfit the data. However, by practical application of the method to several examples over the past year, I realized that this is not the case because the fitting of the cross section is done in the short energy loss range while the background is fitted by the structure in a much wider energy range. So, I have come to the conclusion that it is a very useful and rather general method to improve the accuracy of the analysis and that it could be used quite widely as also demonstrated in videos 11, 13, and 14.

11. Using_2 the external cross section facility

Applied to HAXPES. Analysis of HAXPES is nothing different from ordinary XPS, but the larger IMFPs opens up for analysis of deeper lying structures (~100 nm). The sample studied in this video consists of a stack of materials with quite different inelastic scattering cross sections (Al, Ti, and AlGaN). Optimizing the cross section with the facility is shown to improve the accuracy of the analysis considerably. It is also shown how a mixture of cross sections (Al and Universal cross sections with different weights) can also be applied and when done carefully this gives a slightly better agreement with the nominal structure.

12. Nano-Particles_1

The video summarizes some examples where Quases analysis was applied to determine the size and density of nanoparticles. It is also shown how it is easily applied to study the gradual embedding of NPs in a polystyrene substrate as a function of time and temperature.

It is further demonstrated that even very **weak and noisy peaks** can be analyzed to give valuable quantitative information. This is of course generally valid and not restricted to studies of NPs. This is important to note, not least because one often decides to use a weak peak rather than the most prominent peak if there are interfering peaks from another element in the analyzed energy range.

In the last part of the video, Quases analysis is applied to study coated NPs and it is shown that the structure of both the core and the coating can be determined (see also video 13).

13. Nano-Particles_2

This video shows the steps involved for a detailed analysis of **coated nano particles**. It is shown how deviations from the ideal structure of the coating can easily be determined (i.e. to what extent the core is off center) and it can be determined whether the coating is covering the core NP on all sides. The results are published in the paper (A. Müller et al, 'Determining Non-Uniformities of Core-Shell Nanoparticle Coatings by Analysis of the Inelastic Background of X-Ray Photoelectron Spectroscopy Survey Spectra' DOI: https://doi.org/10.1002/sia.6865)

14. Amb-Press-XPS

XPS taken under **near ambient gas pressure (NAP-XPS)** will have unwanted distortions caused by inelastic scattering of the photoelectrons by the gas molecules. The video shows how Quases can be applied to correct the XPS spectra very accurately for these distortions. The inelastic scattering cross section of the gas (which is needed) is rather complex and it is shown how this can be determined using the software facilities to create external cross sections.

The results are published in the paper (S. Tougaard and M. Greiner 'Method to correct ambient pressure XPS for the distortion caused by the gas' Appl. Surf. Sci. 530, (2020) 147243)