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Developments in Practical Applications of Inelastic Background Analysis to Characterize nano-structures

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Recent advances in practical applications and software for non-destructive characterization of nano-structures by analysis of the inelastic background in photoelectron spectroscopy are discussed.

1. Introduction

The growth in technological applications of nano-structured materials demands non-destructive techniques to characterize elemental depth distributions at the *nm* depth scale. A technique [1] which is increasingly used consists in analysis of the energy distribution of inelastically scattered photoelectrons which depends strongly on the depth distribution of the photoemitting atoms. Nano-structures can be studied up to depths of ~ 8 inelastic mean free paths (IMFP) [1] which with conventional XPS is ~ 5 -10 nm and ~ 100 nm with the high energy photons used in HAXPES. A software QUASES [2] was developed to facilitate the practical use of this method.

Here we review new developments of the technique for improved data analysis and also adaptation of the potentials of the method to the new situation where applications of HAXPES is expected to quickly become widespread with the availability of commercial high energy lab X-ray sources [3,4].

2. Probing deeper with HAXPES

With HAXPES it is possible to study deeply buried structures up to ~ 100 nm or more [5-7]. Fig 1 shows an example where the depth distribution of Ti and Ga atoms in a stack at room temperature are determined by background analysis in the left panels [7]. Note that, although the Ta and Ga peaks can hardly be seen, the analysis is still very convincing and the

background with multiple plasmon structures are accurately modelled over the full 300 eV energy range. The QUASES analysis method is non-destructive and variations during annealing can easily be followed in almost real time. This is illustrated in the right hand panels of Fig. 1, where the quantitative interdiffusion of Ga and Ta atoms as a result of annealing at 550 C, have been determined [7].

A further advantage of HAXPES for background analysis, is that the energy region over which the background can be followed can exceed 1000 eV. Since these electrons have undergone many inelastic scattering events, they originate from atoms at deeper layers and it has been found [6] that the probing depth may reach ~ 20 IMFP.

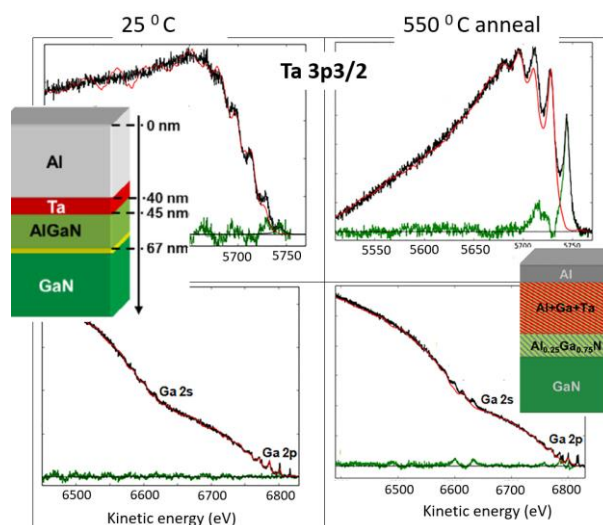


Fig. 1 Non-destructive analysis of the annealing induced diffusion of a deeply buried Ta layer in an AlGaIn structure[3]

3. Optimized cross section for complex structures

For samples with complex structures, the photoelectron may pass regions of materials with varying inelastic scattering properties. In many cases these variations are small but in other cases they may be substantial. This can happen if regions of materials with cross sections dominated by sharp plasmons (e.g. Si, Ge, Al and polymers) occur along with regions with transition metals, which in general have wide and rather featureless cross sections. The situation is more likely to happen with HAXPES because it probes much deeper structures. It was recently found that for such samples the analysis is more accurate when the cross section is modified according to the structure of the sample [5,7,8]. New facilities are now available in the software to interactively fit to the physical scattering properties of the studied material.

4. Elastic scattering correction

It has been found that an approximate correction for elastic electron scattering [9] will enhance the accuracy of the analysis [7]. This correction is small when the studied structures are at depths smaller than ~ 2 IMFP but it can be substantial for deeper structures. Facilities to do this have been implemented in the QUASES-IMFP [2] software.

5. Automated fitting of structural parameters

Automated data analysis is of high importance both in order to save time and also to facilitate analysis by non-experts and computers. To this end, the applicability of both the Powell and the Simplex multidimension minimization algorithms to optimize the model-parameters in the fit to experimental data have been investigated and implemented.

6. 3D-imaging with sub-nm depth resolution

With the smaller lateral size of industrial devices there is also a need for non-destructive 3D-imaging of nano-structured samples. For this, automated data analysis is mandatory due to the huge number of spectra. An algorithm well suited for that was developed ~ 10 years ago [1]. With conventional XPS it was demonstrated [10] that 3D-imaging with sub-nm depth resolution is possible with a lateral resolution of $\sim 10\mu\text{m}$. With HAXPEEM it should be possible to

eventually obtain 3D images with better than 100 nm lateral and 1 nm depth resolution. Such work has been initiated [11]. Here spectral noise is also an issue due to the small areas probed and Principal Component Analysis has proven [10] to be extremely effective for noise reduction.

7. Expected growth in HAXPES applications for routine analysis

Recently, high energy lab X-ray sources have become commercially available [3] and with these it is now possible to perform HAXPES and HAXPEEM in the lab [4]. This opens up for practical industrial applications of these advances in inelastic electron background analysis of nano-structured materials.

8. References

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