Overlayer thickness determination based on XPS no-loss peaks ratio

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X-ray photoelectron spectroscopy (XPS) is attracting considerable interest in surface science and is employed in commercial surface analytical instruments. While qualitative analysis of a XPS spectrum is relatively simple, quantitative analysis is more challenging since the quantification of no-loss peak areas in terms of atomic concentrations is required [1]. The elastic and inelastic scattering cross-sections of electrons at energies 100-1000 eV are of the same order. For lower energies the elastic scattering cross-section increases. Despite this, the majority of electron transport models (e.g. the straight line approximation (SLA)) used for XPS does not provide a rigorous treatment of elastic scattering processes. Instead, semi-empirical corrections are proposed replacing inelastic mean free paths (IMFPs) with so-called effective attenuation lengths (EALs).

In this work, a numerical technique is described, in which the no-loss XPS peaks are modeled by using the radiative transfer equation (RTE). The solution of RTE relies on the discrete ordinate method with matrix exponential [2]. It is suitable for any given singe scattering phase function. No additional assumptions on electron transport in solids are required. The RTE-approach is especially efficient for simulating the isotropization process of an electron beam. A new method for overlayer thickness determination from XPS spectra is proposed. It is based on computing lookup tables for no-loss peak ratios as a function of overlayer thickness by means of the RTE-solver. It provides results for a set of incident and sighting angles and, therefore, is extremely fast. For instance, the computational time required for creating the lookup table for a set of 64 incident and 64 sighting angles is less than 1 minute. Figure 1 illustrates the areas of no-loss XPS peaks for Ni overlayer on Au substrate. The RTE-approach (blue line) is validated against Monte-Carlo simulations (red circles). The agreement within 2 % is obtained. Note that the computations do not involve artificial parameters such as EAL.

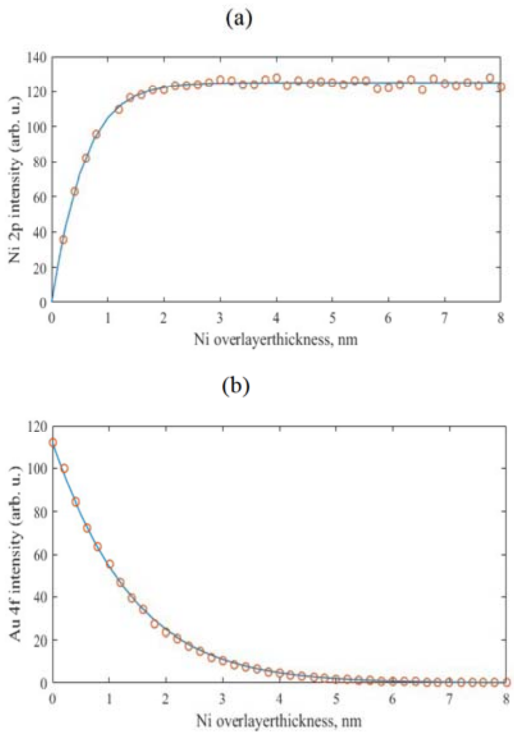

Figure 1. XPS Ni_{2p} (a) and Au_{4f} (b) no-loss peak intensity gross with Ni sputtering on gold substrate compared to Monte-Carlo results from [3]

References

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