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Data treatment for quantitative and high-throughput analysis of soft- and hard- X-ray photoelectron spectroscopies

Hideki YOSHIKAWA

Research Center for Advanced Measurement and Characterization, National Institute for Materials Science, Japan

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X-ray photoelectron spectroscopy (XPS) is a powerful tool for chemical analysis and electronic structure analysis for a variety of materials. It is well-known that XPS is a surface analysis technique which reveals the surface nano-sized thin layers of the materials. However, the quantitative analysis of XPS spectra is often time-consuming because analyzing spectra needs a trial-and-error data-treatment using knowledges on both XPS's surface sensitivity and XPS spectral formative factors (chemical shift, background by multiple inelastic scattering, band-bending or charging of sample surface and so on). In general, more quantitative or more advanced analysis makes its data treatment more time-consuming. For practical use, therefore, the development of more quantitative and advanced analysis needs not only its high functionality but also high-throughput data treatment, which can be realized by new algorithms and softwares. In this report, we show examples of new data treatments of electron spectroscopies.

Firstly, the hard X-ray photoelectron spectroscopy (HAXPES) is recognized as a new useful XPS technique which has a large observation depth over 20 nm. It is well-known that the XPS's high surface sensitivity often brings disadvantages in the analysis of practical materials which have surface contamination or surface degraded layer, because non-damaging ion beam sputter cleaning is difficult for compound materials. The HAXPES overcomes this shortcoming, and the data treatment of HAXPES can be easy if a sample is homogeneous in depth except for an undefined surface layer. On the other hand, if a sample is not homogeneous in depth, the HAXPES analysis is informative but time-consuming. To realize efficient HAXPES analysis, for example, we developed a software to extract non-destructively a band bending in semiconductor from XPS and HAXPES spectra. As an example of the application of this software, HAXPES analysis of the organic light-emitting diode with an electron-injection layer composed of Al cathode and 9,9-dioctylfluorene (50%) and N-(4-(2-butyl)-phenyl)diphenylamine (F8-PFB) revealed that the band bending was created near the cathode at 0 V bias voltage. When a bias over 2V was applied to the device, the band bending was disappeared and a linear potential profile proportional to the applied bias was created.

Secondly, the software to evaluate the band bending from XPS spectra needs the accurate information depth, which is closely related to inelastic mean free path (IMFP), effective attenuation length (EAL) and mean escape depth (MED). It is known that the IMFP is derived from an energy loss function (ELF). Therefore, the efficient and precise evaluation of IMFPs means that the experimental evaluation of ELFs and the transformation from ELFs to IMFPs after considering the dispersion relationship between energy loss and momentum transfer should be efficient and precise. In this report, we also discuss new algorithms to evaluate IMFP and MED efficiently and quantitatively.