[IV-31]

Application of Numerical Method to Angle-Resolved XPS Data

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Angle-resolved X-ray photoelectron spectroscopy (ARXPS) technique provides information on the concentration depth profile of the sample non-destructively, which is useful in many areas of surface research including biomaterials, microelectronics, catalysis, and adhesion. In ARXPS, spectra are collected at various photoelectron take-off angles. Spectra collected at each angle are represented as the Laplace transform of the entire depth profile, so the data must be inverted to generate an estimate of the concentration depth profile. However, the inversion of the Laplace transform cannot generate the concentration depth profile from the ARXPS data unambiguously, because the ARXPS experiment provides data only for a limited range of the concentration depth and the ARXPS data always contain a certain amount of the noise. In this simulation study, a numerical method (singular system approach) is applied to ARXPS data for generating the concentration depth profile. Also, the effect of parameters employed in the numerical method is investigated. The parameters which have considerable effect on the successful application of the numerical method include the number of the data, sampling schemes, and the amount of the noise contained in the data. The gravimetric sampling scheme was reported to provide better results than those from the equidistance sampling design when the initial sampling data point is very close to zero. Since sampling data points in ARXPS measurement are in a limited range, different sampling schemes do not show much significant differences. The effect of the different sampling schemes becomes minor one compared to that of the amount of the noise in the data. The minimum number of the data is determined by the amount of the noise. The data collected at more than the minimum number of take-off angles actually contain redundant information on the depth profile. In this study, the experimental conditions in terms of the number of the data and the sampling design are optimized.