

Experimental Response Function of Photoelectron Spectrometer

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Since the electrons and photons are most easily available particles to probe physical properties of matter, many spectroscopic techniques use these two types of particles. Among the spectroscopic methods using the particles, the photoelectron spectroscopy is a well-established and powerful tool to study electronic structures of the bulk or the surface of solids. The energy-distribution curves of the photoelectrons are closely related with the electronic level density of states of solid systems. In order to interpret electronic structures of solids from the photoelectron spectra we must thoroughly analyze overall effects on the spectral line-shape. Many researchers proposed early the "three step model". The model supposed the photoemission process as the sequences of 1) the optical excitation of a bound electron in an elastic scattering process, 2) the transport of the electron throughout the solid, and 3) the escape through the surface-potential barrier of the sample into the vacuum. These are factorized as a distribution of photoexcited electrons $P(E, \omega)$, a transmission function of $T(E)$, and an escape function $D(E)$ in the following expression

$$I_e(E, \omega) = P(E, \omega) \times T_e(E) \times D(E),$$

where the subscript "e" denotes the elastic process, and thus we consider only the photoexcited electrons with no loss of energy because the background due to the inelastic scattering is independently treated when the spectrum is analyzed. In addition we have to consider the photon source broadening and the electron analyser broadening to make a real spectrum.

To extract the photoexcited spectral weight $P(E, \omega)$ from the energy distribution curve $N(E, \omega)$ of the real spectrum with a photon energy $\hbar \omega$ by the curve fitting procedure, one assumes that all the instrumental and/or the extrinsic factors give a single response function $G(E, \omega)$. Considering the convolution of the signal function $P(E, \omega)$ and the response function $G(E, \omega)$, we express the real spectrum function $N(E, \omega)$ as the following;

$$N(E) = \int P(E - E') \cdot G(E') dE'.$$

Here we omit the photon source frequency ω because the photon energy is normally fixed

in the experiment. For the spectrum of the core line in x-ray photoelectron spectroscopy (XPS), the Doniach-Sunjic line-shape is a well known function adapting well in metallic system. This primary line shape originates from the photoexcitation of an electron. It consists of a lifetime-broadened Lorentzian and the successive modification by the immediate response of the conduction-electron system to the positive photohole which makes an influence on the asymmetric line-shape in the lower kinetic energy range of the spectrum.

On the other hand, the principal factors of the instrumental and/or the extrinsic broadening are the photon source broadening and the analyser transmission broadening. Many researchers used conventionally this response function as a single gaussian shape. This assumption is considerably inappropriate for the precise line-shape analysis since the actual response function of the photon source and the instrument does not have the shape of a single gaussian. Therefore the line-shape analysis with several components could mislead the uncorrect information.

We obtained the numerical response function by the furier transformed deconvolution-method. We selected the core-levels of the noble metal systems, silver and gold since we knows the line-shape parameters (Lorentzian width and asymmetry parameters in the Doniach-Sunjic line-shape function) of the major core-levels of them. In the furier transformed space, we express the energy distribution curve as the following

$$\tilde{N}(\omega) = \tilde{P}(\omega) \cdot \tilde{G}(\omega)$$

where the tilde functions are the inverse furier transformed functions of the original ones. Since we knows the signal function $P(E)$ in the literature and obtains the energy distribution function $N(E)$ in the experiment, we can evaluate numerically the inverse furier transformed instrumental response function $\tilde{G}(\omega)$. Also we can easily get the instrumental response function $G(E)$ by the furier transformation. This response function is independent regardless of the measured samples. The instrument and/or the extrinsic factors only determine the response function. By performing the experiment with the independent samples of which the signal parameters are known, we confirmed the experimental response function. The usefulness of this experimental response function in the line-shape analysis by the curve-fitting convolution procedure must be very powerful. The improved results of the data analysis for other systems will be reported elsewhere later in detail.