# The theory of Photoelectron Yield Spectroscopy

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## 1 Introduction

Photoelectron yield spectroscopy (PYS) is a method for probing occupied state energies, especially ionization potential (IP). In PYS, the total yield is measured as a function of incident light energy. PYS is expected to have an advantage in probing dielectric materials with accuracy because it is not affected by the charging problem and is able to do *in situ* measurements. Absolute value of the IP is found from the threshold energy that the first photoelectron comes out.

The general relational expression which is used for an analysis of the threshold in PYS is as follows.

$$Y(h\nu) \propto (h\nu - \chi)^n \tag{1}$$

Here, $Y(h\nu)$ is the photoelectron yield as a function of incident photon energy $h\nu$, $\chi$ is the threshold energy corresponding to IP and $n$ is a constant exponent (not necessary integer) which depends on the material type (metal, semiconductor, etc). The value of $n$ is advocated independently of a material type of sample as 2 in metal case [1], 1 ∼ 3 in semiconductor case [2] and 3 in organic case [3].

In this study, we derived a simple and general formula of photoelectron spectrum $Y(h\nu)$ which can be applied to every material type and we have checked the behavior of the function near the threshold. Moreover, we found that the density of states near the Fermi level can be obtained by taking the second derivative of the photoelectron yield spectrum.

## 2 Model of the simple and general theory

We introduce the following simple equation for a more general formula of PYS spectrum

$$Y(h\nu) = \int_0^{h\nu-\chi} D(\varepsilon - h\nu)T(\varepsilon)d\varepsilon. \tag{2}$$

Here, $\varepsilon$ is energy of an emitted electron and $D(\varepsilon - h\nu)$ is a density of states of the initial state and $T(\varepsilon)$ is a probability that an electron which was excited overcomes the surface potential barrier and jumps out of the surface.

The physical concept behind formula is that the number of emitted electrons is proportional both to the transmission probability function and the number of electrons which have enough energy to transmit the surface potential. It is shown that the transmission probability is approximately proportional to the energy of emitted electrons near the threshold when the final state electron momentum distribution is isotropic inside the matter.

## 3 Calculation

Results of analytical calculations of the value of $n$ concerning PYS spectrum using our theory are 2, 5/2 and 3 in cases of metals, semiconductors and organic materials respectively. These results nicely agree with previous studies and experiments.

## 4 Analysis of DOS from PYS experiment

Near threshold, the second derivative of our formula (2) is approximately proportional to the density of states :

$$\frac{d^2Y(h\nu)}{dh\nu^2} \approx \frac{1}{4\chi_0}D(-h\nu). \tag{3}$$

$\chi_0$ is the surface potential barrier. This relation suggest the possibility of finding the DOS from PYS experiment, and we have tested this method with PYS data of organic solids.

## References

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