Asymmetry parameter and surface excitation parameter for Ni derived by angle-resolved and energy-resolved PES analysis at SPring-8

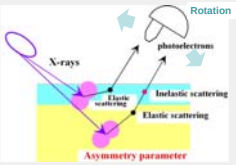
Hideki YOSHIKAWA [1], Hiromi TANAKA [1)3)], Masahiro KIMURA [1)4)], Toshiya OGIWARA [1)], Takashi KIMURA [1)], Sei FUKUSHIMAWA [1)], Kazuhiro KUMAGAI [1)], Shigeo TANUMA [1)], Mineharu SUZUKI [2)], Masato OKUI [1)5)], and Keisuke KOBAYASHI [1)]

[1]Beamline station, National Institute for Materials Science, Japan, [2]ULVAC PHI, INC Japan

Present address: [3]Yonago National College of Technology, [4]Nippon Mining & Metals Co. Ltd., [5]KOHZU Precision Co. Ltd.

Introduction

Quantitative nondestructive depth-profile analysis by angle-resolved high-energy XPS needs the precise knowledge of many factors as follows:



Factors affecting XPS spectra

- multiple elastic scattering effect
- surface excitation and interface excitation
- intrinsic and extrinsic energy loss
- asymmetry parameter
- diffraction effect

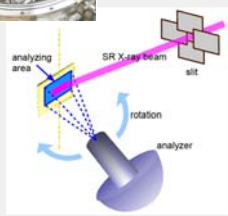
:

How to evaluate these complicated Factors

- Energy-dependent and angle-dependent measurements are useful to evaluate these effects.
  - ① Reflection electron spectroscopy
  - ② angle-resolved XPS with energy-tunable X-rays

Synchrotron Radiation (SR) X-rays

Experiment of angle-resolved and energy-variable XPS



Analyzing area must be larger than the X-ray beam spot on a sample at any rotation angle.

Specification

- Maximum analyzing energy 4800eV
- XPS analyzer rotates around the specimen center

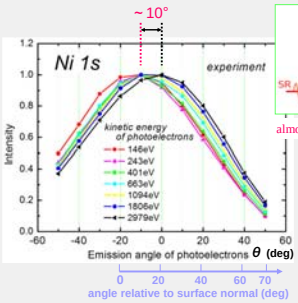
For this, adjustment of the beamline slit is necessary to precise evaluation of XPS factors.

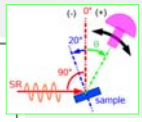
X-ray beam size before shaping : 1 x 2mm

XPS machine

- analyzing area : 3 x 10 mm
- detection angle : ±2 degree
- reproducibility of setting angle < 0.1 degree
- stability of setting angle < 0.01 degree

Experimental result





almost 100% linearly polarized X-ray

Ni 1s binding energy = 8333 eV	
X-ray energy	kinetic energy of photoelectrons
8479.4 eV	146.4 eV
8575.7 eV	242.7 eV
8734.4 eV	401.4 eV
8996.1 eV	663.1 eV
9427.6 eV	1094.6 eV
10139.0 eV	1806 eV
11312.0 eV	2979 eV

Multipole term of asymmetry parameter

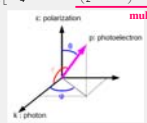
Asymmetry parameter

Case 1 : excited by linearly polarized light

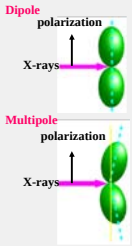
$$\frac{d\sigma_\nu}{d\Omega x}=\frac{\sigma_\nu}{4\pi}\left[1+\frac{\beta}{2}(3\cos^2\theta-1)+\underbrace{(\gamma\cos^2\theta+\delta)\sin\theta\cos\varphi}_{\text{multipole}}\right]$$

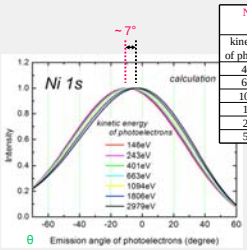
Case 2 : excited by unpolarized or circularly polarized light

$$\frac{d\sigma_\nu}{d\Omega x}=\frac{\sigma_\nu}{4\pi}\left[1-\frac{\beta}{4}(3\cos^2\xi-1)+\underbrace{\left(\frac{\gamma}{2}\sin^2\xi+\delta\right)\cos\xi}_{\text{multipole}}\right]$$



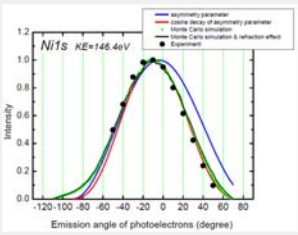
Multipole shape

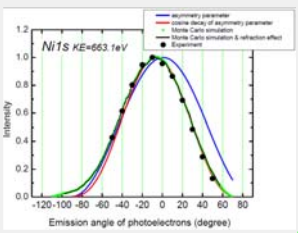




Ni 1s binding energy = 8333 eV, δ is roughly -7x10⁻⁵		
kinetic energy of photoelectron	β	γ
401.4 eV	1.988	- 0.123
663.1 eV	1.985	+ 0.080
1094.6 eV	1.981	+ 0.282
1806 eV	1.974	+ 0.571
2979 eV	1.963	+ 0.900
5000 eV	1.943	+ 1.31

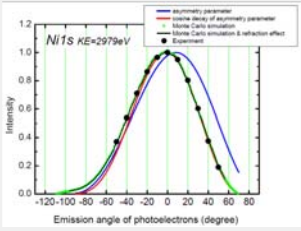
Monte Carlo analysis of angle-resolved and energy-variable Ni 1s photoelectrons





Experimental result

Monte Carlo result



Monte Carlo simulation based on

(1) atomic potential : Dirac-Hartree-Fock potential

(2) IMFP : TPP-2M

(3) asymmetry parameter calculated by Trzhaskovskaya et al. [Atomic Data Nucl. Data. Tables 77 (2001) 97]

(4) with refraction effect

Conclusions

(1) Peak shift of angle-resolved and energy variable Ni1s photoelectrons is successfully described by multipole effect of asymmetry parameter. This means *Multipole effect* is not negligible.

(2) Result of Monte Carlo simulation with plural inelastic and elastic scattering events is extremely good agreement with experimental results .

Surface excitation effect

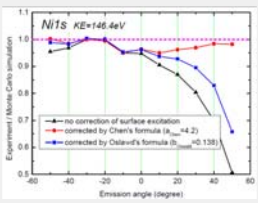
Surface excitation parameter (SEP)

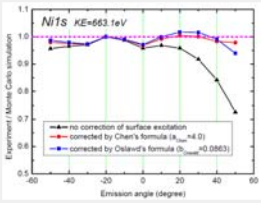
Chen's formula

$$P_s(E,\theta)=\frac{a_{Ch}}{\sqrt{E}\cdot\cos\theta}$$

Oswald's formula

$$P_s(E,\theta)=\frac{1}{b_{Os}\sqrt{E}\cdot\cos\theta+1}$$





Energy (eV)	Chen's parameter a
146.4	4.2
242.7	4.3
401.4	4.2
663.1	4.0
1094.6	3.8
1806	3.6
2979	1.5

Conclusion

Angular dependence of surface excitation for Ni was well described by not Oswald's formula but Chen's formula. Strictly speaking, dependence of SEP on electron energy was a little bit larger than Chen's formula.