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NATIONAL STANDARD OF THE PEOPLE'S REPUBLIC OF CHINA

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Surface chemical analysis - Electron spectroscopies - Minimum reporting requirements for peak fitting in X-ray photoelectron spectroscopy

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foreword

This document is in accordance with the provisions of GB/T 1:1-2020 "Guidelines for Standardization Work Part 1: Structure and Drafting Rules of Standardization Documents"

drafted:

This document is identical to ISO 19830:2015 "Surface Chemical Analysis Electron Spectroscopy X-ray Photoelectron Spectrum Peak Fitting Report"

this requirement":

This document adds a chapter "Normative References":

Please note that some content of this document may be patented: The issuing agency of this document assumes no responsibility for identifying patents:

Introduction

The X-ray photoelectron spectroscopy (XPS) spectra obtained on the surface of many materials are complex, and often contain overlapping or indistinguishable

peak: Insufficiency of resolution may be due to instrument parameters, X-ray linewidth, the natural linewidth of the transition, or a combination of all factors: therefore,

It is often necessary to mathematically fit some or all of the peaks in the XPS spectrum to determine the position of each component peak contained in the envelope of each peak:

placement and strength: Generating an overall peak envelope and quantifying the individual chemical states present is often the first step in the identification of chemical states: Therefore, divide

The analyst must confirm the position (for chemical state determination) and peak area (for accurate quantification) of each peak reported after the peak fit:

The mathematical method applies model peak and background shapes, and the defined

parameters are variable in order to obtain the best fit to the experimental data: Most common

The peak shape of the model peak is a combination of Gaussian and Lorentzian functions:

The parameters that should be reported after peak fitting are mostly those that define those curves: Other factors are selected by the analyst to ensure peak fit processing

The results conform to the chemically meaningful description of the peak envelope or minimize the time required for the fitting process: Actions performed by the analyst include:

--- select parameter values to be fixed in the fit;

--- Determine the range of variable parameter values in the fit;

--- Mathematically associate one parameter value with another parameter value:

Peak fitting is a purely mathematical process to obtain quantitative and qualitative results that may be related to the chemical properties of the analyzed surface: The fitting result will depend on

Depending on the analyst's choice of parameters and constraints, the choice can affect the analyst's interpretive conclusions from the peak fitting results: Therefore, report

These parameters and constraints are important: This will allow other analysts to do the following:

--- Assess the reliability and validity of conclusions drawn from peak fitting;

--- Repeating the peak fitting process on the same data set can get the same results;

--- Repeating the peak fitting process on data obtained from similar samples allows for efficient comparison of data sets:

Most software packages for XPS data processing include peak fitting routines: These programs allow the operator to select the appropriate parameters to

and fitting with the required constraints: It is likely that the software will provide an output that reports this information and facilitates copying for other

The output of the spectral fitting process: Such output will facilitate reporting of appropriate parameters:

This document does not provide instructions for XPS peak fitting or for correlating peak fitting processing results with the chemical properties of the surfaces being analyzed: fact

Above, in the examples in this document, the fit shown does not represent the only method by which a fit can be performed, or even the best method for peak fitting: This

These examples are for illustrative purposes only:

Surface Chemical Analysis Electron Spectroscopy X-ray

Basic Requirements for Peak Fitting Reports for Photoelectron Spectra

1 Scope

This document specifies how to report peak fits of X-ray photoelectron spectroscopy and their results:

This document applies to the fitting of a single spectrum or a set of related spectra, such as a set of related spectra acquired in a depth profiling test:

This document provides a list of parameters that should be reported in order to achieve reproducible peak fitting or to fit and compare multiple spectra:

This document does not provide operating instructions for peak fitting, nor the fitting steps that should be taken:

2 Normative references

There are no normative references in this document:

3 Terms and Definitions

The following terms and definitions apply to this document:

3:1

Inelastic background, inelastic

Due to single or multiple inelastic scattering processes, particles originally at one energy are now emitted at lower energies and appear more intense in the spectrum

degree distribution:

[Source: ISO 18115-1, 4:50]

3:2

Shirley background, Shirley

The background calculated when fitting the measured spectrum at kinetic energies above and below this peak or meaningful peak, such that the background at a given kinetic energy is the same as

The total peak area at higher kinetic energies above background is a fixed proportion of the composition:

[Source: ISO 18115-1:2010, 4:54]

3:3

Tougaard background,Tougaard

Intensities obtained using a differential inelastic scattering cross-section model with respect to energy loss and a three-dimensional distribution model of emitting atoms in the surface region

distributed:

[Source: ISO 18115-1:2010, 4:57]

3:4

passenergy

The average kinetic energy of the measured particle in the energy dispersive region located in the energy analyzer:

[Source: ISO 18115-1:2010, 4:325]

3:5

peak fitting

Steps to adjust the spectrum produced by peak synthesis to match the measured spectrum: