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XPS Study of Multilayer Multicomponent Films

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Abstract

In the paper, we propose an XPS-based quantitative method for depth profile analysis of chemical and phase composition of multi-component and multi-layer samples. The method includes: (1) new method for background subtraction accounting for depth non-uniformity of electron energy losses; (2) new method for photoelectron line decomposition into elementary peaks, which accounts for physical nature of the decomposition parameters; (3) joint solving of both background subtraction and photoelectron line decomposition problems; (4) criterion for assessing of line decomposition accuracy; (5) simple formula for layer thickness extraction for multi-element and multi-layer sample. We apply the developed method for analysis of multilayer niobium oxide and sub-oxide films before and in course of ion milling.

Keywords: XPS; Chemical and phase analysis; Depth profiling; XPS background subtracting; XPS line decomposition; Niobium oxide

1. Introduction

X-ray Photoelectron Spectroscopy (XPS) is one of the most demanded methods of the surface analysis [1]. XPS allows extracting elemental and phase composition of the analyzed surfaces. For that, after background subtraction, position of the peaks formed by inelastically and elastically scattered photoelectrons in the XPS spectrum is determined. Intensities of those peaks are interpreted into the relative concentrations of the elements. The standard method for interpretation of XPS data is based on the assumption about uniform distribution of the elements across the whole depth of analysis. However, in reality sample surface is always non-uniform and can be represented as consisting of layers. Failure to account for that leads to significant errors. For example, assume a sample has on its surface a layer of thickness d_1 of material other than the the rest of the sample. In such case, following the Bouguer law, intensity of the peaks formed by the photoelectrons under that surface layer will be reduced by the factor of $\exp(-d_1/\lambda_1)$, where λ_1 is electron mean free path in that surface layer. In case of XPS with Mg/Al-anode X-ray source, electron mean free path is of the order of a few nanometers. Consequently, even as thin as 1 nm surface layer will noticeably misrepresent the concentrations calculated by the standard mean concentration method.

For analysis of multilayer samples, more sophisticated calculation approach is needed. In paper [2], relationships for elements' relative concentrations in a layer were derived. However, for that one needs to assume the layer model and solve a non-linear system of equations for extracting of layer thicknesses. Analytic solution of such system of equations is pre-

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