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Applied Surface Science

Volume 257, Issue 3, 15 November 2010, Pages 887-898

Resolving surface chemical states in XPS analysis of first row transition metals, oxides and hydroxides: Sc, Ti, V, Cu and Zn

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<https://doi.org/10.1016/j.apsusc.2010.07.086>

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Abstract

Chemical state X-ray photoelectron spectroscopic analysis of first row transition metals and their oxides and hydroxides is challenging due to the complexity of the 2p spectra resulting from peak asymmetries, complex multiplet splitting, shake-up and plasmon loss structure, and uncertain, overlapping binding energies. A review of current literature shows that all values necessary for reproducible, quantitative chemical state analysis are usually not provided. This paper reports a more consistent, practical and effective approach to curve-fitting the various chemical states in a variety of Sc, Ti, V, Cu and Zn metals, oxides and hydroxides. The curve-fitting procedures proposed are based on a combination of (1) standard spectra from quality reference samples, (2) a survey of appropriate literature databases and/or a compilation of the literature references, and (3) specific literature references where fitting procedures are available. Binding energies, full-

width at half maximum (FWHM) values, spin-orbit splitting values, asymmetric peak-shape fitting parameters, and, for Cu and Zn, Auger parameters values are presented. The quantification procedure for Cu species details the use of the shake-up satellites for Cu(II)-containing compounds and the exact binding energies of the Cu(0) and Cu(I) peaks. The use of the modified Auger parameter for Cu and Zn species allows for corroborating evidence when there is uncertainty in the binding energy assignment. These procedures can remove uncertainties in analysis of surface states in nanoparticles, corrosion, catalysis and surface-engineered materials.



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Keywords

XPS; Peak fitting; Transition metals; Oxides

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