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Fitting Strategies for Metallic and Partially Oxidized Al 2p Spectra Containing Suboxides.

Aluminum, a reactive metal, rapidly reacts with oxygen to form a protective aluminum oxide layer. It has three electrons in its valence shell, allowing it to form oxidation states of Al+1 and Al+2, with Al+3 being the most stable oxidation state.

Film deposition of metallic aluminum (99.99% pure aluminum pellets from Sigma Aldrich) through thermal sublimation under ultra-high vacuum conditions was done on silicon substrates (100). The background pressure in the processing chamber was 1.5×10-7 Torr and the pressure during sublimation was 6.5×10 6 Torr. The initial oxidation stages were achieved by exposing the surface to a precisely controlled ultra-pure oxygen atmosphere with varying gas dosages from 1 ×103 L to 1×107 L (1 L ≡ 1×10 6 [Torr][s]). The metallic and oxidized film was characterized using an X-ray photoelectron spectroscopy (XPS) instrument with a monochromatic source (1487.6 eV, XR5 from ThermoFisher) and a 7-channeltron hemispherical spectrometer (Alpha110, from ThermoFisher) assembled by Intercovamex.

Robust analysis techniques for peak fitting ARXPS data from Al 2p and O 1s, including the block approach and simultaneous fitting, as well as background modeling with the active approach, Shirley-Vegh-Salvi-Castle (SVSC), and the Two-Parameter Tougaard background [1], were employed to determine the chemical composition and surface structure during the initial stages of oxidation of pure metallic aluminum samples. It was observed that the layer oxide growth model incompletely replicates the behavior seen in ARXPS spectra, whereas the growth behavior of oxides through protrusions with aluminum sub-oxides does. The oxidation of metallic aluminum involves the formation of an Al+3 oxide layer along with deep protrusions and an Al+1 and Al+2 interface layer between the metallic aluminum and the protrusions.

Keywords

Photoemission Spectra, Chemical Composition, Peak Fitting

Reference

[1] A. Herrera-Gomez, M. Bravo-Sanchez, O. Ceballos-Sanchez, M.O. Vazquez-Lepe, Practical methods for background subtraction in photoemission spectra, Surf. Interface Anal. 46 (2014) 897–905.

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Author approval

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