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Perspective article

A perspective on two chemometrics tools: PCA and MCR, and introduction of a new one: Pattern recognition entropy (PRE), as applied to XPS and ToF-SIMS depth profiles of organic and inorganic materials

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ABSTRACT

X-ray photoelectron spectroscopy (XPS) and time-of-flight secondary ion mass spectrometry (ToF-SIMS) are much used analytical techniques that provide information about the outermost atomic and molecular layers of materials. In this work, we discuss the application of multivariate spectral techniques, including principal component analysis (PCA) and multivariate curve resolution (MCR), to the analysis of XPS and ToF-SIMS depth profiles. Multivariate analyses often provide insight into data sets that is not easily obtained in a univariate fashion. Pattern recognition entropy (PRE), which has its roots in Shannon's information theory, is also introduced. This approach is not the same as the mutual information/entropy approaches sometimes used in data processing. A discussion of the theory of each technique is presented. PCA, MCR, and PRE are applied to four different data sets obtained from: a ToF-SIMS depth profile through ca. 100 nm of plasma polymerized C_3F_6 on Si, a ToF-SIMS depth profile through ca. 100 nm of plasma polymerized PNIPAM (poly (*N*-isopropylacrylamide)) on Si, an XPS depth profile through a film of SiO_2 on Si, and an XPS depth profile through a film of Ta_2O_5 on Ta. PCA, MCR, and PRE reveal the presence of interfaces in the films, and often indicate that the first few scans in the depth profiles are different from those that follow. PRE and backward difference PRE provide this information in a straightforward fashion. Rises in the PRE signals at interfaces suggest greater complexity to the corresponding spectra. Results from PCA, especially for the higher principal components, were sometimes difficult to understand. MCR analyses were generally more interpretable.

1. Introduction

Material characterization and analysis play a central role in the advancement of essentially all materials, i.e., in the semiconductor industry [1], and for nanomaterials [2], separation devices [3,4], data storage materials [5], hydrophobic coatings, [6] etc. For many materials, the most important area of interest is its *surface* because the surface, based on its physical and chemical properties, interacts directly with its surroundings. For example, catalysis, tribology, wetting, adhesion, corrosion, adsorption, biological signaling and transport, separation science, device failure, and sensing often depend on what is happening in the outermost 0.1–1 nm of a material. Different analytical techniques provide information about surfaces at different length scales. X-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy (AES) probe ca. 0.5–10 nm into surfaces, time-of-flight secondary ion mass spectrometry (ToF-SIMS) is sensitive to ca. 2–3 nm into a material, and low energy ion scattering (LEIS) [7,8] is sensitive to the outermost monolayer of a material. Very often it is a combination of analyt-

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