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Computer simulation of XPS analysis of nanocomposite metal/plasma polymer thin films

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X-ray photoelectron spectroscopy is a widely used technique for analysis of thin films. Most of the XPS signal comes from the depth of the first few nanometers, where the relative elemental composition of the film can be directly measured, but the bulk properties of the film is much harder to obtain using XPS. This is particularly true in the case of nanocomposites, where the "matrix" often overcoats the top layers of the "filler" and the elemental composition of the films obtained by XPS underestimates the amount of filler. Finding a dependence of the apparent XPS composition of the film on the real bulk filling factor and size of the filler nanoparticles would be beneficial.
The authors have developed two computer models that simulate the apparent XPS signal of the matrix and of the filler in the form of nanospheres. Both models use a simulated structures of the film that is randomly generated for various combination of filling factor and size of the particles. The current study is focused on metal/plasma polymer nanocomposite films. The models take into account differences in the electron mean free path in various materials, random positions of the particles of the filler and their size distribution.
The simple geometrical model is based on the calculation of the volume of the filler in the matrix in several consecutive horizontal "cuts" of the films, each being taken into account with some effective electron mean free path coefficient. The total XPS intensity ratio of the filler vs. matrix is then calculated.
The second model directly calculates the intensity of each element of the film by virtual "probing" the film in an evenly-spaced grid. The intersections of the probing line with the edges of the nanoparcticles are calculated and the signals of each materials along the probing line are integrated.
The results of the simulations are compared with experimental data obtained using various methods on a model plasma polymer / metal system.

Keywords
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