Development of a self-consistent approach to study the 3D morphology of a thin film

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Two pertinent problems often arise when studying the morphology of a thin film exposed to treatments such as growth, ion erosion, or oxidation: (a) the evolution of the film roughness during process and (b) the evolution of the depth-distribution of the dielectric constant of the film. Formerly, these problems were solved independently using simplified assumptions. To perform a quantitative analysis of the film roughness it is typically assumed that (a) the film density is constant over depth and (b) the substrate roughness remains unchanged during film growth or erosion. However, reality might contradict each of these assumptions. Likewise, during the reconstruction of the dielectric constant profile from X-ray scattering measurements, the effect of interfacial roughness on the reflectivity is usually neglected or described in a simplified manner, e.g., by introducing Nevot-Croce or Debye-Waller factors to modify the contribution of each interface to the amplitude reflectivity.

While roughness influences the reflectivity of a thin-film, a variation of the dielectric constant with depth will also modify the wave field inside the film and, hence, alter the scattering pattern. In this respect, questions arise (a) regarding the modification of the depth-distribution profile of the dielectric constant extracted from reflectivity measurements when taking roughness into consideration and, conversely (b) regarding the modification of the film roughness parameters when accounting for the depth-distribution of the dielectric constant.

In this paper, we investigate the possibility of extracting film morphology information at the same time over depth (reconstruction of the dielectric constant profile) and in the lateral direction (roughness parameters). The approach is based on a simultaneous analysis of the reflectivity curve and of a set of scattering diagrams measured at various grazing angles of an X-ray probe beam. A computational iterative procedure has been developed, which considers the roughness effect during reconstruction of the dielectric constant profile and, vice versa, the depth-distribution of the dielectric constant during determination of the Power Spectral Density functions describing the film roughness. Using this approach, the quantitative analysis of the morphology of a tungsten film after growth, erosion, and oxidation will be presented. The iterative procedure will be demonstrated to converge quickly allowing to describe precisely the whole set of experimental data.