

Ion Beam Induced Effects in Sputter Depth Profiling

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Summary: Sputter depth profiling /1/ has become one of the main areas for the use of surface analysis instruments such as AES, XPS, SIMS etc. because they are either operating with a primary ion beam (SIMS) or they can be easily combined with that facility (AES, XPS). Understanding the principle of the technique of sputter depth profiling is rather straight forward: Similar to sand-blasting in surface finishing of machinery parts, energetic particles impinging on a solid material abrade a thin surface layer of it and expose the deeper lying layers. In case of ion (or atom) bombardment this process is called sputtering.

It is obvious that there are two ways of getting analytical information about the composition of a sample as a function of depth, i.e. the depth profile: Either we analyze the material sputtered away (e.g. in SIMS, SNMS) or we analyze the newly generated (instantaneous) surface (e.g. in AES, XPS) as a function of the ion dose or -for constant ion current density- of the sputtering time. If the measured elemental signal intensity is proportional to the concentration in the first atomic layer and sputtering would proceed in a layer-by-layer fashion with constant sputtering rate (=idealized depth profiling), the measured raw data (i.e. elemental intensity as a function of sputtering time) already would be proportional to the in depth distribution of the respective element. To obtain a quantitative result, we only need two "sensitivity" factors: one for the calibration of the concentration scale (e.g. counts per second for one atomic percent of the respective element in a certain matrix) and one for the calibration of the depth scale (e.g. in seconds of sputtering time for 1 nm sputtered depth). The result obtained in this way is at best approximately correct. In general there exists a considerable deviation between the measured profile and the true, original depth distribution.

The above mentioned difference has many causes which can be categorized in instrumental factors, ion-solid interaction effects (and effects depending on the peculiar nature of the sample). For example, instrumental factors are

insufficient vacuum, wrong adjustment of the analyzed spot and sputtered area, varying ion current density in the latter etc.. Special sample characteristics which often cause insurmountable obstacles for successful profiling are, for example, lateral inhomogeneities (precipitates), electrically insulating properties, high sensitivity to electron and ion bombardment and to slight temperature increase which enhances pronounced effects of diffusion, segregation and decomposition.

Most important for the correct interpretation of depth profiling data and their quantification is consideration of the fundamental effects of ion beam-sample interaction which may cause change in composition and topography ("roughness"). /1/ When an energetic ion hits the sample surface, it penetrates into the sample by pushing away the sample atoms, very similar to billiard game hard ball interactions. If the displaced atoms have enough kinetic energy, they may cause displacement of another sample atom by hitting it and so forth. In each step, a characteristic amount of energy is lost and further displacement stops when the energy transferred is below the threshold displacement energy (typically 15-25 eV). The direction of momentum transfer depends on the Rutherford scattering parameter and is quickly randomized. Therefore, a certain probability exists that momentum is transferred to an atom in the surface layer in the direction away from the surface. If the transferred energy is

above the surface binding energy (typically 1-3 eV), this surface atom leaves the surface, it is sputtered away. One can easily imagine that the fraction of the totally dissipated energy which is used for sputtering is rather small, usually about a few percent or less. The main amount of the ion energy ends up in defect formation, which cause a practically random displacement in the collision cascade described above. This nearly random displacement is therefore called mixing or atomic mixing.

Of course, vacancy and interstitial defect formation at first means breaking up of chemical bonds which may lead to decomposition of chemical compounds (and/or to the formation of new ones). Furthermore, it causes radiation enhanced diffusion which enhances atomic mixing, i.e. randomizing the concentration within the mixing zone. However, if there exist other chemical driving forces such as interfacial free energy of segregation for one component, the respective element is enriched at the outer surface (or at the inner interface with the undistorted bulk). The case of surface segregation is often found to occur together with preferential sputtering of the component, causing a typical elemental distribution within the mixing zone with a minimum below the first surface layer /2/.

Ion beam induced topographical effects are a frequently observed source of depth resolution degradation in depth profiling. /3/. Two different phenomena can be distinguished: First, the fundamental effect of the statistical nature of sputter emission and secondly the effect of local variations of the sputtering yield within the analyzed spot. The latter are mainly due to crystalline orientation in polycrystalline metallic materials or to any kind of other structural or chemical defects, even in single crystals. Generally, the crystalline effect induced roughness increases with sputtered depth and leads to typical interface broadening of more than 10 nm. It is effectively diminished by high ion incidence angle (>70 deg.) or completely reduced by using sample rotation during

profiling /3/. In contrast, the statistical sputtering induced roughness saturates after an initial increase at typical values of about 2-5 monolayers, i.e. 0.5-1.5 nm. Therefore, it is only of importance in very high resolution depth profiling.

Knowledge of how the above mentioned effects show up in depth profiling results is necessary for theoretical modeling the depth resolution function which can be used for deconvolution or reconstruction of the original distribution by measured profile simulation /4,5/. Recently, a simple model based on the three most important parameters atomic Mixing, Roughness and Information depth (MRI-model) was successfully tested for AES depth profiles of GaAs/AlAs superlattice structures /5/.

During the past two decades, many researchers have contributed to an improved understanding of ion beam induced effects in sputter profiling. Although the more complicated effects of the interplay of mixing, radiation enhanced diffusion and segregation are not yet sufficiently well understood, the currently attained state of knowledge allows general predictions for optimized sputter profiling conditions with respect to specific samples /1/.

References:

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