Argon Monatomic and Gas Cluster Ion Beam XPS Depth Profiling of Metal Oxides and GaAs: Experimental and Modelling Studies

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Metal oxides are employed as thin films and coatings for electronic, optical, catalytic, sensor, tribological, biomedical etc. applications. Determination of the chemical composition of such thin films and coatings as a function of depth by XPS depth profiling is very important in optimising growth conditions and properties. However, the use of monatomic argon ion beams to generate the XPS depth profile is well known to result in preferential sputtering of oxygen for most metal oxides. It has generally been regarded by the XPS community that the degree of preferential sputtering of during depth profiling cannot be reliably predicted. TRIDYN is a Monte Carlo program based on the binary collision approximation, which models the Ar⁺ ion beam induced sputtering and considered both mass difference effects and surface binding energies. The TRIDYN code has been modified to consider the effect of attenuation length affecting the XPS analysis depth of different compounds. XPS depth profiles at Ar⁺ incident energies of 500 eV and 3 keV have been compared with TRIDYN simulations for different metal oxide thin films: TiO₂, V₂O₅, Nb₂O₅, Ta₂O₅ and Al-doped ZnO. The results show good agreement between the experimental and simulated results.

GaAs is an important bulk and thin film semiconductor material for functional devices. The preferential sputtering of As under argon gas cluster ion beam (GCIB) bombardment with argon clusters of different average energy per atom (E/n) has been studied. Molecular Dynamics (MD) modelling has also been performed. GCIB conditions for minimising As preferential sputtering and observed changes in surface morphology following GCIB bombardment will be discussed.