PLATHINIUM
PLASMA THIN FILM INTERNATIONAL UNION MEETING
13-17 September 2021
VIRTUAL MEETING
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GROM / Thin films growth and modelling

Multi-scale modelling of sputtered deposited TiN, ZrN, HfN and TiAlN thin films at oblique angle incidence

C. Mastail, R. Mareus, F. Nita, A. Michel, G. Abadias
Institut Pprime, UPR 3346, CNRS-Univ. Poitiers-ENSMA, Poitiers (FR)

Abstract content

The deposition of thin films by condensation of vapor fluxes at oblique angles (oblique angle deposition (OAD)) leads to the development of columnar, tilted columns, large porosity and increased specific surface area. This route is advantageous for applications in optics, catalysis or bio-sensors. The work carried out here aims to better understand the influence of the angle of incidence and the deposition parameters (pressure P, temperature T) on the morphology of thin films of transition metal nitride (TMN) deposited by OAD. The employed methodology relies on both experimental (reactive magnetron sputter-deposition) and multi-scale computational modelling (DFT calculations and Monte Carlo codes; SRIM, SIMTRA and MODENA). The studied systems are group IVb binary TMNs (TiN, ZrN, HfN) and the ternary alloy TiAlN, promising materials for plasmonic applications. The crystal structure, texture and growth morphology are studied by X-ray diffraction, SEM and AFM imaging, and some of their properties (electrical resistivity and wettability) evaluated. The films exhibit a strongly columnar growth, and a biaxial crystallographic texture corresponding to the formation of pyramidal facets. The inclination angle of the columns b increases with the inclination angle of the substrate a and is correlated to the inclination angle y of the (111) crystal planes. The greatest variations are observed for HfN due to a more directional flux of particles. In the case of TiN, the relation b (a) shows a saturation phenomenon for a> 65 ° for high pressure , and a shift of + 10 ° when T increases from 25 ° to 500 ° C. The use of the MODENA code, based on a kinetic Monte Carlo model on a rigid lattice, and including deposition and diffusion events, makes it possible to qualitatively reproduce the trends observed experimentally, and highlights the preponderant role of the angular distribution of the particle flux on the tilt of the columns. DFT calculations are performed on ZrN and HfN systems to determine the energy landscape of (100) and (110) surfaces providing access to adsorption sites and diffusion barriers of metallic and nitrogen species, comparatively to TiN. These data show greater diffusivity on the (100) surface than on (110) one, and a different surface reactivity of nitrogen depending on the chemical and crystallographic nature of the system. The knowledge gained from these DFT calculations will subsequently improve the MODENA code by considering the specific energy barrier values for each studied system.