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Simulations of oxide films growth deposited by magnetron sputtering and evaluation of their morphology and optical properties

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Introduction

In order to simulate the growth of oxides thin film by vacuum deposition methods, a model based on kinetic Monte Carlo (kMC) approach on a three-dimensional lattice has been developed. The model takes into account deposition of different species, metallic and reactive. Both metallic and reactive fluxes may consist of atoms as well as ions having their own energy and angular distributions. Effects of deposition of energetic particles are also taken into account. These effects are energy transfer from the projectiles to the film, sputtering of the film as well as re-deposition.

Simulation model

 Deposition of two species with their own specific fluxes

Film morphology \rightarrow optical properties

Simulation of TiO₂ film growth by magnetron deposition on non flat substrate

- Deposition of energetic particles energy transfer to the film
- Characterization of the film density, roughness, X-ray diffraction, reflectance

In order to get:

- Film structure
- Morphology
- Properties (roughness, hardness, optical properties, ...)



Experiments (left) by J.Dervaux et al. (Umons). Simulations (right) by NASCAM



- Number of atoms: up to 10^7 ;
- Substrate size: up to 100x100 nm²;
- Simulation time: 1 day in a ballistic mode for maximum of simulation parameters.





Oxide mode

Upper right

Plasma simulations + Film growth simulations + Film analysis

Center,



TiOx optical properties vs film morphology



Upper right, porosity = 4%porosity = 15%



Evolution of morphology with oxidation degree









 O_2 inlet flow : 2sccm; Incident flux: O/Ti = 0.5Porosity = 7%

 O_2 inlet flow : 4sccm; Incident flux: O/Ti = 6.5Porosity = 7% O_2 inlet flow : 6sccm; Incident flux: O/Ti = 50Porosity = 11%

 O_2 inlet flow : 8sccm; Incident flux: O/Ti = 8700 Porosity = 15%

The tilting angles become smaller with the rise of a partial oxygen deposition flux .

- Ti flux is directional
- Oxygen flux is uniform.
- \rightarrow High partial oxygen coatings have lower directionality





Conclusions

A three-dimensional kinetic Monte Carlo code has been developed to simulate the growth of non metallic thin film by vacuum deposition methods and evaluation of film properties. Comparison with TiO₂ films deposited by magnetron sputtering was chosen. The presented model is able to predict the stoichiometry of the film as well as its morphology as a function of the parameters of Ti and O flows to the substrate and the relative amount of oxygen in the deposition chamber. It is shown that the metallic flux forms the skeleton of the structure and the flux of a reactive gas serves for its « decoration » and only slightly influences the final morphology.

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