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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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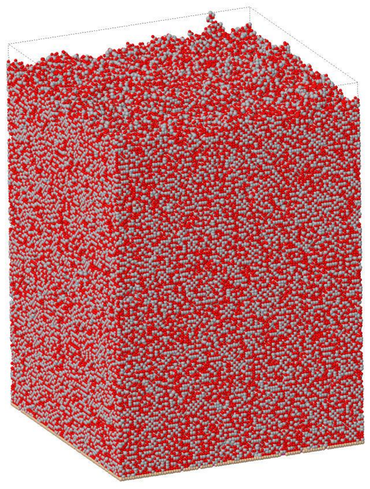
Introduction

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.

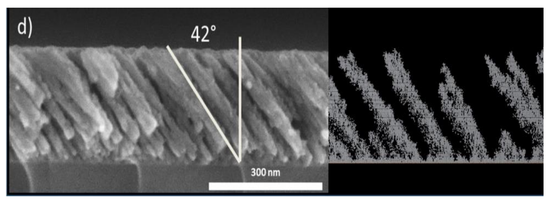
Simulation model

- Deposition of two species with their own specific fluxes
- 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, …)

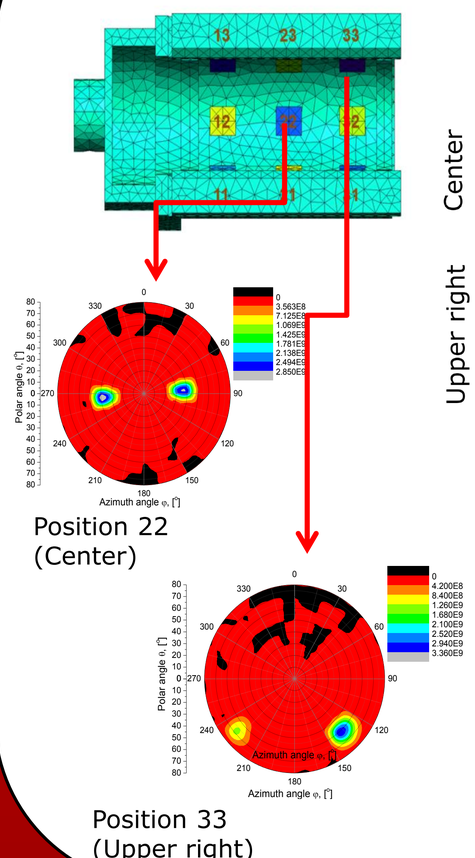


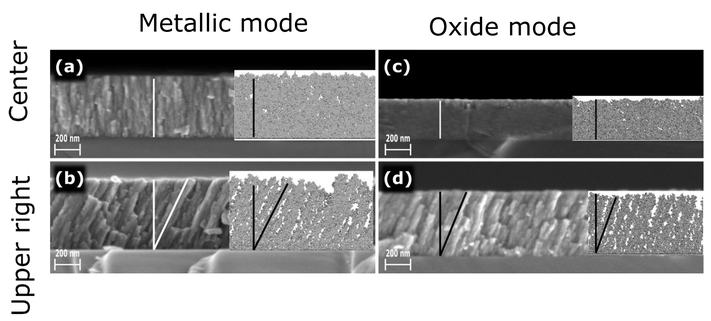
- Number of atoms: up to 10^7;
- Substrate size: up to 100x100 nm^2;
- Simulation time: 1 day in a ballistic mode for maximum of simulation parameters.

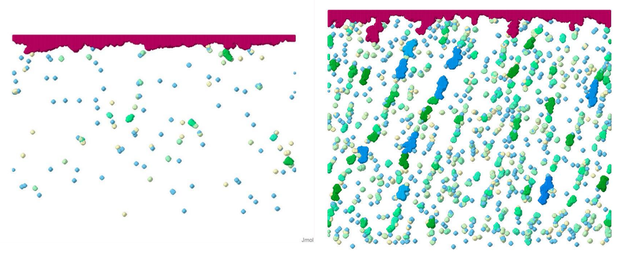
Experiments (left) by J.Dervaux et al. (Umons).
Simulations (right) by NASCAM

Film morphology → optical properties

Simulation of TiO_2 film growth by magnetron deposition on non flat substrate

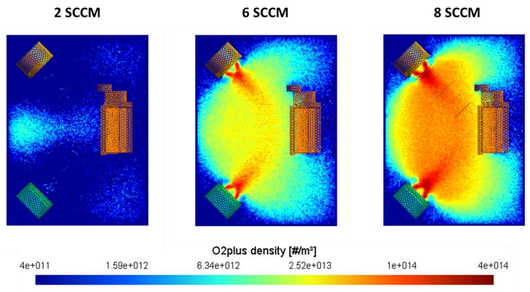




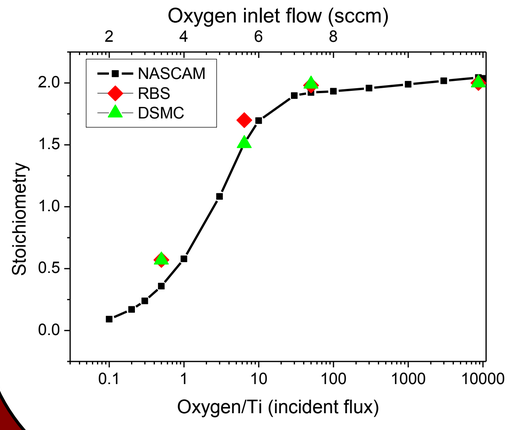


Plasma simulations + Film growth simulations + Film analysis

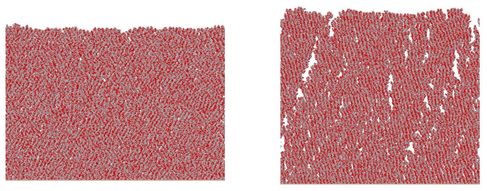
TiOx film stoichiometry vs Oxygen inlet flow



DSMC simulations: software from A. Pflug, IST, Germany



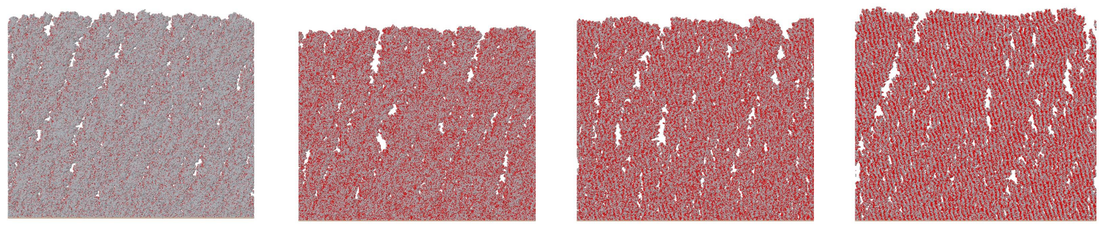
TiOx optical properties vs film morphology



Center,
porosity = 4%

Upper right ,
porosity = 15%

Evolution of morphology with oxidation degree



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

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

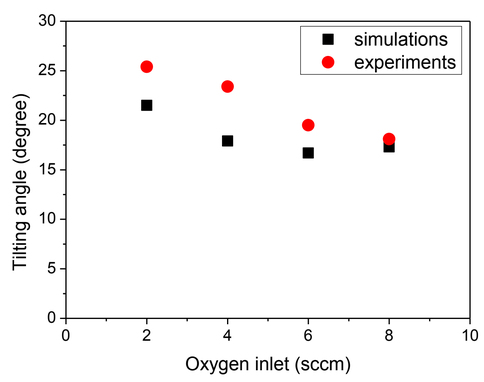
O_2 inlet flow : 6sccm;
Incident flux: O/Ti = 50
Porosity = 11%

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.

→ 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 TiO_2 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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