PO1006

Kinetic Monte Carlo simulations of thin film growth deposited by reactive magnetron sputtering and evaluation of morphological properties of the film.

Pavel Moskovkin, Romain Tonneau, Stephane Lucas

University of Namur, Namur, Belgium

pavel.moskovkim@unamur.be

A three dimensional kinetic Monte Carlo (kMC) model has been developed in order to simulate the growth of oxides thin film by vacuum deposition methods. The model takes into account simultaneous deposition of metallic and reactive species. Both metallic and reactive fluxes may consist of atoms as well as ions, each flux is characterized by its own energy and angular distributions.
During the simulation of deposition particles (metallic and reactive atoms and their ions) are considered to be randomly thrown towards a substrate with the velocity according to given energy and incident angle distribution functions. Metallic atoms are supposed to be attached with the sticking probability equals to 1. Sticking coefficient of reactive species depends on the local stoichiometry around the location where the reactive atom hit the film. Reactive atoms are supposed to be attached only if the local composition of the film is under stoichiometric. Effects of momentum transfer from the energetic particles to the film are also taken into account.
The presented kMC model has been applied to the growth of TiO_2 film deposited by a magnetron sputtering on a curved substrate. The properties of the film have been studied at different locations at the substrate. It has been showed that the morphology of the film is the function of the position on the substrate. Depending on the position the film can either exhibit tilted columnar growth or not. Also it has been shown that the roughness of the film is not uniform across the substrate but depends on the location. The simulation results have been compared with the experimental data and the good agreement between them has been found.

Keywords
kinetic Monte Carlo
simulations
film growth
reactive sputter deposition
Titanium oxide