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Simulation of thin film growth as deposited by magnetron sputtering and evaluation of their morphology, optical and mechanical properties

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Among the computational methods to mimic real experiments, one can cite Kinetic Monte Carlo (kMC) that has been well described by many authors. kMC can be used for the modeling of different processes at the surface such as growth of films during deposition, post deposited development of films, etc at atomic scale level.
A three dimensional kMC code (called NASCAM – Nano SCAle modelling) has been developed [1, 2] for simulations of deposition and evolution of surface structures at room and elevated temperatures. The code includes simultaneous deposition of atoms of different kinds. It takes into account angular and energy distribution of depositing species as well as energy transfer effects during the deposition. Substrate can be specified as a squared or a hexagonal lattice, textured or not, and angular and energy distribution of incident deposited atoms can also be varied. Substrate is necessarily fixed. It can be rotated or undergo oscillations which is especially helpful for simulating film growth at glancing angle deposition. Also the code can be used to simulate the multilayer growth.
In the present work, we present the latest development and their benchmarking with experimental data. The main results will be focussed on the method developed to evaluate how the deposition conditions affect mechanical properties of Ti films deposited by HIPIMS and DC magnetron, on the optical properties of Si/Mo multilayered EUV films and on the porosity of Glancing Angle Deposited Ti and TiO2 films.
References

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