Atomistic modelling of thin film growth with realistic input data obtained from reactor-scale process simulation

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ABSTRACT

Low pressure thin film deposition processes such as magnetron sputtering involve different physical mechanisms acting on vastly different time and length scales. The global process kinetics of the reactor and spatial distributions of film thickness and film stoichiometry can be usually described within particle based or continuous models of gas and precursor transport and plasma discharge [1]. In contrast, predicting the intrinsic properties of the growing film such as crystalline phase composition, morphology etc. requires to apply computational material modelling on atomistic scale. For realistic predictions of the film structure by atomistic modelling it is crucial to provide realistic input data in terms of particle fluxes, as well as their energy and angular distribution functions. By setting up a multi-scale simulation chain it is possible to feed the output of reactor scale simulation into atomistic models [2]. Using this multi-scale approach we present atomistic computations of intrinsic TiO₂ films grown by reactive magnetron sputtering. Molecular Dynamics [2] and kinetic Monte Carlo method [3] are applied with initial conditions obtained from different process conditions by particle-based reactor scale modelling. The results are compared with scanning electron and atomic force microscopy of the film morphology and surface texture.

REFERENCES