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Study of continuous and pulsed deposition of thin metal films by atomistic computer modelling

Rudolf Hrach[1], Vera Hrachova[1]

[1]Charles University, Prague 8, Czech Republic

rudolf.hrach@mff.cuni.cz

When depositing thin metal films on dielectric substrates, the three-dimensional island growth occurs. The complete growth mechanism involves a number of atomic scale processes, both increasing the speed of growth and decreasing it, resulting even in dissolution of small clusters. By decreasing the temperature or increasing the deposition rate the nucleation rate of the clusters can be increased and vice versa. Besides these two basic experimental parameters, there exist further physical parameters as kinetic energies of impinging atoms, state of the substrate, etc., one of the most important being the duration of the evaporation process. This idea is used in the pulsed laser deposition and pulsed plasma deposition techniques, which belong to important technologies. When analyzing these techniques, it was found that the computer simulation, especially the kinetic Monte Carlo method, is extremely useful for the study of growth processes on a microscopic level.
The present contribution is devoted to the study of physical processes taking place during thin film growth by an atomistic computer modelling. The basic technique is the kinetic Monte Carlo approach, used both for the preparation of simulated structures and for their analysis. Information about some processes for the stochastic description of film growth are taken from the literature, the most important parameters, however, are calculated by the molecular dynamics simulation and used as input data for the Monte Carlo model. The main purpose of this study is the discussion of basic mechanisms of the initial stages of film growth in both continuous and pulsed regimes.

Keywords
pulsed deposition
continuous deposition
film growth
atomistic modelling