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Computational study of pulsed depositions of metal films

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When depositing metal films on dielectric substrates, a three-dimensional growth occurs. The complete mechanism involves a number of atomic scale parameters, the basic being substrate temperature and deposition rate. Besides them the kinetic energies of impinging atoms, state of the substrate and the duration of the evaporation process are important physical parameters. This idea of variable deposition times is applied in the pulsed laser deposition and pulsed plasma deposition technologies. The type of deposition technique influences profoundly the composition and energies of impinging particles.
For the study of initial growth stages the combination of experimental and computational approaches is very useful. The contribution is devoted to the analysis of main physical processes taking place during nucleation and early stages of film growth. For this purpose two methods of computational physics were applied - atomistic computer simulation and image processing of micrographs of resulting films. In the atomistic modelling of metal film growth the combination of two techniques was used: the nucleation process and the initial island growth were simulated by the molecular dynamics approach, while the simulation of further growth stages was performed by the kinetic Monte Carlo method. The combined molecular dynamics & kinetic Monte Carlo approaches were used both for the preparation of simulated structures and for their analysis. The further approach of computational physics was the image analysis, applied both on the results of simulation and on experimental data. The main purpose of this study was to analyse the influence of basic mechanisms of the initial stages of film growth in both continuous and pulsed regimes. The main differences in laser deposition or vacuum evaporation and plasma deposition techniques are included into the molecular dynamics part of the complete atomistic model.

Keywords
pulsed plasma deposition
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image processing