Simulation study of nucleation, growth and coalescence of palladium nano- clusters on thin film of MgO(100)

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Abstract

The dynamic process of the formation of the system Pd /thin MgO (100) surface is investigated by developing many programs using Fortran software. This simulation is based on rate equations and includes processes of nucleation, surface diffusion of adatoms, growth and coalescence of islands in the case of thin films growth in Volmer–Weber mode. The nucleation kinetics is interpreted according to the theory of random nucleation. It shows a good agreement with the experimental result time dependencies of island density. The phenomenon of coalescence is explained via island migration process. It is essentially described by surface atom diffusion and the surface coverage. It is important to notice the influence of the deposition temperature, which modifies the clusters coalescence time. It is clearly seen that the coalescence occurs more rapidly when the substrate temperature is high.

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