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Kinetic Monte Carlo Simulation of Metallic Nanoislands Grown by Physical Vapor Deposition

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Abstract. We report kinetic Monte-Karlo (KMC) simulation of self-assembled synthesis of nanocrystals by physical vapor deposition (PVD), which is one of most flexible, efficient, and clean techniques to fabricate nanopatterns. In particular, self-assembled arrays of nanocrystals can be synthesized by PVD. However size, shape and density of self-assembled nanocrystals are highly sensitive to the process conditions such as duration of deposition, temperature, substrate material, etc. To efficiently synthesize nanocrystalline arrays by PVD, the process control factors should be understood in detail. KMC simulations of film deposition are an important tool for understanding the mechanisms of film deposition. In this paper, we report a KMC modeling that explicitly represents PVD synthesis of self-assembled nanocrystals. We study how varying critical process parameters such as deposition rate, duration, temperature, and substrate type affect the lateral 2D morphologies of self-assembled metallic islands on substrates, and compare our results with experimentally observed surface morphologies generated by PVD. Our simulations align well with experimental results reported in the literature.

AMS subject classifications: 82B24, 82B26, 82D20, 82D25, 82D80

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1 Introduction

Thin film technology is the underlying basis of a wide range of applications ranging from microelectronics to the emerging field of nanotechnology. In particular, self-assembly of

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nanoscale metallic islands on various crystalline materials, or amorphous substrates such as SiO_2, present a strong interest for nanotechnology applications. However, synthesis of functional crystalline nanostructures require a fine control of the nanocrystalline morphology for which, in turn, the dependence of the morphology on the deposition process conditions should be well understood.

The basic physical mechanisms behind the nucleation and growth of deposited films have been extensively addressed in the literature. At the early stages of deposition, incident atoms randomly impinge on the substrate at a given rate, and then the adsorbed atoms can re-evaporate, aggregate, or diffuse [1]. Coalescense of adatoms results in nucleation of tiny nanoislands on the substrate. Islands containing more adatoms than a critical nucleation number [2, 3] give rise to relatively stable nanocrystals, whose size increases due to the arrival of new adatoms at the surface [4]. The evolution of growing islands can be described by kinetic rate equations [4, 5]. For relatively early stages of deposition, some of the rate equations can be solved analytically. The corresponding solutions, known as scaling laws, relate the number density of stable nuclei with the various process and material parameters, as it has been addressed in detail by Venables and coworkers [4–7]. For example, the density of stable islands N in a hypothetical steady state regime is given by,

$$N = An_0 \left(\frac{R}{v}\right)^p \exp\left(\frac{U}{kT}\right), \tag{1.1}$$

where A is a dimensionless constant, n_0 is the density of adsorption sites at the surface, R is the deposition rate in ML/sec, v is the fundamental frequency, T is temperature, U is the activation energy, and the power p is a parameter depending on the critical nucleation size i. The asymptotic dependence of p on i is usually described by $p = i/(i+2)$ [7,8].

The scaling laws have proven to describe well the density of stable nuclei at early stages of deposition. Of major interest for applications, however, are detailed morphologies that develop at later stages of the process, when the nuclei grow into nanocrystalline islands. Thus, the experimental morphologies shown in Figs. 1 and 2 demonstrate that the shape of deposited metallic islands depends of the substrate. As it can be seen in Fig. 1, under typical conditions, metal islands deposited by PVD techniques on amorphous substrates such as SiO_2 undertake smooth droplet-like shapes [9]. At later stage of deposition, some of these patterns resemble percolation networks (see the last picture of Fig. 1(a)). In contrast, when a metal is deposited on a crystalline substrate [10–12], the islands adopt more regular "crystal-like" shapes, as shown in Fig. 2. The crystalline morphology persists when temperature increases, which is evident form the images in the figure. It is clear that such differences cannot be captured by the density and/or the average size of islands provided by the scaling laws, and require a more detailed consideration. With continuing deposition, the islands start merging and the pattern evolves into a continuous thin film. These late stages of nanocrystalline synthesis also require appropriate simulation approaches capable to account for the changing surface morphology.