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Abstract. Our aim is to we review different models of surface growth processes. Then we focus on the calculation of the surface roughness for the amorphous thin film growth represented by a one-dimensional deterministic field equation. On the base of numerical simulations, better understanding of the amorphous thin film growth process is available. The temporal evolution of the surface roughness of the surface morphology with parameter data has been presented. The effect of the parameter is significant on the height profile, on the mean average height profile and on the surface roughness.

INTRODUCTION

Surface roughness has a huge impact on many important phenomena. Typical examples of spatiotemporal pattern formation in systems driven away from equilibrium can be found in physical, chemical and biological processes such as in hydrodynamic systems in pure fluids and mixtures, in patterns of solidification fronts, in optics, in chemical reactions and in excitable biological media [1]. While on micro- and macro scales one can control the processes by special devices, on nano scales such instruments are absent or their use is extremely expensive. Therefore, the investigation of self-organization and self-assembly provide promising mode to understand basic physical principles and mechanisms. The understanding of these processes can allow us to extend the use of such technique to a large variety of fabrication processes, to create new electronic devices, sensors and tailored surfaces; moreover, to controllably modify chemico-physical properties of the surface by tailoring the nanoscale morphology during patterning and to optimize certain film properties like roughness and coarsening. In many industrial applications a thin film of a solid material needs to be deposited on a solid semiconductor substrate. This deposition can be made by different methods, e.g., by ion beam sputtering, Physical Vapor Deposition (PVD) or Chemical Vapor Deposition (CVD), and during the growth process atoms of the film stick to the atoms of the substrate at its surface. Usually, the growing film does not remain planar during its growth and various kinds of surface structures are developed. The types of these structures depend on physical characteristics of the materials as well as on the growth conditions. The main objective is to introduce deterministic equations that describe physical phenomena and their solutions are most likely received from the initial condition and will remain valid even after a long time. Surfaces can be smooth but the same surface can also be rough. Surfaces with "ideal" topography, e.g., prepared by fracture or by some growth process, have been studied intensively for many years [1, 2, 3]. An important question is how we can describe the morphology and how to study surface and interface dynamics.

Mathematical approach

In the mathematical approach, it is important to incorporate the uncertainty of the parameters into the model. The main sources of uncertainties are difficult to predict. These include the elastic interaction at atomic level, surface

state changes and others. The irregular surfaces are characterized by partial differential equations together with free boundary conditions. To find analytical solution to these partial differential equations is usually impossible, the applied numerical algorithms are generally unstable, and therefore variation methods have to be used. With this approach, the singular geometries can also be treated.

The theoretical base is the system of partial differential equations. The deterministic equations of motion are usually non-linear differential equations. They are sometimes supplemented by stochastic members representing temperature or instrumental noises. In the experiments on macro scale stochastic forces are negligible. Some aspects of self-assembly of quantum dots in thin solid films are considered. Nonlinear evolution equations describing the dynamics of the film instability that results in various surface nanostructures have been analyzed in the literature [4, 5, 6]. Pattern formation is analyzed by means of amplitude equations.

Reports on the nano sized surface patterns of solid substrates are dated back to the 1960s. In 1956 Navez et al [19] observed the phenomenon, that bombarding a glass surface with an ion beam of air, the bombardment produced a new morphology depending mainly on the incidence angle of the ion beam. The obtained surface is covered by wavelike structures (ripples). Some authors tried to find analogies with macroscopic phenomena such as sand ripple structures formed by wind. The observed formations in sand dunes and in clouds are very similar to the features observed on the glass modified by ion bombardment [7] when air and sand come into contact. Air and sand can be moving at very different speeds. The boundary between them can develop complex wavelike structures and ripples that merge or split at different time position. The morphologies of sand dunes are qualitatively similar to that obtained by sandblasting. The same experiment as in [8] compared with sand ripples observed in the desert in paper [9]. One of the typical features of quantum dots is that they formed spontaneously due to the instability of a thin solid film deposited on a solid substrate. Therefore, one can talk about self-assembly of quantum dots having various shapes: regular, as faceted pyramids; irregular, as small crystals with many facets in various orientations; rounded, as cones [10]. When an array of quantum dots formed on the surface of a solid film is kept at a fixed temperature, the dots can either exhibit coarsening or not. During coarsening the larger dots grow at the expense of the smaller ones so that the average dot size increases in time. In the absence of coarsening, the dot size distribution does not essentially evolve at all. The mechanisms that govern the shape of quantum dots, the dynamics of their formation and the evolution of the quantum dot arrays are expressed in several models.

Theoretical predictions for surface structures are derived by partial differential equations involving the derivatives of a time dependent height function of the surface, describing film growth at a mesoscopic level. Numerous conservative continuum equations have subsequently been proposed [4], since in many practical situations the dominant surface relaxation mechanism is surface diffusion, with vacancy formation and particle desorption being quite negligible. Usually such models admit main contributions related to both local dynamics, chemical reactions type of birth and deaths processes, and mass transport [6]. In testing the validity of the theory it is important to identify the right terms of the evolution equation.

(i) To study of non-equilibrium surface growth the Edwards–Wilkinson (EW) model lattice was introduced for studying the fluctuations in a surface, growing by random deposition of particles with immediate relaxation to nearest-neighbour sites. The EW equation, for the thickness h of the thin fluid film, is written as

$$h_t(x, t) = \nu \nabla^2 h + \eta(x, t), \tag{1}$$

where ν denotes the surface tension, and η is the stochastic contribution to the surface fluctuations. Note that the linear evolution equation (1) is mathematically ill-posed, unbounded growth of short wavelength models appear.

(ii) The Kardar, Parisi and Zhang (KPZ) model [5] is a very well-known example of the growth process, suggested a continuum equation which does not conserve particle number, and is therefore applicable to cases where desorption and/or vacancy formation, but not surface diffusion, are the dominant surface relaxation mechanisms.

It was introduced in the context of studying the motion of growing interfaces for connections between polymers and lattice gases in [5]. Experimental observations caught the imagination are published for many applications. For example, physical phenomena modeled by the KPZ class include turbulent liquid crystals, crystal growth on a thin film, facet boundaries, bacteria colony growth, paper wetting, crack formation, and burning fronts [1].
The time derivative of the height function depends on three factors: smoothing (the Laplacian), rotationally invariant, slope dependent, growth speed (the square of the gradient), noise (e.g., space-time white noise)

$$h_t(x, t) = \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \eta(x, t), \tag{2}$$

where η is the noise term and ν and λ are non-zero parameters.

(iii)   One widespread example of the Molecular Beam Epitaxy (MBE) model, where material is slowly evaporated on the surface at sufficiently high temperature. The growth process of surface formations is regularized by surface diffusion. The evolution equation for the shape of the film surface can be written

$$h_t(x,t) = -K\nabla^4 h + \lambda_2 \nabla^2 (\nabla h)^2 + \eta(x,t), \tag{3}$$

where K and λ_2 are parameters. The smoothening term $-K\nabla^4 h$ expresses the surface diffusion. This expresses the evolution of a thin epitaxial film in the case when the film instability is caused by the epitaxial stress, the film surface energy is isotropic, and the film is thin enough.

(iv)   The step instabilities can also be described by the evolution equations, two different types of instability may appear [11]. The step bunching occurs while steps are straight, i.e., the dynamics can be described by 1+1 dimensional equations. In the presence of large desorption it can be modeled by

$$h_t(x,t) = -\nu h_{xx} + \gamma h_{xxx} - K h_{xxxx} + \lambda [h_x]^2, \tag{4}$$

where γ and ν are parameters and $h = h(x,t)$ is the rescaled step shape in stepwise direction x. The term $-\nu h_{xx}$ is responsible for the instability, the second term expresses the surface energy and surface diffusion, the third nonlinear term is proportional of the coarsening dynamics at long time [12].

(v)   In the the step meandering instability, the steps do not stay straight and start wandering. The dynamics of meandering depends on the asymmetry in the attachment. In the presence of strong evaporation the Kuramoto-Sivashinsky (KS) equation is used

$$h_t(x,t) = -\nu h_{xx} - K h_{xxxx} + \lambda [h_x]^2, \tag{5}$$

which one is obtained from (4) with $\gamma = 0$. It is the typical equation of the spatio-temporal chaos. KS equation is derived for both electrochemical deposition (ECD) and chemical vapor deposition CVD.

(vi)   In case of vanishing desorption and weak symmetry, the growth process and the rise of coarsening pattern are modeled by the conserved Kuramoto-Sivashinsky (CKS) equation.

$$h_t(x,t) = -\nu h_{xx} - K h_{xxxx} + \lambda_2 [h_x]^2_{xx}. \tag{6}$$

The term $-\nu h_{xx}$ is responsible for the instability, the nonlinear term $-\lambda_2 \left[h_x^2\right]_{xx}$ is proportional to the flux. Experiments suggest that CKS describes the surface dynamics for MBE.

The boundary conditions indicate the stress and the displacement continuity at the film-substrate interface. The governing equation is considerably simplified if the small-slope approximation is used, assuming that the slopes of the emerging surface structures are small.

SURFACE ROUGHNESS

A common feature of most non-equilibrium interfaces is that their roughening follows simple scaling laws [13]. This phenomenon is also observed experimentally. Here we define the mean height function $\bar{h}(t)$ at the time t for $t \in [0, T]$ by

$$\bar{h}(t) = \frac{1}{|\Omega|} \int_\Omega h\, dx$$

where $|\Omega|$ is the area of $\Omega = [0, L]^2$. At the surfaces the perpendicular fluctuations can be characterized by the surface roughness

$$w(t) = \sqrt{\frac{1}{|\Omega|} \int_\Omega \left|h(x,y,t) - \bar{h}(t)\right|^2 dx}$$

for $t \in [0, T]$.

Numerical Results

The one-dimensional deterministic field equation

$$h_t(t, x) = -h_{xx} - h_{xxxx} + (h_x)^2 - r(h_x)^2_{xx}, \tag{7}$$

is examined numerically which equation is a form of equation (4) after rescaling. We note that r the parameters of the experimental setup, the details of kinetics and the deposition process are involved. The one-dimensional equation (7) is solved with using Fourier spectral collocation in space and the fourth order Runge-Kutta exponential time differencing scheme for time discretization.

The numerical solution for the height profile h for the variants of parameters r will be presented. The visualization of the cross section of the spatio-temporal evolution of the surface of the film calculated from the nonlinear growth equation (7) will be shown for different values of parameter r. The mean interface width profile $w(t)$ is investigated.

Conclusions

Based on the growth equation the better understanding of the amorphous thin film growth process is available. The temporal evolution of the surface roughness of the surface morphology with parameter data is presented. The effect of the parameter is significant on the height profile, on the mean average height profile and the surface roughness.

Acknowledgements

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