

Universal Power Exponent in Network Models of Thin Film Growth

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Abstract— Understanding the growth dynamics of physical processes in thin film growth is of great interest due to many practical applications such as device fabrication in microelectronics, optoelectronics, micro-electro-mechanical systems (MEMS), and nano-electro-mechanical systems (NEMS). In our previous work [1], we developed a network model to study the growth dynamics of thin films and nanostructures. In this model, we used a grid network model along with Monte Carlo simulation methods to study shadowing and re-emission effects. In this paper, we use a cluster-based network model with Monte Carlo simulation methods to study shadowing and re-emission effects. Monte Carlo simulations are used to grow films and dynamically track the trajectories of re-emitted particles. Our recent studies showed that a cluster-based model better captures the shadowing and re-emission effects in the growth process and reveals a power-law behavior in the corresponding network's degree distribution. In this paper, we extended our model to different growth techniques and performed simulations for normal incidence, oblique angle, and chemical vapor deposition (CVD) techniques. Each deposition method leads to a different dynamic evolution of surface morphology due to different sticking coefficients involved and different strength of shadowing effect originating from the obliquely incident particles. We observed that a universal pattern emerges in the network model of the thin film growth process.

Keywords— **Thin film, Grid-based network, Cluster-based network, Degree distribution**

I. INTRODUCTION

Networks are present in many aspects of our world. Study of such networks has become one of the rapidly growing research areas. These networks are compared, analyzed for various mathematical and topological properties. Such studies are highly interdisciplinary. While our existence depends on many of complex systems of networked behavior and we must understand how network structure affects the robustness and characteristics of them. Numerous studies have been carried out to study the dynamics and measurement of the networks. Among these there is a particular focus on networks derived from real data involves community structure, degree distributions, and hubs. These are studied along with various existing models of networks like small-world [2,3,4], scale-free models [5,6,7], and community structures [8,9]. Quantitative analysis allows us to classify the real networks into major categories, thus allowing us to focus on particular theories and analysis in their study.

In order to explore existence of network behavior during thin film growth, 3D Monte Carlo simulations that consider shadowing, re-emission, surface diffusion, and noise effects were developed in earlier work [10]. These effects simulate the evolution of surface topography, and also, the simulation environment allows us to record the trajectories of re-emitted atoms. Qualitative network behavior can easily be realized in these simulated morphologies as the trajectories of re-emitted atoms “link” various surface points. It can also be seen that larger sticking coefficients lead to fewer but longer range re-emissions, which are mainly among the peaks of columnar structures. Therefore, these higher surface points act as the “nodes” of the system. This is due to the shadowing effect where initial particles preferentially head on hills. They also have less chance to arrive down to valleys because of the high sticking probabilities. On the other hand, at lower sticking coefficients particles now go through multiple re-emissions and can link many more surface points including the valleys that are normally shadowed by higher surface points. When the sticking coefficient is large enough, the peaks can grow larger to form a columnar morphology.

II. CLUSTER VS. GRID-BASED MODELS

When developing a network model of the surface morphology, we treat each column as a “cluster” corresponding to a node of the network. During a re-emission, the particles travel from a hill to valley and cause smoothing effects. These non-local interactions among the surface points of a growing thin film originating from shadowing and re-emission effects can lead to non-random preferred trajectories of atoms/molecules before they finally stick and get deposited. For example, during re-emission, the path between two columns where a particle bounces off from the first and head on to the second can define a “network link” between the two columns/clusters. Our network model approach, aims to capture these non-random sequences of re-emission. The size and shape of these columns or clusters change dynamically as the thickness of the film grows.

In our previous work [1], every lattice on the thin film is considered to be a node, which we called the *grid-based model*. This does not provide a dynamic property to the nodes in grid model. By treating the set of lattice points within a column (which is determined after some image processing techniques) as a “cluster”, we developed a *cluster-based network model* [11] where each network node corresponds to a cluster/column. In the cluster-based network model, the nodes are dynamic; and this helps us better understand the

growth dynamics of thin films. Due to columnar structures formed on the surface, we predict that cluster based network model will provide better insight on shadowing effect.

III. RESULTS AND DISCUSSION

In this paper we present the effects of various physical conditions on the network characteristics. One of the most important factors in the thin film growth is angle of incidence, which is the angle at which the particles are released on to the film. Different angles result in different growth structure and dynamics on the thin film. We used three different incidence: 0° , 85° and 90° . Another parameter in the simulations was the sticking coefficient, which can play a major role in the shadowing and re-emission effects. In our study we have used two different sticking coefficients: 0.3 and 0.9. Another property of thin film growth we studied is the film thickness. The thickness is measured in lattice units. One lattice unit is considered to be the thickness of a particle. For this study, we have collected and analyzed data for three different thicknesses: 11, 51, and 101. At these thicknesses, we take a snapshot of the film and these three factors determine a network model [1] to characterize the physical properties of the thin film, e.g., the number, height and width of the hills and valleys formed, and the distances between them.

Two different networks are created using this data, according to cluster-based or grid-based models. In the cluster-based network, each hill and valley is treated as a node of network and the path of particles bouncing between these clusters are treated as links. During the film growth, a snapshot of the film is taken at various thicknesses and the movement of the particles is recorded. A network graph is created using this information and degree distribution is calculated. Following table illustrates power trendline equations for various scenarios discussed above.

TABLE I
DEGREE DISTRIBUTION OF CLUSTER-BASED AND GRID-BASED NETWORKS

Data Series	Cluster-based Network Equation	Grid-based Network Equation
A00_S03_d11	$y = 585.92x^{-2.227}$	$y = 1.7616x^{-5.719}$
A00_S03_d51	$y = 644.43x^{-2.362}$	$y = 1.7072x^{-5.707}$
A00_S03_d101	$y = 862.96x^{-2.616}$	$y = 2.2367x^{-6.022}$
A00_S09_d11	$y = 823.47x^{-2.411}$	$y = 2.1642x^{-5.614}$
A00_S09_d51	$y = 886.27x^{-2.472}$	$y = 2.3031x^{-5.452}$
A00_S09_d101	$y = 788.57x^{-2.24}$	$y = 2.5075x^{-5.483}$
A85_S03_d11	$y = 357.43x^{-2.059}$	$y = 0.0755x^{-1.759}$
A85_S03_d51	$y = 300.41x^{-1.893}$	$y = 0.0892x^{-1.761}$
A85_S03_d101	$y = 357.43x^{-2.059}$	$y = 0.0755x^{-1.759}$
A85_S09_d11	$y = 172.83x^{-1.729}$	$y = 0.0488x^{-1.643}$
A85_S09_d51	$y = 132.74x^{-1.727}$	$y = 0.0313x^{-1.601}$
A85_S09_d101	$y = 101.11x^{-1.945}$	$y = 0.0306x^{-1.626}$
DEP_S03_d11	$y = 1060.6x^{-2.378}$	$y = 0.013x^{-1.915}$
DEP_S03_d51	$y = 1113.8x^{-2.444}$	$y = 0.0134x^{-1.822}$
DEP_S03_d101	$y = 914.53x^{-2.314}$	$y = 0.0133x^{-1.818}$
DEP_S09_d11	$y = 470.63x^{-2.113}$	$y = 1.7933x^{-4.46}$
DEP_S09_d51	$y = 547.22x^{-2.174}$	$y = 0.7607x^{-2.683}$
DEP_S09_d101	$y = 585.92x^{-2.227}$	$y = 0.7201x^{-2.704}$
NODEP_S03_d11	$y = 397.39x^{-2.215}$	$y = 0.0743x^{-1.751}$

NODEP_S03_d51	$y = 344.08x^{-2.062}$	$y = 0.0898x^{-1.766}$
NODEP_S03_d101	$y = 358.76x^{-2.04}$	$y = 0.0743x^{-1.751}$
NODEP_S09_d11	$y = 462.16x^{-2.111}$	$y = 0.0502x^{-1.658}$
NODEP_S09_d51	$y = 592.03x^{-2.235}$	$y = 0.031x^{-1.595}$
NODEP_S09_d101	$y = 603.13x^{-2.166}$	$y = 0.0309x^{-1.631}$

Each entry under data series pertains to a particular scenario. For example A00_S03_d11 represent data set for angle 0° (A00), sticking coefficient 0.3 (S03) and thickness of 11 (d11). From the table, it can be noticed that the power exponent stays mostly the same (i.e., around -2) in the cluster-based model. Since, the exponent does not change when the factors like sticking coefficient, angle of incidence and thickness of film are changed, the cluster-based model captures a universal behavior in the thin film growth network. But same behavior is not seen between two networks. When the selection criteria for nodes is changed from grid-based to cluster-based, there is a significant change in the exponent, i.e. between -1.5 and -6.0.

While the grid-based model captures different properties in the way nodes are identified, the cluster-based model hides some of the local interactions within the lattice points in a cluster. Thus, the cluster-based model will help researchers identify global behavior of thin film and avoid any noise that might be originating due to local interactions. This comparison of degree distribution between two networks sheds light on various factors that would impact the characteristics of thin film growth phenomenon.

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