ABSTRACT

of the thesis entitled

Study of aggregation models, cluster connectivity and kinetics of surface roughening in pulsed laser deposited thin films

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Abstract

Aggregation is an irreversible physical process in which basic unit (molecules or micro/nano particles) stick together, to build characteristic structures, called aggregates. The study of growth models has become an important area in statistical mechanics. There are several reasons behind this interest. The most important reason is the experimental relevance of growth models. Early growth models were proposed to describe various experimental situations like tumor growth, colloidal aggregation etc however, many experimental realizations of growth models are now known and are studied by experimentalists. Another reason is the complexity involved. History plays an important role in growth. The end product depends on certain configuration of the past. Thus growth is non-Markovian process and it is not in general possible to simply write down a partition function or generating function. New ideas were needed and this has fascinated workers in this field. Growth models allow simulation of the growth patterns on computer. These computer programs are often rather simple and yet generate aggregates, which strikingly resemble, in many aspects, to aggregates in reality.

It has been recently realized that the growing interface exhibits a new type of dynamical scaling, a scaling which is intimately related to the geometric form. The surface and interface roughness also controls many important physical and chemical properties of the grown films. For instance, interface in field-effect transistors (FET) or tunnel junctions have to be extremely smooth to guarantee homogeneous insulator thickness; on the other hand the so-called giant magneto resistance (GMR) effect in magnetic multilayers is enhanced by a certain degree of interface roughness. The surface roughness also plays an important role in wetting and de-wetting. Thus characterization of a surface of the thin films in terms of interfacial roughness has paramount importance from scientific and technological viewpoint. Proper control of the surface properties requires an understanding of the underlying growth mechanisms, which can be achieved by detailed structural analysis of surfaces prepared under various growth conditions. Very often the phenomenon of growth front roughening occurs under conditions far from-equilibrium. One important outcome of the dynamic scaling hypothesis is the existence of the universality in which the essential features of the roughness evolution depend only on certain symmetries and the dimensionality of the system and not on the detailed interaction.

The present study deals with the cluster growth using computer simulation and study of their microscopic features like connectivity etc. The simulation results are substantiated using experiments on similar systems. Afterward, study has been focused on the macroscopic aspect of the interface generated using simulated interfaces and interfaces developed in the physical vapor deposition process. In the following section we discuss the summery of each chapter.

Chapter 1: Introduction and motivation

In this chapter we present a brief discussion on aggregation phenomenon and their geometrical characterization in terms of fractal dimension and self similarity. Brief review of different growth models, the surface properties and fractal dimensions of the aggregates grown is also presented. Some experimental realizations of these growth models are also discussed. Motivation for this research work is stated in the last section.

Chapter 2: Segregation of two seed growth patterns with fractal geometry

In this chapter we present the 2-dimensional generalized diffusion-limited aggregates (g-DLA), grown from two proximal nucleation seeds placed at distance *d* lattice units on a square lattice and investigate the probability *p(d)* that these aggregates get connected. For the purpose of growing the g-DLA we use sticking probability model as proposed by Banavar *et al.* [Phys. Rev. A, **33**, 2065 (1986)]. We vary the sticking probability to get a range of aggregate geometry from fractal to compact one. Segregation phenomenon is also demonstrated experimentally for viscous fingering patterns with two injection points and for electrochemical deposition grown on two cathodes.

Chapter 3: Scaling properties of surfaces of aggregate grown by modified growth models

In this chapter we have presented dynamic scaling of rough surface. Method to calculate the scaling parameters is described by taking the example of rough interface grown using two models viz. generalized diffusion limited aggregation (g-DLA) and Modified Ballistic Deposition (MBD). We use g-DLA to generate an interface patterns on a line substrate. In the second model two variants namely, Nearest Neighbor BD (NNBD) and Next Nearest Neighbor BD (NNNBD) is used to construct a rough interface on a line substrate. The simulated rough interfaces are characterized using dynamic scaling approach.

Chapter 4: Kinetics of surface roughening in pulsed laser deposited Ag thin films on Si(100) substrate

The scaling exponents characterize the local structure of rough surfaces making it possible to classify various surface growth phenomena into discrete universality classes. Thus these scaling exponents provide us with a convenient measure regarding growing surfaces and can be used for the comparisons between experimental data and theoretical model systems. However, the exponents may vary strongly with parameters associated with experimental systems. Thus, the scaling relation is usually applied to self-affine or self-similar surfaces grown under the conditions where kinetic limitation dominates, it is of interest to examine the behavior of scaling exponents for metallic thin films deposited by the Pulsed Laser Deposition (PLD) technique on Si(100) substrate.

In this chapter, surface roughness and surface morphology of pulsed laser deposited (PLD) silver (Ag) thin films, grown on a single crystal substrate of Si(100), as a function of deposition time, has been investigated using atomic force microscopy (AFM) technique. The dynamic scaling approach is used to analyze the surface topology of PLD grown films. Height-height correlation function is used to determine the value of scaling exponents. Interestingly it is seen that the exponents values are in close agreement with the value obtained for simulated interface using g-DLA ($\alpha' = 0.01$) (studied in Chapter 2).

Chapter 5: Kinetics of surface roughening in pulsed laser deposited ZnO thin films on Si(100) substrate

In this chapter we have investigated surface roughness and surface morphology of pulsed laser deposited (PLD) ZnO thin films, grown on a single crystal substrate of Si(100), as a function of deposition time using atomic force microscopy (AFM) technique. The dynamic scaling approach is used to analyze the surface topology of PLD grown films. Height-height correlation function is used to determine value of scaling exponents. The value of the exponents suggests that ZnO growth is anisotropic. The c-axis growth as seen in the X-ray diffraction, support the argument.

Future scope of the research is given at the end of thesis.

Publications:

1. Segregation of fractal aggregates grown from two seeds.
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   Physical Review E 75, 051401 (2007).
2. Growth temperature and N_2 ambient pressure dependent crystalline orientations and band-gaps of pulsed laser deposited AlN / (0001) sapphire thin films.
   Shas M. Jejurikar, A. G. Banpurkar, **Deepak N. Bankar**, and K. P. Adhi; L. M. Kukreja
   Journal of Crystal Growth 304, 257 (2007).
3. Surface morphology studies of pulsed laser deposited highly c-axis oriented swift heavy ion irradiated LSMO thin films.
   M. S. Sahasrabudhe, **Deepak N. Bankar**, A. G. Banpurkar, K. P. Adhi, S. I. Patil Ravi Kumar.
   Nuclear Instruments and Methods in Physics Research B 263,407 (2007).

4. Growth Kinetics Study of Pulsed Laser Deposited ZnO Thin Films on Si (100) Substrate.
   Deepak N. Bankar, Suhas M. Jejurikar, K. P. Adhi, A. V. Limaye and A. G. Banpukar
   AIP Conf. Proc. 1391, 101(2011).
5. Study of growth kinetics of pulsed laser deposited silver thin films.
   Deepak N. Bankar, Shashikant D. Shinde, K. P. Adhi, A. V. Limaye and A. G. Banpurkar
   National Symposium on Pulsed Laser Deposition of Thin Films and nanostructured materials (PLD-2011).
6. Scaling properties of surfaces of aggregate grown by modified growth models.
   Deepak N. Bankar, A. V. Limaye and A. G. Banpurkar
   (Under preparation)

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