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# SURFACE GROWTH MODELS FOR MORE THAN ONE SPECIES: A REVIEW

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## Abstract

The progress in the understanding of the surface growth problem in the case of deposition of more than one species is reviewed and lines of action to be followed are suggested. Unfortunately very few works regarding this problem are carried out although it is common in the growth of real materials to find more than one deposited component. The use of discrete models by allowing several growth processes and the interaction between different particles will introduce a new insight into the dynamics of the surface roughening, especially in (2+1)-dimensions, where the results can be compared with those of the experimental observations. It is shown in many simulations that a new universal behaviour is observed in the growth of composites. The recent methods of dynamic scaling that lead to distinguish between local and global exponents, will assist to categorize growth processes into universality classes. It has been argued that the numerical simulation models as well as the numerical solutions of the growth equation in a general form will introduce a better understanding of the film growth of alloys. The interplay between different growth mechanisms will also allow to investigate the main processes that are responsible for the origin of the surface roughening which is monitored in many experiments.

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# I. INTRODUCTION

The growth of surfaces and interfaces remains a challenging problem in physics. It attracts much more interest due to its technological importance since many properties of real materials depend on the presence of surface and interface roughness. It is a hope to make a smooth surface to obtain optimum material properties. However, during the growth of materials the surface becomes undesirably rough. In order to avoid such kind of morphology, the basic physical effects and the processes that lead to the development of surface roughness must be well understood. Apart from technology, most rough surfaces are formed under conditions that are far from equilibrium. Therefore, the study of this phenomena has a relevant importance in the understanding of nonequilibrium statistical mechanics at the fundamental level [1–7].

It is well known that a stochastically growing surface exhibits scaling behaviour and evolves to a steady state without a characteristic time or length scale. Therefore, a scaling concept allows to connect measurable quantities with some scaling relations through some exponents, which in turn lead to the definition of what is the so-called universality classes. The scaling approach as well as other methods of analysis such as discrete models, continuum growth equations and experiments are used to classify different systems and growth processes into some certain universality classes [5].

Simple discrete growth models have played a major role in the understanding of the nature of surface roughness since they mimic the essential physical parameters and eliminate less important details. Therefore, computer models represent a crucial link between theory and experiments, where two important aspects should be taken into consideration: kinetics and morphology. Kinetics helps to understand how surfaces evolve with time while morphology provides a clear interpretation of the first aspect.

Although surface growth models have been extensively studied in the past, most of previous studies have dealt with the growth of deposited components of only one kind. The growth of two or more species is common in modern technology where little is known about the kinetic roughening [8–10]. Therefore, the study of such problems has a great interest since it gives a new insight into the dynamics of roughening as well as the morphological structure. The connection between computer models of more than one species with both experiments and theory will allow to understand how surface roughness is originated in the system of alloys. It also allows to define universality classes that the growth processes may belong to. In addition, it helps to distinguish a new universal behaviour that might exist.

Most studies of composite growth have been carried out in (1+1)-dimensions. However, in order to be closer to the real systems, one needs to perform simulations in (2+1)-dimensions. Another important fact is that there are still disagreements about the classes of the universality and it might be expected to find a new universal beahviour [8,11]. In addition, the stochastic growth equations in (2+1)-dimensions in general cannot be solved analytically except for the linear theory which is the simplest case. Apart from the linear theory, there is no agreement about analytical solutions [5]. Therefore, numerical solutions of those equations are required. The numerical solutions will allow to test the interplay between all the mathematical terms, which express growth processes, in the differential equations and compare with experiments and models [12]. This indeed will allow to get a clear picture to understand the main processes that are responsible for the roughening and how the interchange between each other will lead to a certain morphology.

The organization of this paper is as follows: in section two the dynamic scaling concept is introduced. In section three the general form of the growth equation is given, where different universality classes are special cases of the general form. In section four, different growth models for two species are reviewed. The discussion is presented in section five. Finally the conclusion is found in section six.

## II. DYNAMIC SCALING

It appears that stochastically growing surfaces, which are self-affine fractals, exhibit scaling behaviour. Scale invariance will allow to find the scaling relations between the important measured quantities. These relations will help to define the universality classes where the differences between many growth processes can be distinguished. Therefore, starting with an initially flat substrate and defining the surface width $W(L,t)$ by

$$W^2(L,t) = \frac{1}{L^{d-1}} \sum_r [h(r,t) - \overline{h_L(t)}]^2 \tag{1}$$

where $L$ is the system size, $h(r,t)$ is the height of the surface at position $r$ and time $t$, $\overline{h(t)}$ is the average height at time $t$, and $d-1$ is the surface dimension, the scaling law [13] is given by

$$W(L,t) = L^{\alpha} f(t/L^{z}) \tag{2}$$

The scaling function $f(x)$ behaves as

$$f(x) = \begin{cases} x^{\beta} & x << 1 \\ L^{\alpha} & x >> 1 \end{cases} \tag{3}$$

where $\alpha$ is the roughness exponent which characterizes the roughness of the saturated surface, $z$ is the dynamic exponent and $\beta = \alpha/z$ is the growth exponent that characterizes the short time dynamics of the roughening process. The exponents $\alpha$, $\beta$ and $z$ determine the universality classes.

So far the attempts have been made under the assumption of scale invaraince. A similar behaviour is expected for the surface width $w(l,t)$ defined in a box of lateral size $l << L$

$$w^2(l,t) = \frac{1}{l^{d-1}} \sum_r [h(r,t) - \overline{h_l(t)}]^2. \qquad (4)$$

It is expected that $w(l,t)$ scales in the same way as (2) and takes the form

$$w(l,t) = \begin{cases} t^\beta & t << l^z \\ l^\alpha & x >> l^z \end{cases} \qquad (5)$$

However, in many models and growth equations, it has been found that the local surface width behaves for intermediate time ($l << t << L$) as $w(l,t) \sim l^{\alpha_{loc}} t^{(\alpha - alpha_{loc})/z}$ with $\alpha_{loc} \neq \alpha$. This phenomena is known as anomalous scaling [14], (for models of more than one species, this phenomena has not been seen up to now. However, for the proposed models (of sections $IV$ and $V$), anomalous scaling may be found and hence to define $\alpha_{loc}$ will assist to define the universality classes). Two processes can be defined according to anomalous roughening which are super-rough ( $\alpha > 1, \alpha_{loc} = 1$) and intrinsic anomalous roughening ($\alpha_{loc} < 1, \alpha > \alpha_{loc}$). Recently [15], a new dynamic scaling approach was introduced where the dynamic scaling behaviour was investigated by calculating the structure factor (power spectrum)

$$S(k,t) = \langle \widehat{W}(k,t) \widehat{W}(-k,t) \rangle \qquad (6)$$

where $\widehat{W}(k,t) = \sqrt{L^{d-1}} \sum_r [h(r,t) - \overline{h_L(t)}] e^{ikr}$. The structure factor scales as

$$S(k,t) = k^{-(2\alpha+1)} s(kt^{1/z}) \qquad (7)$$

where the scaling function has the form

$$s(u) = \begin{cases} u^{2(\alpha - \alpha_s)} & u >> 1 \\ u^{2\alpha+1} & u << 1 \end{cases} \qquad (8)$$

Here, $\alpha_s$ is the spectral roughness exponent. The general case of scaling is [15]

$$\begin{array}{ll} \alpha_s < 1 \Rightarrow \alpha_{loc} = \alpha_s & \begin{cases} \alpha_s = \alpha \Rightarrow \mathrm{Family - Vicsek\ scaling:\ (1)} \\ \alpha_s \neq \alpha \Rightarrow \mathrm{Intrinsic - rough} \end{cases} \\ \alpha_s > 1 \Rightarrow \alpha_{loc} = 1 & \begin{cases} \alpha_s = \alpha \Rightarrow \mathrm{Super - rough} \\ \alpha_s \neq \alpha \Rightarrow \mathrm{unknown\ \ class} \end{cases} \end{array} \qquad (9)$$

The scaling law (9) [15] shows a general form that can be used in order to define universality classes in different growth processes. It is expected that the use of discrete models for composites may lead to define a new universal behaviour [8,11] especially in $(2+1)$-dimensions. These new universalities can be identified by different scaling exponents. The definition of more than one exponent will contribute to the efforts in order to categorize all growth processes into universality classes.

## III. GROWTH EQUATIONS

A very successful tool for understanding the behaviour of the different growth processes are stochastic differential equations. In many cases the obtained equations cannot be solved analytically. Therefore, numerical solutions must be made in order to define the scaling exponents [12]. It will also allow to extract the required information to understand the main growth processes which are involved in the system of different kinds of deposited components.

The general form of the growth equation is

$$\frac{\partial h}{\partial t} = \upsilon \nabla^2 h + \frac{\lambda}{2}(\nabla h)^2 - K\nabla^4 h - \lambda_1 \nabla^2 (\nabla h)^2 + \eta \tag{10}$$

where $h$ is the surface height at position $r$ and time $t$ and $\eta$ is the noise that determines the fluctuations of the deposition processes around the mean value of the deposition rate. The first term in equation (10) expresses the relaxation due to either deposition or desorption [5]. The second term is the Kardar-Parisi-Zhang (KPZ) [16] term that describes the lateral growth and overhang/void processes. The third term was suggested by Mullines for surface diffusion [5]. The fourth one was proposed by Villain to encounter the inhomogeneous concentration of the diffusing particles on the surface [5]. The coefficient of the first term is defined as $\nu = -Fb$, where $F$ is the mean deposition rate and $b$ is the difference between the typical range of the interatomic forces and the equilibrium distances of the adatoms to the surface [5,12]. It is sometimes called a "surface tension". The coefficient $\lambda$ is positive because of the volume increase due to the oblique incidence. The coefficients $K$ and $\lambda_1$ must be negative and they are related to the diffusion length as the first coefficient [5,12].

According to eperimental observations, main growth processes can be included in the discrete models and in the corresponding growth equations. In this case the interplay between different growth processes will help to interpret the experimental evidences of surface roughness in real growth systems. Many universalities can be derived from equation (10) according to the growth processes that are either observed in experiments or tested by means of computer models. For models that capture relaxation processes as well as lateral growth like ballistic deposition, solid on solid and restricted solid on solid the following equation can be written

$$\frac{\partial h}{\partial t} = \upsilon \nabla^2 h + \frac{\lambda}{2}(\nabla h)^2 + \eta \tag{11}$$

which is the KPZ equation [16]. This equation cannot be solved analytically in (2+1)-dimensions. The one loop renormalization group analysis indicates that there are still inconsistent values for the exponents that determine the KPZ universality class in a dimension higher than $(1+1)$. This in fact motivates to study the kinetic roughening by means of simulation models. For the random deposition model with surface relaxations, one can get the Edwards-Wilkinson (EW) [17] equation

$$\frac{\partial h}{\partial t} = \upsilon \nabla^2 h + \eta \tag{12}$$

This equation can be solved and gives expononents that determine the EW universality. Other processes can be grouped in the classes to describe the growth by molecular beam epitaxy (MBE), Wolf-Villain (WV), Das Sarma-Tamborenea (DT) and others [5]. These universalities can be described by either linear or non-linear equations, like

$$\frac{\partial h}{\partial t} = -K\nabla^4 h - \eta \tag{13}$$

and

$$\frac{\partial h}{\partial t} = -K\nabla^4 h - \lambda_1 \nabla^2 (\nabla h)^2 + \eta \tag{14}$$

It should be noted that in the case of the deposition of more than one species linear and nonlinear terms might be introduced to incorporate growth processes that are observed in experiments. In reference [12] the authors introduced an approach to describe the growth processes that are observed in real experiments [18] by numerical solution of the growth equations. In this case the numerical solution of the growth equations will be the most powerful tool as well as the computer simulations to understand clearly the nature of film growth.

## IV. MODELS FOR BINARY SYSTEMS

Surface evolution is influenced by several factors. It is impossible to mimic all in one model. However, discrete models allow to describe the microscopic mechanisms that lead to surface roughening by capturing only the important physics of the problem. They also represent an essential link between theory and experiments. For models that are composed of more than one species, few studies towards the understanding of the nature of the roughening in such systems, are carried out. In these studies simple rules for the interaction between different particles are maintained. Previous studies can be classified according to the used models and growth processes. These models are random deposition with surface relaxation, solid on solid, restricted solid on solid and submonolayer growth models.

### A. Random Deposition Model with Surface Diffusion (RDD)

It is common in growth processes to find local diffusion of newly arriving particles along the surface of the deposited material. RDD model for two species is introduced in order to incorporate surface relaxation, where simple rules of interaction between different species are allowed [19]. In (1+1)-dimensions the study shows that the RDD belongs to the EW universality class, although there is a small deviation for the calculated values of the exponents from those of EW. The dynamic scaling and the morphology in (2+1)-dimensions [20] indicate that the model does not belong to any of the known classes. In addition an unstable morphology is observed.

### B. Ballistic Deposition Model (BD)

The BD model represents an example of well studied growth models where overhangs processes are allowed. In reference [21] a model with two kinds of particles, sticky and sliding, was introduced. This model interpolates between a diffusive model and the usual BD one. The results reveal that in the case that diffusion is dominant the model belongs to EW universality while in the case that overhang is dominant the model belongs to the KPZ universality. In a series of studies [9,19,20,22], a BD model is introduced for two kinds of interacting species. The study in (1+1)-dimensions suggested that the model may not belong to the KPZ class. In (2+1)-dimensions, it is shown that the model does not belong to the KPZ universality for all conditions of the deposition. In reference [23], the BD model is proposed for two species with next nearest neighbour interactions. This study shows a different result than those observed with only nereast neighbour interactions as well as a non KPZ universal behaviour.

### C. Ballistic Deposition Model with Surface Diffusion (BDD)

The BD model captures the essential features of processes such as vapor deposition. However, it does not provide an adequate representation of diffusion on the surface. Therefore, to simulate deposition as realistically as possible, both diffusion and overhang processes must be included [24,33]. Thus different kinds of species and different growth processes yield different kinetics and morphology. The studies in (2+1)-dimensions [8,25] show that the model neither belongs to KPZ nor EW classes, whenever overhang or diffusion is dominant, respectively.

### D. Solid on Solid Model (SOS)

The numerical simulations of the SOS model for two species has been carried out in (2+1)-dimensions [26,27] motivated by experimental observation of atomic ordering in alloy films. The study shows that the interplay between the domain growth and the surface roughening leads to a non-EW-universal behaviour although the main processes are deposition and diffusion. However, the study is limited to the case of the growth of binary alloys of the concentration $\mathrm{A}_{0.5}\mathrm{B}_{0.5}$.

### E. Restricted Solid on Solid Model (RSOS)

Influenced by phase ordering in binary systems, a study in (1+1)-dimensions in the context of the RSOS model has been carried out [10,28,29]. It has been argued that there is no new universal behaviour in this dimension and the model belongs to the KPZ universality. However, the authors expect in (2+1)-dimensions that the extension of the model might give something new.

Even though the studies regarding the growth of alloys were designed to include processes such as deposition and surface relaxations, there could be evaporation processes in the real growth as well [30,31]. The effect of desorption on surface roughening is rarely studied either experimentally or by discrete models. Previous numerical studies are performed in (1+1)-dimensions only.

### F. Models for Submonolayer Deposition

Towards the understanding of surface evolution problem, it is of importance to figure out a correct picture regarding the early time behaviour. Therefore, the study of the dynamics of island formation represents an essential step in order to gather more information about the main growth processes in systems of composites. Although a work concerning such problems is necessary, there is only one recent work by Kotral et. al [32]. In this work the authors studied the dynamics of island formation for two species model.

## V. DISCUSSION

In the previous sections, it has been shown that although the problem of the growth of more than one deposited components is of great importance, unfortunately, there are very few studies regarding such problem. These few studies are carried out in the context of simple simulation models that capture simple rules for the interactions between different kinds of the deposited species. Many of these studies were done in (1+1)-dimensions where no comparison with experiments can be achieved. To simulate real growth processes, one should perform simulation in the (2+1)-dimensions. In addition to the dimension, it seems that the different growth processes, which are involved in this case, are more complicated than the well studied problem of only one kind of deposited particle. However, to investigate the origin of roughness and how much it is affected by the interactions between different kinds of particles on the surface, further studies are required to produce a better understanding of the film growth of more than one species. In order to study a problem like that not only the questions like how many growth processes are presented and how big is the effect of the interaction between deposited particles should be answered but also how much the phase order in the growth of many species is effective. It is of importance to study growth-induced ordering and the evolution of the domain size on the surface. To answer the addressed questions it appears that a study of all factors together is recommended to reach a level of knowledge which allows to interprete real experimental observations. This kind of study should be carried out by using the standard approaches such as discrete models and solution of the growth equations taking into account several growth processes that are monitored experimentally or those that are expected to lead to a certain morphology.

Discrete growth models are used on the microscopic level to explore the growth phenomena. There is a wide variety of models that are used to simulate growth for a single component deposition. These models can be generalized to be used for more species deposition. This should be achieved taking the simplicity of the models into account where the essential physics must be included. However, the results of simple models with simple rules of interactions between different particles show in many cases a deviation from those that are obtained by the same models for a single particle. They show a different universal behaviour. To identify this new universal behaviour more studies are required with a wide variety of models allowing all possible rules of interactions between deposited particles. For example, evaporation processes are not included in models like RDD, BD , BDD and SOS. Also the rules according to which the different processes of growth occur should be introduced in these models with possible extension of the interaction to include more neighbours. In addition, it should be taken into account that the presence of atomic ordering should play a certain rule in the surface roughening during the film growth. Another process which is relevant in higher dimensions than (1+1) is the overhang [33]. This kind of process should be introduced in the simulations.

One of the important growth techniques is MBE. Many models in the context of the RSOS model are used to study the kinetic roughening in case of only one deposited component as well as the investigation of the main sources of unstabilities and mound formations [34] that are observed in real experiments. In general, introducing models for more than one species will help to illustrate the origin of the roughening in MBE as well as the unstable morphologies and mounds [35]. Besides, it will allow more inspections about the origin of roughening either normal or anomalous that are found in many techniques. Also, studies regarding the growth in early time should be achieved in case of mixture deposition. In this case there should be answers for main questions like: what is the typical size of an island and how many are there? What is their morphology? How do these quantities change with the coverage or with the flux?.

Recent approaches of scaling that helped to identify several growth exponents will give a great improvement. Therefore, it is recommended to further study the deposition of more than one species to measure several quantitities of interest. This will allow to categorize the growth processes into different universality classes. In accordance with the study of discrete models there should be other studies for the numerical solutions of the growth equations in order to measure how much the exchange between different growth processes influences the final morphology. A comparison between results of both simulation models and numerical solutions of the equations with those of experiments is possible in order to interpret real observations.

## VI. CONCLUSION

The review shows that the knowledge of the growth of more than one species is not very deep. This may be due to the complexity of the problem and the computational limits. However, such studies are necessary to understand the origin of the kinetic roughening at the microscopic level in a wide range of the growth processes. It is also necessary to perform numerical simulation in (2+1)-dimensions in order to compare with experiments. It is suggested that numerical solution of the growth equations will help towards a better understanding of the problem since in many cases analytic solutions are not found. The advantage of the numerical solution is that it allows to test the interplay between different terms and how much is the weight of each process among all of them. Recent dynamic scaling approaches will greatly contribute to the effort of classification of the main growth processes into universality classes.


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