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Scaling behavior and morphological properties of the interfaces obtained by the multilayer deposition process

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ABSTRACT

The aim of the present work was to study numerically the scaling behavior and the morphological properties of the interfaces generated by the multilayer deposition process. We have noticed that, in the case where the ratio of the surface diffusion coefficient to the deposition rate reaches high values $D/F >> 1$, the interface consists of mound structures. By using the dynamic scaling, we have shown that the height–height correlation function scales with time t and length l as $G(l,t) \sim l^{\alpha} f(t/l^{\alpha/\beta})$ with $\beta = 0.25 \pm 0.05$ and $\alpha = 0.51 \pm 0.02$. These exponent values are equal to the ones predicted by the Edwards–Wilkinson approach. Besides, our results are in agreement with the growth system of Cu/Cu(100) at 300 K which has been characterized in more detail by a combined scanning tunneling microscopy and spot profile analysis — low energy electronic diffusion study. Moreover, by considering two different methods, we have examined the fractal aspect of the obtained interfaces.

1. Introduction

During the last two decades, the growth dynamics and formation of the roughing interfaces have received a lot of attention. So, many theoretical, numerical and experimental investigations have been developed on the subject in order to understand the roughening process of fluctuating interfaces. When the interface grows, it roughens because of to thermal fluctuations; the origin of the randomness arises essentially from the random nature of the deposition and the diffusion processes [1–7]. The Family–Vicsek [7] scaling is one of the models which can describe the dynamic growth of these interfaces in various other physical, chemical, or biological systems, ranging from bacterial growth to diffusion fronts. However, when the atoms or molecules impinge randomly on a substrate, they form strong chemical bonds at a periodic array of localized adsorption sites [8] and then the substrate constitutes a heat bath providing thermal energy to the adsorbed atoms. In the case where desorption process is neglected, the adsorbed atoms diffuse across terraces on the substrate, and formed islands by attractive interactions. Continued deposition can produce complicated submonolayer patterns and multilayer morphologies. These processes can be naturally described within the framework of atomistic lattice–gas models [3,4]; homoepitaxial growth [5–8] constitutes a large domain where the diffusion process of the adatoms leads to a development of largely strain-free adlayers or multilayer films. There is a large number of studies focusing on the characterization of rough interfaces using diffraction methods, both for single interface [9,10] or multilayer [11]. The main result is that diffraction methods are able to separate the dynamical and static properties of interfaces. The morphology of experimentally observable interface can be conveniently described by fractal concepts. It has been suggested that the remarkable similarity at high-magnifications of amorphous silicon, germanium, pyrolytic graphite, thick metal films or the cauliflower can be understood if one assumes that the surface is fractal. Hence, they proposed that the growth mechanism involved in the formation of some of the thin film morphologies must lead to self-similar morphologies [12].

In our investigation, the principal goal is to study the kinetic growth and the scaling properties of the interfaces obtained by the multilayer deposition process in a model in which we attempt to take into account the mound morphology. The rest of the paper is structured as follows: in the second section, we present our investigation model and we define some physical quantities. In the third one, we present and discuss our calculation results concerning the kinetic growth of the width of the wedding cake structures and some morphological properties of these interfaces. The obtained values of the growth and the roughness exponents are compared to the ones predicted by the Edwards–Wilkinson equation. Finally, we summarize this work in the Summary and conclusion section.

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2. Model and method: scaling approach of the interface

It was shown that when the ratio of the diffusion coefficient to the deposition rate tends to infinity (i.e. $D/F \to \infty$), the interface has a mound morphology [13,14] (see Fig. 1). Microscopically, this structure originates essentially from the existence of an additional energy barrier near the step edges. This additional potential barrier usually called the Ehrlich–Schwoebel barrier [15,16] prevents atoms from descending from the atomic layer on which they have been deposited [13]. Consequently, the concentration of adsorbed atoms on top of two-dimensional islands is increased. Such that second-layer nucleation occurs well before the first-layer has been completed. This process repeats itself in subsequent layers giving rise to a mound structure of islands on top of islands.

The dynamic scaling approach is an effective tool for characterizing the temporal evolution of most interface phenomena and for identifying the universality classes to which the different models belong. One of the most important quantities used to characterize the scaling of the interfaces is the global width parameter $\sigma(L,t)$ defined as:

$$\sigma(L,t) = \left(<h^2> - <h>^2\right)^{1/2} \tag{1}$$

where the function $h(x,t)$ gives the interface height at time t and position x. L is the system size and $< >$ denotes a spatial average over the whole system. It has been shown in Ref. [7] that the width of an interface scales with time t and system size L as:

$$\sigma(L,t) \sim L^{\alpha} f\left(t/L^{\alpha/\beta}\right). \tag{2}$$

The function $f(x)$ satisfies the following equations: $f(x << 1) \sim x^{\beta}$ and $f(x >> 1) \sim const.$ The two exponents α and β are called the roughness and growth exponents, respectively. The invariance property under the scale transformation implies that there is no characteristic length scale in the system besides the system size, and thus all scales obey the same physics law. Hence, the scaling behavior of the interface can be obtained by measuring the local width over a window of size $l \ll L$ at the interface,

$$\sigma(l,t) \sim \begin{cases} t^{\beta} \text{ if } t << t_c(l) \\ l^{\alpha} \text{ if } t >> t_c(l) \end{cases}, \tag{3}$$

where

$$t_c(l) = l^{\alpha/\beta}. \tag{4}$$

The present model is usually applicable for systems obtained by the epitaxial process which present a mound morphology and Family–Vicsek scaling behavior.

In this work, we consider a flat surface with an integer lattice of sites (i,j) with an integer height variable $h(i,j,t)$ defining the position of the surface above (i,j). At time zero, the atoms are randomly deposited with a constant flux F. Atoms arrive on the surface and hop to neighboring sites provided that they remain within the same layer (the deposition and the diffusion processes characterized by the diffusion constant D take place simultaneously). However, when the adatom arrives to the limit of the layer, it does not fall down because it should overcome the Ehrlich–Schwoebel barrier which avoids the diffusion ($D = 0$) (see Fig. 1). We mention that the only physical parameter, in our system, is the ratio D/F. Here, we consider the case $D/F \gg 1$, where the long-ranged lateral correlation can be observed [13] and the interface consists of mound structures.

Scaling arguments [17,18] and simulations [13,17,19,20] show that the diffusion length of the deposited atoms l_d, which is the typical distance traveled by an atom before it can be incorporated into an island or step, scales as:

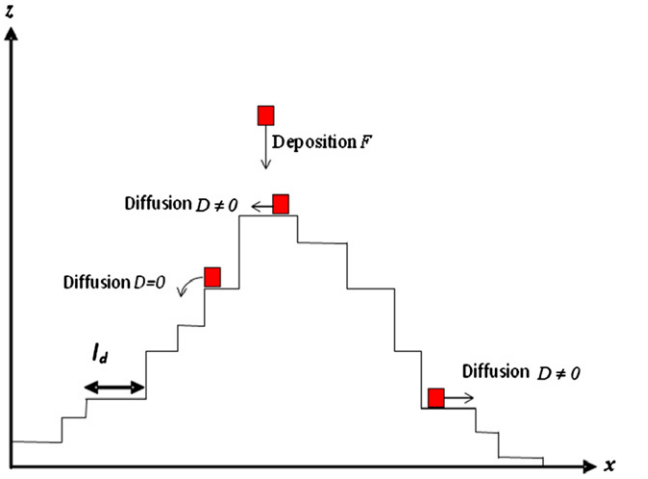

Fig. 1. Schematic of interface formation obtained by the multilayer deposition process.

$$l_d \sim (D/F)^{\delta_d} \tag{5}$$

where δ_d is an exponent whose value is determined by the actual mechanism of island formation,

$$\delta_d = \frac{1}{4 + d_f}. \tag{6}$$

Here d_f is the fractal dimension of the generated interface.

3. Results and discussion

The study of the scaling behavior and the morphological properties of the interfaces are important for obtaining detailed information on the growth mechanisms and the crystal growth to name just two. For our numerical simulation used for this specific study, we have considered a square lattice with $L \times L$ sites on which the atoms are deposited randomly with flow constant F. In this case, we have fixed the ratio D/F at 10^8, and we calculate the time evolution of the height at each site (i,j). In Fig. 2, we present an image system in the x-direction for a system part

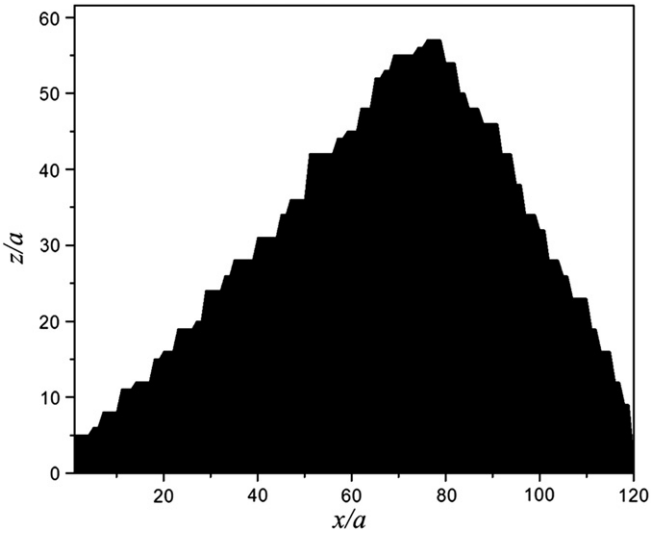

Fig. 2. Image of the system in the x direction obtained after 3754 deposited atoms. The x and z coordinates are normalized by the lattice constant a.