Growth model with a finite number of orientations on a linear substrate

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The aim of this work is to present a simple model for studying the texture formation during the electrodeposition process. Monte Carlo simulations are used to describe the formation of the deposits, and the scaling concepts are employed to characterize their growth and roughness properties. In this model particles are randomly deposited with an orientation chosen from a discrete set of possible directions. The final orientation of the deposited particle is determined by its interaction with the first neighboring particles and by the temperature of the substrate. Particle interactions are chosen according to the q-state ferromagnetic Potts model Hamiltonian. Simulations were performed on $(1+1)$ dimensions, and for several values of temperature and substrate size. The results of the simulations lead to different behaviors for the model at low and high temperatures. At high temperatures, the scaling exponent $\beta=0.5$ was found, which characterizes a pure random deposition model. However, at low temperatures, we observed that after a given time interval, particles start orienting in a fixed direction and the interface width saturates just during a time window. Suddenly, a fluctuation makes the interface width increase again, that is, we never observed a full saturation. On the other hand, at zero temperature, the system reaches an absorbing state with all the layers occupied by particles oriented in the same direction. At zero temperature we found $z=1.90$, $\alpha=1.80$, and $\beta=0.99$ for the dynamic, roughness, and growth exponents, respectively. The scaling exponents are consistent with a self-affine behavior of the model and they are in agreement with the well known Family-Vicsek scaling relation.

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I. INTRODUCTION

In the recent years a lot of attention has been devoted to the study and understanding of the deposited structures formed by electrodeposition [1–4]. The texture of the electrodeposits has attracted the interest of researchers since it is known that some deposits of metallic materials such as copper, silver, and iron have fiber textures [5–7]. A change in texture can give to the deposits different mechanical properties, such as wear resistance, corrosion [8].

Properties associated with the different textures are related to the distinct crystallographic planes seen on the electrodeposits [9]. In this sense if the electrodeposit texture is controlled during the electrodeposition process, material properties could be improved. Then, it may be relevant to direct the deposition in order to obtain a desired crystallographic plane. However, this can be a matter of considerable labor because the phenomenon of electrodeposition is very complex and involves a lot of variables, as for example, solution concentration, ion diffusion, types of substrate and electrolyte, nucleation rates, etc.

In this work we propose a simple model for the deposition of particles to be studied by Monte Carlo simulations and using the Metropolis prescription [10] to map the texture evolution during the electrodeposition process. We have also considered in this study the application of the finite size scaling arguments to describe the surface growth. The scaling laws of the self-affine surfaces have been observed in many different growth processes such as molecular beam epitaxy, electrodeposition, bacterial growth [11–14], etc. Apart from the intrinsic technological interest, the understanding of the solid growth is of a considerable interest, because it can provide us with important clues to the way in which complex structures are formed in nature through the aggregation of simple ones. For most of the kinetic models, the surface growth is accompanied by the fluctuations of the height interface. This property is defined by

$$W^2(L,t)=\frac{1}{L^2}\sum_{\vec{r}}\left[h(\vec{r},t)-\overline{h}(t)\right]^2, \tag{1}$$

where $h(\vec{r},t)$ is the height at the site position $\vec{r}$ and time t. The fluctuations of the height interface, also called surface width, increase as a power law $W\propto t^{\beta}$ at short times, and after long times, reach a steady state and behave as $W\propto L^{\alpha}$, which depends on the lattice size L. There is also an exponent z related to the crossover time t_c between the two regimes, which is defined by $t_c\propto L^z$. Based on these behaviors, Family and Vicsek [15] proposed the general scaling relation for the surface width,

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

where $f(x)$ is a scale function, which must satisfy the following asymptotic properties: if $x\ll 1$, $f(x)\propto x^{\beta}$ and if $x\gg 1$, $f(x)$ is constant. The exponents α, β, and z are not independent and they are related by $\beta=\alpha/z$.

For the model we consider in this work, we assume a random deposition of particles over an initially flat substrate. After adsorption, the main axis of the particle will be oriented in a given direction, chosen from a set of q directions parallel to the surface. As we will see in the following section, the deposition does not take into account the existence of overhangs, and it is known in literature as the solid on solid restriction [16]. All sites below the new incorporated site are necessarily occupied according to the SOS constraint. However, the final orientation of the particle is not

completely random, the new adsorbed particle relaxes to a given direction, which minimizes its free energy. This minimization depends on the interaction energy with its neighbors and on the temperature of the substrate. In order to describe the finite set q of possible orientations we consider a ferromagnetic Potts model [17] to account for the interactions. In this way, if a pair of nearest neighbor sites is in the same direction (state) there is no cost in energy.

In the following section, we will present the model, the variables we have defined, and the details of the Monte Carlo simulations, to describe the time evolution of the surface growth. In Sec. III we present the results of our simulations applied to growth in $(1+1)$ dimensions, and we compare them with the results we have found for a similar model previously studied in $(2+1)$ dimensions [18]. We also determined the behavior of the growth exponent as a function of the number of orientations and temperature. Finally, in Sec. IV, we present our main conclusions.

II. MODEL AND MONTE CARLO SIMULATIONS

We take as our substrate a linear chain of size L. The formed deposit is a two-dimensional structure, so we have a growth model on $(1+1)$ dimensions. Initially all the sites of the linear chain are empty, and we start depositing the next layer just after all the sites of the actual layer have been occupied. We considered periodic boundary conditions in the direction perpendicular to the growth surface. The whole process proceeds as follows. An empty site is randomly chosen on the current layer and a particle is deposited there. Then, the particle looks for the best orientation, which is selected according to the orientation of its first neighbors and the substrate temperature. The interaction energy between a particle at the site i and its nearest neighbors is given by

$$E_i = J \sum_{\langle ij \rangle} [1 - \delta(O_i, O_j)], \tag{3}$$

where the sum is over the nearest neighbors of the site i, and O_i is the orientation of the particle axis at this site. The variable O_i can take one of the values in the set $(1,2,\ldots,q)$, $\delta(O_i, O_j)$ is the Kronecker delta function, and $J>0$ measures the degree of relative orientation of the axis of the particles at the sites i and j. For example, if the particles at the sites i and j are oriented in the same direction the energy is zero, otherwise, in the case of different orientations, the energy is J. For the deposition onto a linear substrate, the maximum number of neighbors of a given site is three (two nearest neighbors in the actual layer, and one neighbor just below this layer).

When the particle arrives at the top of the ith column, we compute the value of E_i for each one of the q orientations that would be possible at this column. As the maximum number of neighbors is three the possible values of E_i are 0, J, $2J$, and $3J$. Then, we select the orientation having the lowest energy and that corresponding to the first excited level. Following this, we determine ΔE, which is defined as the difference of energy between the first excited and the local ground state level. So, we always have $\Delta E > 0$. According to the Metropolis prescription, the first excited level will be chosen with probability P, where P is given by the Boltzmann factor $P = \exp(-\Delta E/k_B T)$. Otherwise, we choose the level of lowest energy. In the calculation of P, T is the temperature, which is measured in units of J/k_B, and k_B is the Boltzmann constant. If more than one state (orientation) belongs to the selected energy level, then we choose, with the same weight, what will be the resulting orientation of the particle deposited. This works very well at low temperatures, where the probability to find states with energy larger than $2J$ is very small, and only the first excited state is of interest. On the other hand, at intermediate and high temperatures, we calculated the probability for each one of the orientations and the selected direction for the particle was done according to the heat-bath algorithm. This is particularly useful when the number of orientations, q, is large.

We recorded the orientations inside each layer, which corresponds to a unit of time in our Monte Carlo experiment, and we defined a variable that gives the mean orientation per layer, $S_l(t)$. Then, the mean orientation in the layer l at the time t is

$$\langle S_l(t) \rangle = 1/L \sum_{i=1}^{L} O(i,t). \tag{4}$$

We also calculated the fluctuations in the orientation, around the mean value $S_l(t)$, as a function of the time t and linear size L. It is defined by the following root mean square:

$$W_l(L,t) = \sqrt{\frac{1}{L} \sum_{i=1}^{L} [O(i,t) - \langle S_l(t) \rangle]^2}. \tag{5}$$

For each lattice size L, we can follow in time the evolution of these layer fluctuations during the growth process, that is, we write

$$W(L,t) = \sum_{j=1}^{t} W_l(L,j). \tag{6}$$

We will show in the following section that the function $W(L,t)$ exhibits a self-affine behavior, and the growth exponents can be calculated from the scaling relation of Family and Vicsek. While $W(L,t)$ can saturate at a finite temperature for the same model in $(2+1)$ dimensions, the saturation is possible only at zero temperature in $(1+1)$ dimensions. We have started our deposition process with an initial condition of a flat substrate, and the simulations were performed for lattices of size $L=100$, 200, 300, 400, 500. Depending on the size of the lattice, we need to consider up to 200 statistically independent samples in order to get reliable values for the averages of interest. We present explicit results for the number of orientations, $q=2$, 3, 4, and 5.

III. RESULTS

In Figs. 1(a) and 1(b) we plot the function $W(L,t)$, for $L=300$, $q=2$, at $T=0$ and at very high temperatures, re-

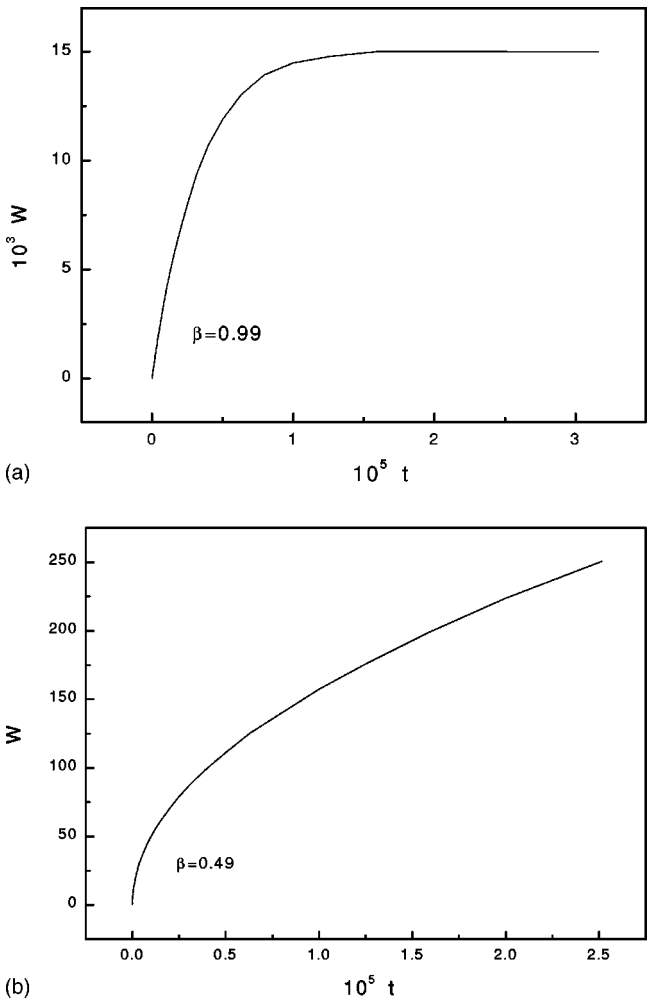

FIG. 1. Root mean square of the function W as a function of time t, measured in MCs, for $q=2$, $L=300$, and average over 150 samples. (a) $T=0$, where saturation is observed, $\beta=0.99$. (b) High temperature ($T=3$) where the surface width does not saturate, $\beta=0.49$.

spectively. Figure 1(a) shows that $W(L,t)$ saturates at zero temperature, and in this case it is possible to calculate the roughness exponent α associated with the steady state. After a saturation time, where each sample of the ensemble acquires a well defined texture (a fixed orientation for the particle axis), W becomes constant. For this zero temperature the growth exponent is $\beta=0.99\pm0.01$. For the other orientations the values we found for β are the same. We have also measured the exponents α and z. We have found that for all the q orientations considered, $\alpha=1.80\pm0.15$ and $z=1.90\pm0.15$. That is, the exponents related to the growth and saturation are not sensitive to the number of possible orientations of the particles over the substrate. Once we have reached the saturation regime, all the new deposited particles will be oriented in the same direction. On the other hand, Fig. 1(b) shows that at high temperatures the function $W(L,t)$ does not saturate, and only the growth exponent β can be defined. We have found $\beta=0.50\pm0.01$, which is typical of a random deposition model. The new adsorbed particle relaxes almost independently of its neighborhood, and we did not observe

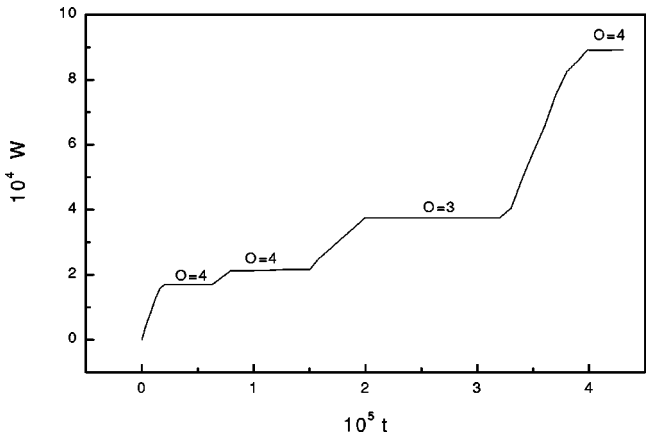

FIG. 2. Root mean square of the function W as a function of time t, measured in MCs, for $q=5$, $L=200$ for a selected sample. $T=0.085$, and the surface width does not saturate. The symbols O over the plateaux represent the orientations of the particles. For this very low temperature, $\beta=0.99$.

any characteristic texture for any sample of the ensemble at high temperatures. The behaviors at $T=0$ and at high temperatures are very similar to those seen in $(2+1)$ dimensions [18]. However, there is an important difference in the behavior of $W(L,t)$, in $(1+1)$ and $(2+1)$ dimensions, at low temperatures. While saturation is observed for the model in $(2+1)$ dimensions, for the model in $(1+1)$ dimensions saturation occurs only at zero temperature.

For instance, in Fig. 2, we can see the behavior of the function $W(L,t)$ at a very low temperature, but different from zero. This figure exhibits a typical route followed by any sample. The roughness does not saturate, despite the presence of some plateaux of variable time extent, where the layers contain particles oriented in the same direction. That is, the system reaches a well defined texture. Therefore, for some time windows, we observe some quasisteady states where the deposited particles exhibit the same orientation. However, for this low-dimensional system, fluctuations appear and some high energy states are populated. Depending on the fluctuation sizes, the system can eventually change from one orientation to a different one. In Fig. 2, where $q=5$ orientations are considered, we indicate over the plateaux some of the orientations seen in the interval $0<t<4\times10^5$. Then, in the region of the plateaux we have an apparent saturation. In this figure the first plateau appeared at $O=4$ orientation, then after some fluctuations the system returned to $O=4$ orientation (second plateau). Sometimes, strong fluctuations occur and the system is taken from a given orientation to a different one, as that happening between $1.5\times10^5<t<2.0\times10^5$ in Fig. 2. We have also calculated the growth exponent β at the initial times where we have a flat substrate and from a given plateau as $(W-W_O)\approx(t-t_O)^\beta$. In this expression t_O is the instant where we are leaving a given plateau whose interface width is W_O. For all the cases studied we found $\beta=0.99\pm0.01$, the same value as that at zero temperature. We cannot calculate the other exponents because the system never reaches an absorbing state as in the $(2+1)$ dimensions. At very low temperatures in

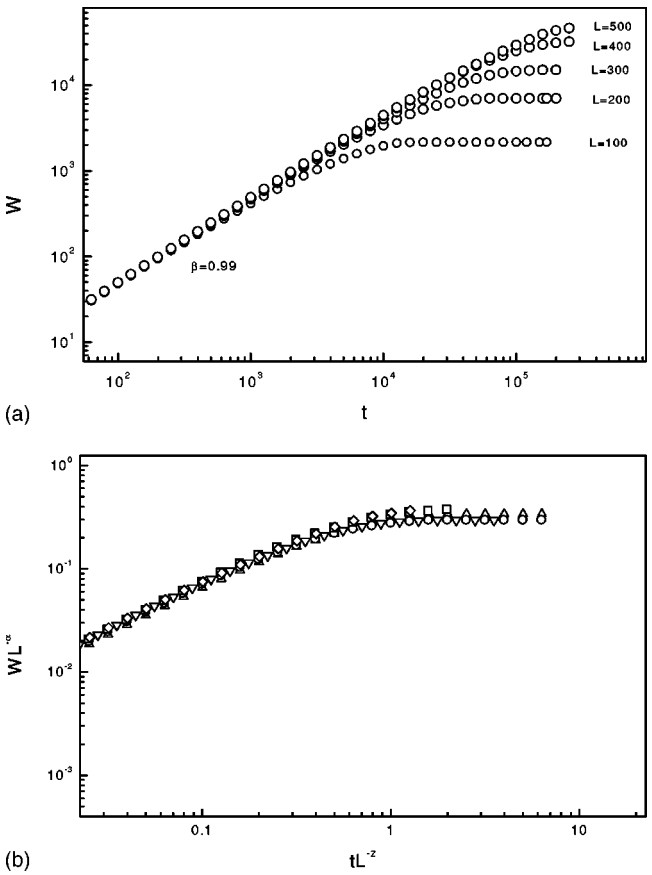

FIG. 3. (a) Surface width W as a function of time t, measured in MCs, for $q=2$, $L=100$, 200, 300, 400, and 500, and $T=0$. Averages are over 150 samples. (b) Data collapse of (a) according to the Family-Vicsek scaling relation. Diamonds ($L=500$), squares ($L=400$), down triangles ($L=300$), circles ($L=200$), and up triangles ($L=100$).

$(2+1)$ dimensions, the fluctuations in the orientation are only of short range, and do not allow the system to escape from the absorbing state.

Figure 3(a) is a typical plot of the function $W(L,t)$, for $q=2$, for all the studied lattice sizes at zero temperature where the saturation is observed. The data of Fig. 3(a) can be collapsed into a single curve that fits very well to the Family-Vicsek scaling relation. Then, Fig. 3(b) shows the data collapse, and from which we can find the critical indices for the growth. For the $q=2$ case of Fig. 3(b), the best values of the exponents that allow this fitting are $z=2.00$ and $\alpha=1.90$. As expected from the Family-Vicsek scaling law, the exponents α, β, and z are not all independent. As we can see from our data $\beta=\alpha/z$.

Finally, in Fig. 4, we show the values we have found for the growth exponent β as a function of temperature and q. We observe that the behavior of this exponent as a function of temperature is almost insensitive to the values of q. For temperatures less than 0.25, $\beta=0.99\pm0.01$, however, it is a decreasing function of T and, at high temperatures, the exponent becomes 1/2, as for the random deposition model. As we have pointed before, for any temperature different from zero, the fluctuations do not allow for a saturation of the surface for the times of observation we have considered. Therefore, this growing system does not exhibit a texture with a well defined orientation of the deposited particles at any finite temperature.

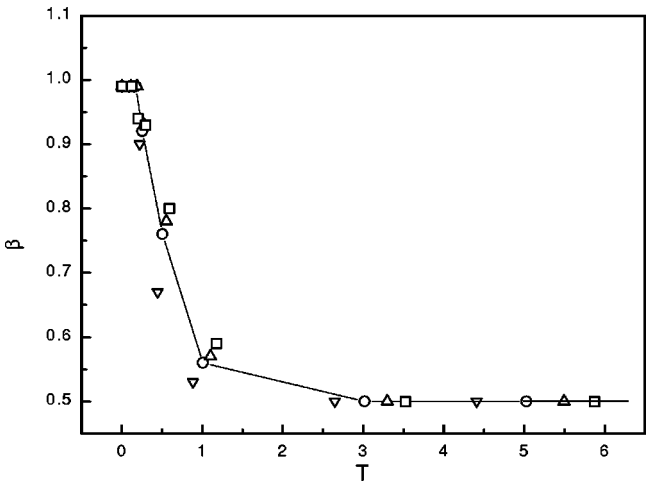

FIG. 4. Behavior of the growth exponent β as a function of T for different values of the number of orientations q. Squares ($q=5$), Down triangles ($q=4$), circles ($q=3$), and up triangles ($q=2$). The line is just a guide to the eyes.

IV. CONCLUSIONS

We have considered a very simple model to describe the texture evolution of the deposits formed by electrodeposition processes. In our model particles are randomly deposited onto a substrate, and they locally relax with their main axes pointing in a given direction. The final orientation depends on the substrate temperature and interaction energy with the neighboring particles. The lowest energy states of the system correspond to nearest neighbor particles oriented in the same direction. The model is mimicked by a Potts model of q states, where q gives the possible directions for the orientation of the particles. We recorded the orientations for each line and calculated the mean orientation and fluctuations as a function of time, size of the system, and number of orientations. We have investigated the cases $q=2$, 3, 4, and 5 for the lattice sizes $L=100$, 200, 300, 400, and 500. At zero temperature this growth model satisfies the well known Family-Vicsek scaling relation for all the values of q, and our estimate for the exponents α and z is $\alpha=1.80\pm0.15$ and $z=1.90\pm0.15$. The growth exponent that characterizes the system behavior at the initial times is $\beta=0.99\pm0.01$. At high temperatures we noted that the surface width does not saturate, and the system does not exhibit a texture with a well defined orientation of the deposited particles. In these cases the layers are occupied for all the possible orientations, which is characteristic of the random deposition model, where we found $\beta=1/2$ for the growth exponent. On the other hand, at low temperatures, the system never enters into an absorbing state, with a well defined texture. We observed quasisteady states just during short time intervals. Fluctuations in orientation in this $(1+1)$ system are always present

at any finite temperature, which prevent the system from reaching an absorbing state. We have also seen that the increase in the surface width when we left any plateau with a well defined orientation is given by $\beta = 0.99 \pm 0.01$, the same growth exponent as that found at zero temperature.

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