Surface Properties of a Selective Dissagregation Model

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Abstract

The scaling properties of one-dimensional surfaces generated by selective disaggregation processes are studied through Monte Carlo simulations. The model presented here for the deconstruction process takes into account the nearest neighbors interaction energies. This interactions are considered to be the energy barrier the detaching particle has to overcome in order to desorb from the surface. The resulting one-dimensional surface has self-affine properties and the scaling exponents of the surface roughness are functions of the interaction parameter $J/kT$, where $J$ is an interaction energy, $k$ is the Boltzmann constant and $T$ is the temperature. The dependence of the width exponents on the interaction parameter is analyzed in detail.

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There are three fundamental physical processes that give rise to the morphology of a surface: deposition, surface diffusion and desorption. The characteristics of the interfaces generated by the combination of deposition and surface diffusion have been well studied during the past decades \[1–3\]. In particular for growth models, particles are added to the surface and then are allowed to relax by different mechanisms. Many of this models have been shown to lead to the formation of self-affine surfaces, characterized by scaling exponents. From a theoretical point of view, the studies dedicated to the self-affine interfaces generated by growth models can be considered to follow two main branches. The studies about the properties of discrete models and the studies about continuous models. The first ones where dedicated mainly to the study of the properties of computational models in which the growth proceeds on an initially empty lattice representing a d-dimensional substrate. At each time step, the height of the lattice sites is increased by units (usually one unit) representing the incoming particles. Different models only differ on the relaxation mechanisms proposed to capture specific experimental characteristics. Then, the models are classified according to the values of the scaling exponents in several universality classes. The continuous models, on the other hand, are based on stochastic differential equations of the type \[4\]

\[
\frac{\partial h}{\partial t} = F - \nabla \cdot j + \text{noise},
\]

in which \(h(r, t)\) is the thickness of the film deposited onto the surface during time \(t\), \(F\) denotes the deposition rate and \(j\) denotes the current along the surface which in turn depends on the local surface configuration. When the surface current represents some experimental nonlinear equilibrium processes it gives rise to different types of nonlinear terms. The \(\text{noise}\) term corresponds to the fluctuations in the growth rate and, in general, is assumed to be uncorrelated. The differential equations are solved, either numerically or analytically (when it is possible), and the scaling exponents are determined. If the values of the exponents are similar to those of the discrete models, it is said that both (discrete and continuous models) belong to the same universality class, although the formal connection between both approaches is still an open question.

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Desorption or detaching processes, despite its technological importance, have not received the same attention. Maybe because they were considered to be the reciprocal of the growth models and no new characteristics were expected to appear.

There are many technological processes depending on the details of the etching phenomena and only recently few of them have been modeled in order to understand the phenomena at an atomic level [5]. As an example, corrosion is among the most important disaggregation processes, because its economical importance. A basic fact is that the corrosion attack is more intense at high temperatures and strongly depends on the type of material under attack. It would be desirable to take into account these characteristics in basic desorption models. In this paper we present a discrete disaggregation model, which can be considered as a generalization of a recently reported model [6]. We claim that our model is much more realistic than previous ones because we incorporate an interaction parameter proportional to the nearest-neighbor energies. The main characteristic of the model presented here is the dependence of the values of the scaling exponents on the interaction parameter.

It is well known that most chemical reactions that take place at a surface or interface, as well as those processes that lead to particles removing, are activated processes. The particle has to overcome an energy barrier in order to detach. In a first approach, this energy barrier could be consider to be proportional to the number of bonds the particle has at its location on the surface. Then, the energy barrier could be written as \( nJ \), where \( n \) is the number of nearest-neighbors of the particle and \( J \) is the bonding energy. Following this line, it is usual to represent the probability for a particle to overcome a barrier of height \( nJ \) as

\[
p_{(n)} = \exp(-nJ/kT),
\]

where \( T \) is the temperature and \( k \) is the Boltzmann constant. In our model, the resulting self-affine interface shows different values of the scaling exponents for different values of \( J/kT \), as a consequence of the dependence of the desorption probability on the interaction parameter.

In our computational model, the surface is represented by an one-dimensional array of integers specifying the number of atoms in each column. In order to maintain the solid-on-solid characteristic of the model the detaching processes will not give rise to overhangs.
The simulations were carried out in the following way: each column of the one-dimensional array is initially filled enough in order to allow the deconstruction process to take place during the whole simulational time, i.e., no column height must become negative at the end of the simulation. By initially filling all columns with the same amount of atoms the the simulations start with a flat surface at $t = 0$. In order to simulate the selectivity of the deconstruction process, a column $K$ is picked at random. Then, the site with the greatest number of open bonds is selected among the site $s(K)$ lying at the top of the column $K$ and the sites $s(K - 1)$ and $s(K + 1)$ at the top of each of the neighbors columns. After selecting the column with the greatest number of open bonds, the detaching probability for the particle at the top of the selected column is calculated as $p(n) = \exp(-n J/kT)$. The particle is detached from the selected position if a random number $r$ is less than $p(n)$.

Then, the detaching probability depends on the number of nearest-neighbors $n$ of the atom in the direction $x$ running parallel interface, i.e, in our model $n = 0, 1$ or 2. The interaction energy corresponding to the neighbor in the direction $y$, perpendicular to the interface, is not taken into account since it is present in all detaching atoms. In this way the atom with less neighbors $n$ has the greatest probability to desorb from the surface.

Following the studies realized to growing models we expect that the surface generated by the above described process presents self-affine properties. Then, we are mainly interested in the scaling properties of the width (or roughness) defined as

$$\omega(L, t) = \left[ \langle h^2(x, t) \rangle_x - \langle h(x, t) \rangle_x^2 \right]^{1/2},$$

where $\langle \cdot \rangle_x$ denotes average over the entire lattice size $L$, $h(x, t)$ is the height of the column at position $x$, $\langle h(x, t) \rangle_x$ is the average surface height and $t$ is the time, roughly proportional to the number of removed monolayers $m$.

As for a growth processes we assume that the roughness obeys the Family-Vicsek scaling law [7], valid for self-affine interfaces,

$$\omega(L, t) = L^\alpha f \left( \frac{t}{L^z} \right),$$

where $\alpha$, $z$ and $f$ are universal scaling exponents.
being $\alpha$ the roughness exponent because $\omega \sim L^\alpha$ when $t \gg L^z$ and $\beta$ the growth exponent because $\omega \sim t^\beta$ when $t \ll L^z$. In our case there is, of course, no growth but an exponent $\beta$ can be defined in the same way. $z = \alpha/\beta$ is the dynamic exponent.

In our model, the relevant characteristic is the dependence of the scaling exponents $\alpha$ and $\beta$ on the interaction parameter $J/kT$ and this characteristic in investigated in detail here. The exponent $\beta$ was determined by measuring the slope of the log-log plot of $\omega(L,t)$ vs $t$ at early times and the results presented below were obtained for systems sizes of $L = 5000$. On the other hand, the exponent $\alpha$ was determined using the correlation height-height correlation function defined as $c(r,\tau) = \langle [h(x,t) - h(x + r, t + \tau)]^2 \rangle_{r,\tau}^{1/2}$. The correlation function is known to scale in the same way as the width $w(L,t)$; in particular for $t \gg L^z$ and for $r \ll L$ the correlation function behaves as $c(r,0) \sim r^\alpha$. Results presented below for the exponent $\alpha$ where obtained by measuring the slope of the log-log plot of $c(r,\tau)$ vs $r$ in the limit $r \to 0$. For all the presented values of the interaction parameter $J/kT$ the used lattice size was $L = 1000$ because the correlation function calculation must be done at long times in order to allow the width to reach the saturation value. Averages where taken over the necessary independent runs to reduce the statistical error below 0.4% in all the simulations.

In Fig. 1 a log-log plot of the interface width versus time is presented. Time is advanced by $1/L$ when a particle at the upper monolayer is asked to detach. In Fig. 1 the upper points with the label RND where obtained by removing the particle at the top of randomly selected columns. Its slope is 0.5 and is presented as a reference. The other plots corresponds to the behavior of the width for various increasing values of the interaction parameter $J/kT$. It can be seen that the slope is smaller for larger values of $J/kT$. This behavior is quantitatively verified by the plot in Fig. 2. In this graphic, the values of the exponents $\beta$ are plotted as a function of $J/kT$. The values for $\beta$ were obtained from the slopes of the lines fitting the log-log plot of the points of the width vs time. Although only few values of $J/kT$ are plotted, clearly there is a continuous variation of the exponent $\beta$ with the interaction parameter. It can be seen that the value of $\beta$ deceases as the interaction parameter increases but, after
certain crossover, a limiting value $\beta \approx 0.26$ is reached and the exponent does not decrease for further increments in $J/kT$. The height-height correlation function for long times is plotted in Fig. 3 for the same values of $J/kT$ as shown in Fig. 1. The dependence of the slope of $c(r,0)$ on the interaction parameter is evident. The values of the exponent $\alpha$ were obtained from the slope of the lines through the points for $r \to 0$. The values of $\alpha$ are plotted in Fig. 4 as a function of $J/kT$. As for $\beta$, the same limiting effect can be observed, and also the value of the exponent decreases as the interaction increases for the lowest values of the parameter.

The presented results can be interpreted in several ways. For fixed $J$, these results show that below certain temperature the scaling properties of the interface do not change. For fixed temperature it can be seen that materials with greater interaction energies present more resistance to etching. However, these are not linear effects. On the other hand, the behavior of the width of the surface is in agreement with the intuitive picture of a corrosion process, for instance. The roughness of the surface tends to decrease with increments of the interaction parameter indicating that if the interaction energy is large or the temperature is low, the surface is less affected by the attack, but eventually exponent $\beta$ reaches a saturation value.

In summary, the model presented here capture the basic behavior of chemical disaggregation processes and show how the self-affine characteristics of the surface are affected by the inclusion of an interaction parameter. The model cannot be associated to any known continuous model because there is a parameter that continuously control the value of the scaling exponents. No continuous model shows this characteristic. In continuous growth models the values of the exponents are independent of any parameter involved in the stochastic differential equations. A possible equivalent discrete growth model would be a deposition model in which the particles sticks at the sites with the smaller number of bonds. However this will result in an unrealistic deposition model. The model presented here incorporates a realistic physical parameter, the interaction $J/kT$, which appears usually in many atomistic processes and, since the values of the scaling exponents depend on this parameter, the
model does not fall in any known universality class. There are interested extensions of the present work that can be pointed out; the inclusion of next-nearest-neighbors interactions (competitive and not competitive) and the case of deconstruction in 2+1 dimensions. These cases are under study and the results will be published elsewhere.
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FIGURES

FIG. 1. Plot of the interface width $w(L, t)$ versus time in log-log scale. The slope through the upper points with the label RND is 0.5. The other points correspond to the simulation results of the deconstruction model, for various values of $J/kT$, using $L = 5000$.

FIG. 2. The exponent $\beta$, measured from the slopes through the points plotted in Fig. 1 as a function of $J/kT$.

FIG. 3. Height-height correlation function $c(r, 0)$ as a function of $r$ for various values of $J/kT$ plotted in a log-log scale. The correlation function is measured using $L = 1000$ after the saturation value of the width was reached.

FIG. 4. The exponent $\alpha$, measured from the slopes through the points plotted in Fig. 3 in the $r \to 0$ limit, as a function of $J/kT$. 

Figure 1
Figure 2
Figure 3
Figure 4