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Dynamic Scaling Theory of $A+B \rightarrow 0$ Surface Reaction

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We study several sapects of the irreversible depositions of two different species of particles on a surface with $A+B \rightarrow 0$ chemical reactions. Two types of reaction are considered in $1+1$ dimensions. The anlaytic results are obtained if the reation occurs only when a A (or B) particle deposits on the top of a B (or A) particle (vertical reaction). The surface width grows like the random deposition model ($\beta=1/2$) but the average height scales as $t^{1/2}$. When the horizontal reactions occur in adition to the vertical reactions, the surface width saturates in the long time limit and we find numerically $\alpha=1/2$ and $\beta=1/4$. This model can be mapped exactly to the Edwards-Wilkinson model with uncorrelated random desorptions.

In recent years considerable interests have developed in a variety of growing rough surfaces. Various natural and industrial dynamical processes lead to the formation of rough surfaces.[1,2] Crystal growth, spray painting and coating, biological growth, vapor deposition, and electroplating are a few examples. However, because these are stochastic processes involving nonequilibrium many-body effects, the standard approaches of statistical mechanics are not suitable for describing the surface growth problem. It has been recognized that the deposit has a compact structure with a well-defined density, while its growing surface exhibits a self-affine[3,4] fractal geometry and naturally evolves to a steady-state having no characteristic time or length scale. This has led to the development of a dynamical scaling approach[3,5] for describing growing rough surfaces. The surface of the deposit can be described in terms of the following scaling form,

$$w(L,\ t)=L^{\alpha}f\left(\frac{t}{L^{z}}\right) \tag{1}$$

where w is the surface width, t is time and L is the lateral size of the deposit. The scaling fuction $f(x)$ is defined by

$$f(x)\sim\begin{cases} x^{\beta} & x\ll 1 \\ \text{const}x\gg 1 \end{cases} \tag{2}$$

with the dynamical exponent $z=\alpha/\beta$. The study of simplified numerical models aimed at underatanding the dynamics of growing surfaces have been done. In $1+1$ dimensions, simulations give $\alpha\simeq/1/2$ and $\beta\simeq/1/3$ for the ballistic model[3,6] and Eden model.[7,8] By introducing surface diffusion in the random deposition model,[3] it has been found numerically that $\beta\simeq/1/4$ and $\alpha\simeq/1/2$. A theory of deposition processes by Edwards and Wilkinson[9] is able to predict the values of α, β, and z for the random deposition model with surface diffusions. By solving a linear Langevin equation in $1+1$ dimensions, they obtained exactly the values of the exponents $\alpha=/1/2$, $\beta=1/4$ and $z=2$ which is in excellent agreement with simulations.[3] This work was later extend by Kardar et al.[10] who took into account the possibility of lateral growth. They showed that the values of exponents $\alpha=1/2$, $\beta=1/3$ and $z=3/2$ in $1+1$ dimensions.

One motivation for this work is to construct models of growing rough surface where some elementary reactions may occur on the deposited surface. We study the random deposition model on one dimensional substrate in which particles are depositied from above onto a line of L sites. But impinging particles are mixture of two different species, A and B, with probabilites P_A and $P_B=1-P_A$, respectively. On depositions, adjacent $A-B$ pairs react and desorb from the surface. In order to keep models simple enough to investigate, either analytically or numerically, we first consider the vertical reaction model.

For the vertical-reaction model, the reaction occurs when a A (or B) particle deposits on the top of a B (or A) particle column. Since there are no reactions possible horizintally, the vertical reactions only affect the height of each column independently. Without reactions, the growing rough surface should be described by the random deposition model. The simulation results in Figure 1 show the dependence of the surface width w on h at different values of the probability P_A. Here the averaged deposition height$\langle h\rangle$is definded by the number of deposited particles per each sites. The heights of columns in this case form a Poisson distribution and correspondi-

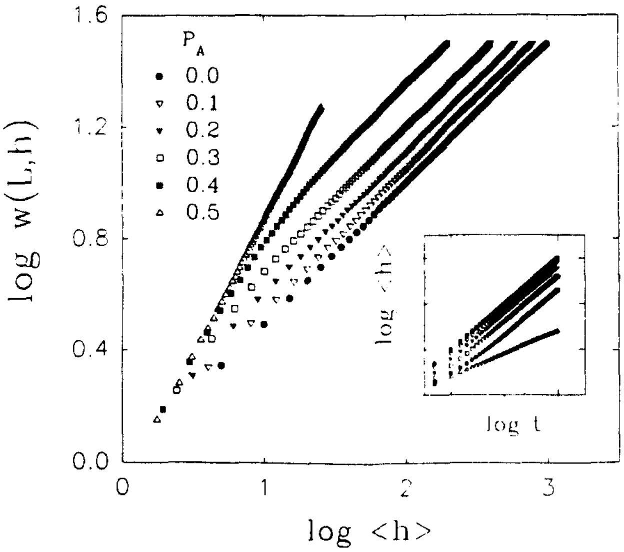

Fig. 1. Plots of the surface width $w(L,h)$ against the averaged deposition height $<h>$ for $L=128$. Dependence of $<h>$ on time t is also shown in the inlet.

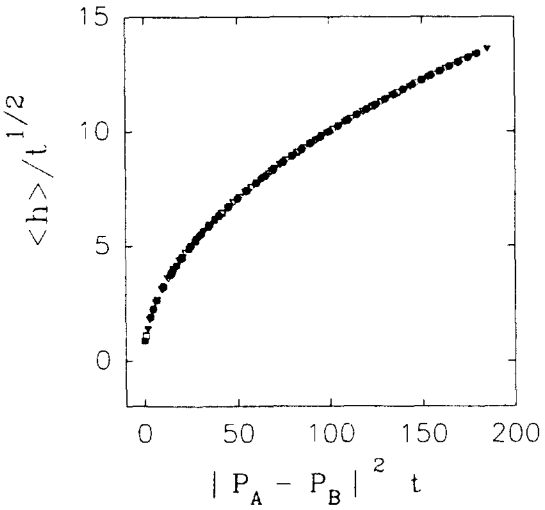

Fig. 2. Scaling plot showing that data for $<h>/t^{1/2}$ plotted against $|P_A-P_B|^2t$ for various values of P_A perfectly fall on a single curve.

ngly the surface width diverges with $<h>$, independent of L. We have found that surface width diverges with $<h>$, independent of L. We have found that $w\sim<h>$ for $P_A=P_B=1/2$ and $w\sim<h>^{1/2}$ for $P_A\neq P_B$. The dependence of $<h>$ on time t is found to be $<h>\sim\sqrt{t}$ for $P_A=P_B=1/2$ and $<h>\sim t$ for $P_A\neq P_B$. Thus in any case the surface width scales as $w\sim t^{1/2}$ to give an exponent $\beta=1/2$. Our vertical-reaction model gives the same result as the random deposition model, but the averaged deposition height scales as $<h>\sim\sqrt{t}$ in the case of $P_A=P_B=1.2$.

We also propose the following scaling form for the average height:

$$<h>=t^{\gamma}f(|P_A-P_B|^{\phi}t) \tag{3}$$

$$f(x)=\begin{cases}\text{const.} & x\ll 1\\ x^{1-\gamma} & x\gg 1\end{cases} \tag{4}$$

In Figure 2 we have plotted $<h>/\sqrt{t}$ against $|P_A-P_B|^{2t}$ for various values of P_A. The curves collapse perfectly on a single scaling function, which confirms the above scaling form with $\gamma=1/2$ and $\phi=1/2$ and $\phi=2$. Since this model does not have any interactions between columns, the height of each column changes independently. If the same (or different) kind of particle is deposited on an existing column, its height increases (or decrease) by unity. This is nothing but a one-dimensional random walk. But if a particle is deposited on a bare site(substrate), a new column beginss to grow; the substrate behaves like a mirror. So the model can be mapped into one-dimensional random walks with a reflection boundary. Using the known probability distribution of random walks with reflected boundary conditions, for the case of $P_A=P_B$ (unbiased random walks), we obtain

$$<h>\sim\sqrt{\frac{2}{\pi}}t^{1/2},\ w\sim t^{1/2}. \tag{5}$$

And for the case of $P_A\neq P_B$ (biased random walks)

$$<h>\sim\sqrt{2t}(P_A-P_B),\ w\sim 2(tP_AP_B)^{1/2}. \tag{6}$$

These analytic results are in an excellent agreement with the simulation result. One can also consider the model with a particle reservoir rather than with a bare substrate. We use a reservior of B particles as a substrate and deposit. A particles from above. This model is equivalent to the random deposition model except that $<h>\sim 0$ when $P_A=P_B=1/2$.

Now we consider the model with the horizontal reactions in addition to the vertical reactions. The impinging particle now looks for its nearest-neighbor sites. If a different kind of particles is found, they react and leave from the surface by the $A+B\to 0$ reaction. When a particle finds B particles both on the target site and the nearest-neighbor sites, the horizontal reaction occurs. For convenience, we use a B particle reservior as a substrate and then deposit particle A with the probability P_A. The simulation results in Figure 3 show the dependence of the surface width $w(L,t)$ on time t, defined by $t=N/L$ where N is the total number of impinging particles. The nearest neighbor interactions invoked by the horizontal reactions tend to smooth out the surface. In the short time region$(1\ll t\ll L)$, $w(L,t)$ varies with t as the surface. In the short time region $(1\ll t\ll L)$, $w(L,t)$ varies with t as

$$w(L,t)\sim t^{\beta}. \tag{7}$$

The slopes from the curves in Figure 3 give $\beta=1/2$ for $P_A=0$ and $\beta=1/4$ for nonzero P_A. Even for very small value of P_A, the exponent β is found to be 1/4 as shown in the inlet of Figure 3. In the long time limit, the surface width begins to saturate to a constant value $w(L,\infty)$ unlike the vertical reaction model. The dependence of $w(L,$

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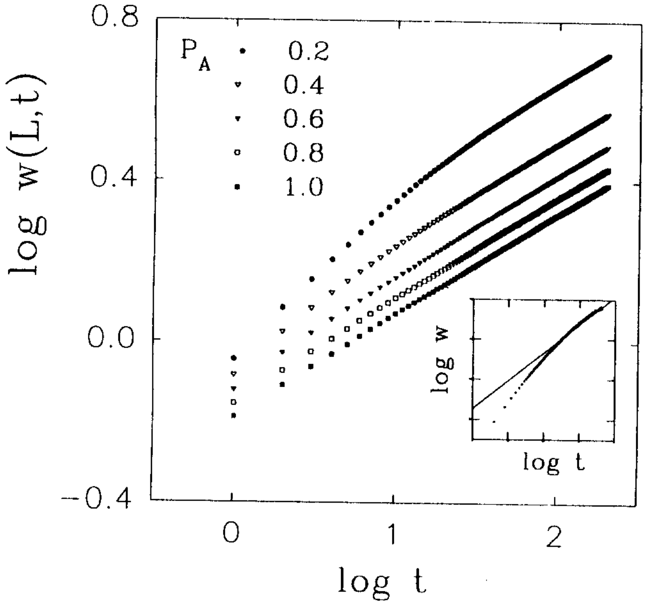

Fig. 3. Time dependence of the surface width $w(L, t)$ for $L=1024$. The case of $P_A=0.01$ in the inlet.

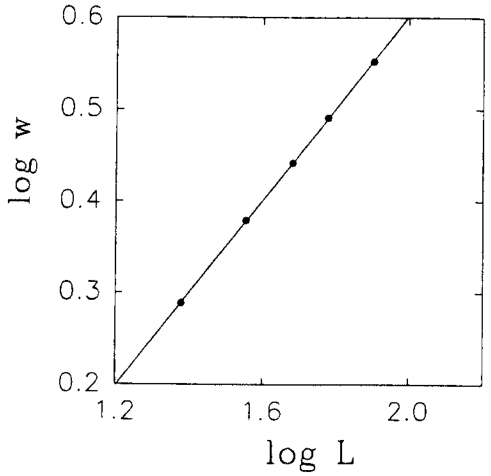

Fig. 4. Size dependence of the saturated surface width $w(\infty, t)$.

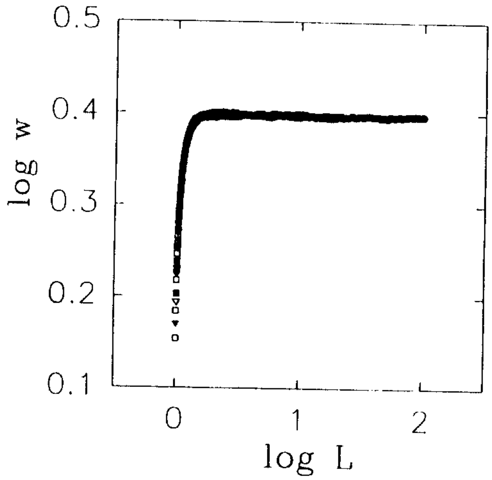

Fig. 5. Scaling plot of $w/L^{1/2}$ against t/L^2 for various system sizes.

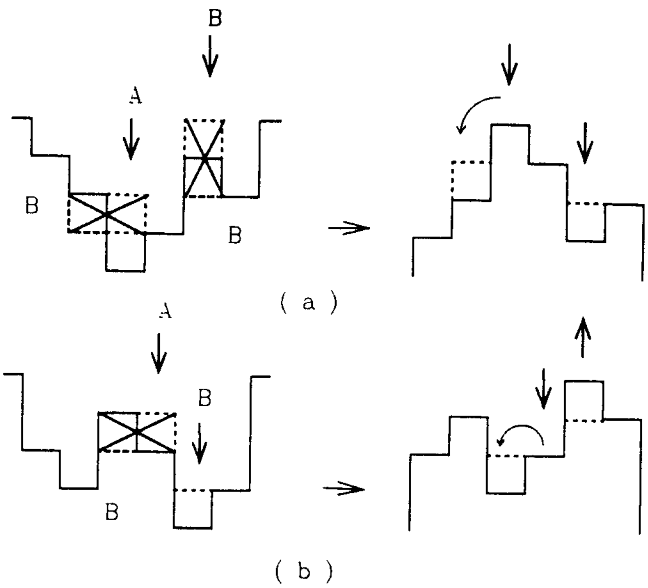

Fig. 6. (a) Mapping to the EW model at $P_A=1$. (b) Mapping to the EW model with random desorptions for nonzero P_B.

∞) on L is shown in a log-log plot in Figure 4. The straight line through the data points indicates that the saturated surface width varies as

$$w(L, \infty) \sim L^{\alpha}, \tag{8}$$

where we estimate the slope of the line, $\alpha=0.505\pm0.002$.

The scaling results of Eqs. (7) and (8) suggest us to fit the data into the well-known dynamical scaling form, Eq. (1). In Figure 5, we have plotted $w/L^{1/2}$ against t/L^2 for various values of L at $P_A=0.5$. The data collapse on a single scaling function almost perfectly.

The above scaling results indicate that our nearest-neighor reaction models (including both vertical and horizontal reactions) at nonzero P_A may belong to the same universality class as the Edwards-Wilkinson (EW) model, which is the random deposition model with diffusion process ($\alpha=1/2$ and $\beta=1/4$). Actually at $P_A=1$, our model can be mapped exactly to the EW model as shown in Figure 6(a). By turning upside down of a surface configuration of our model, we can get a corresponding surface configuration of the EW model. A vertical reaction corresponds to a deposition of a particle without diffusion and a horizontal reaction to a surface diffusion of a particle into a lower site in the EW model. For nonzero P_B, our model is equivalent to the EW model with uncorrelated random desorption processes. A deposition of a B particle on a B-particle reservoir corresponds to a desorption of a particle in the EW model. Our simulation results imply that the uncorrelated random desorption processes in the EW model are irrelevant on the scaling behavior of the rough surface. A trivial limit of our model is obtained at $P_A=0$, which is the pure random deposition model with $\beta=1/2$ and no saturation occurs.

In summary we have studied the surface deposition model with the reactions between two different species of particles. The model with the vertical reactions only exhibits the same critical behavior as the random deposition model but the average height scales differently when $P_A=P_B=1/2$. The model with the horizontal and vertical reactions is found to belong to the same universality class of the EW model with the random deposition process. Extended versions of the present model, for example, with the ballistic depositions or the random depositions with the correlated desorptions are now under investigation. These results will be reported elsewhere.

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