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Power-Law Exponents for a Spreading Front and Growing Interface in an Irreversible Wetting

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Using computer simulations, the power-law behavior of the interface growth of a spreading fluid is studied in a two-dimensional lattice model. The interface width exponent ν and the dynamical exponent k for the evolution of the front are consistent with their dynamical scaling relation. The magnitude of these exponents seems to depend upon the nature of the substrate and the concentration of the carriers of the wetting fluid.

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To describe the evolution of the growing interface in a granular deposit, Edwards and Wilkinson[1] have studied the Langevin equation for the surface profile. Kardar, Parisi, and Zhang[2] (KPZ) have extended it to model the driven interface growth by adding a lowest-order nonlinear term to the Langevin equation, i.e., by the Burgers equation,[3]

$$\partial h/\partial t = D\nabla^2 h + (\lambda/2)(\nabla h)^2 + \xi(x,t)\,, \tag{1}$$

where the height $h(x,t)$ represents the interface profile, D is the diffusion constant, $\xi(x,t)$ is the random noise with zero mean, and λ is the coefficient of the nonlinear term. Using a renormalization scaling, KPZ predicted[2] a remarkable relation between the exponents of the dynamical scaling[4] for the interface width,

$$W(R,t) = \langle h^2\rangle - \langle h\rangle^2 = R^{\chi} W_0(t/R^z)\,, \tag{2}$$

with

$$2\chi = (2-d) + (2-\eta-z)\,, \tag{3}$$

where R is the linear size of the substrate, z and η are the dynamic and hydrodynamic exponents, respectively, and d is the spatial dimensionality. For nonzero λ, KPZ have predicted[2] the growth exponents $\chi = \frac{1}{2}$ and $z = \frac{3}{2}$. Applicability of these results and their verifications to a variety of growth models by computer simulations have attracted considerable interest in recent years.[4-15] We study a computer-simulation model of an irreversible wetting front and we find that the exponents χ/z and $1/z$ are consistent with relation (3) but their magnitude may depend on the microscopic details such as the nature of the substrate and the concentration of the carriers.

We consider a two-dimensional discrete lattice of size $L_x \times L_y$. One end of the lattice, say, the first column, is connected by a source of the wetting fluid while the opposite end, the L_xth column, by an absorbing sink. A fraction p of the lattice site is randomly occupied by particles (the carriers of the wetting fluid) which are in constant stochastic motion. Initially, all the particles and lattice sites are dry, except those in contact with the source where the particles are supersaturated and the occupied sites are wet. A particle becomes supersaturated as soon as it comes in contact with the source. A supersaturated particle wets all the sites along its trajectory and becomes dry when it hits the sink. A dry particle cannot wet a dry site; however, a wet site remains permanently wet—an irreversible wetting. Thus, as the particles execute their stochastic motion, some of them become supersaturated on contact with the source and spread the wetting fluid along their trails. An interface between the wet phase (from the source side) and the dry phase develops as the noisy fluid front moves into the dry lattice. The stochastic geometry of the carrier trails may depend on the concentration of the carriers, their interaction with the host, and the nature of the substrate. Here we address questions such as: How does the interface evolve? How does the front move? How do the microscopic details (the nature of the substrate and the carriers) affect the interface growth and the front motion?

Two types of substrates are considered: (1) the smooth substrate in which there is no interaction between a particle (supersaturated or dry) and its neighboring empty sites and (2) the rough substrate in which the empty sites attract their neighboring supersaturated particles. The wetting density of a supersaturated (dry) particle is assumed to be unity (zero) and, therefore, the total number of supersaturated particles N_s is a measure of humidity; the wetting density of a supersaturated particle is assumed to be unity. To maintain a zero level of humidity, each empty site is assigned a superdry density $\rho_u = -N_s/N_e$, where N_e is the number of empty sites. Apart from the hard-core interaction among the particles, they interact with their neighboring particles and empty sites with a nearest-neighbor interaction which is equal to the product of their densities (see below). Thus, while a supersaturated particle is attracted towards empty dry sites, there is no force between a dry particle and an empty site. A particle and an empty site can interchange their positions if it is energetically possible, as in most Monte Carlo (MC) simulations.[16] The empty sites, in this model, act as the background medium that affects the movement of the supersaturated carriers. Such a repulsive interaction among the supersaturated

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carriers and an attractive interaction between the supersaturated particles and the substrate, along with the random distribution of particles and empty sites, may take into account the effects of the viscous and the capillary forces for the transient spreading trail of the supersaturated carriers. Thus, the wetting fluid spreads along the ramified trails as the capillary forces compete with viscosity which should depend on the concentration of the carriers in this model.

The active zone for the irreversible wetting is the locus of sites on the frontiers of the spreading fluid which is different from the diffusive front of particles in a gradient percolation.[17] One may expect that the width of the interface between the wet and the dry phases (i.e., the roughness of the wet surface) and the growth of the front position R should follow the dynamical scaling (2) which has been remarkably successful in understanding a variety of growth models such as ballistic deposition[4] and the Eden model[8] at least in two dimensions. Simulation results on our irreversible wetting model seem consistent with the KPZ predictions and the dynamical scaling; however, the magnitude of χ/z and $1/z$ exhibits a variation as a function of carrier concentration (at least on a rough substrate).

We have used various sample sizes at almost all carrier concentrations ($p=0.1$–0.9). We use the following method for the hopping mechanism of the particles. A particle at site i and one of its neighboring site j are selected randomly. If site j is empty, then we calculate (a) the interaction energy E_0 with the particle at site i,

$$E_0=\rho_i\sum_k\rho_k\ , \tag{4}$$

where the index k runs over all the neighboring particles and empty sites; and (b) the interaction energy E_1 for a configuration in which the position of the particle is interchanged with the randomly selected empty site. If the change in energy $\Delta E=E_1-E_0<0$, then the particle is moved from site i to site j; if $\Delta E=0$, then the particle's move is allowed with half probability. On the other hand, if site j is occupied, then an attempt to move the particle from site i to site j fails and the particle remains at site i. An attempt to move each particle, once irrespective of their success to hop, is defined as one Monte Carlo time step (MCS). A periodic boundary condition is used for the particle's hop along the transverse (y) direction and the open boundary condition along the longitudinal (x) direction at the source and at the sink. Initially, those particles are supersaturated which are in contact with the source (at the first column) where the wetting front begins; all other particles have zero wetting density. As stochastic motion proceeds, more particles become supersaturated (or charged with the wetting fluid) on contact with the source; a supersaturated carrier becomes dry (or discharged) with zero wetting density on contact with the sink. Since all the particles (except those in contact with the source) are initially dry, the probability of fluid transfer from the source is high and the probability of fluid discharge (i.e., the evaporation) at the sink is very low.

The nonequilibrium state of the fluid flow is sustained throughout the simulation as we limit ourselves to the time regime in which the interface width grows; we discard all the data beyond a time step when the active zone hits the opposite end (the sink) where the interface width begins to decay. In other words, the lattice sites beyond the wetting front (and, therefore, the lattice size along the direction of front propagation) do not restrict the interface growth in our analysis. In our study, the spreading of the fluid is governed by the position of the front and, therefore, the average position of the front R serves as the limiting size, as far as the interface growth is concerned. A number of independent samples (300–500) are used to evaluate the mean front position and the mean interface width (2).

Now, if the dynamical scaling (2) is valid here, then the exponent k with $R\sim t^k$, $k=1/z$, can be evaluated from the slope of the logarithm of the front position versus the logarithm of the time plot. A plot of the estimate of k versus carrier concentration is presented in Fig. 1. As we see that the magnitude of the exponent k lies between 0.60 (around $p=0.5$–0.7) and 0.66 at the extreme concentrations ($p=0.1$ and 0.9), while the predicted value is $\frac{2}{3}$ for other growth models. One should, however, note a nonmonotonic trend in the behavior of the exponent k, a systematic decline followed by a regular increase with p (Fig. 1). The interface width exponent ν in $W\sim t^{\nu}$ can also be evaluated from the log-

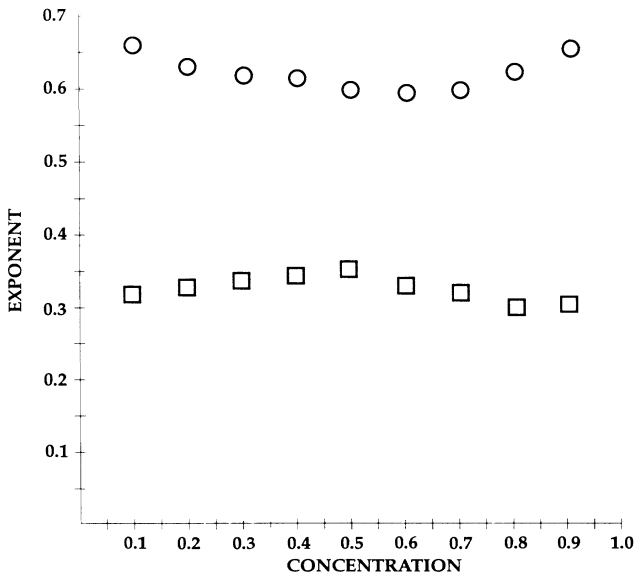

FIG. 1. Exponents for the front motion k (○) and for the interface width ν (□) vs carrier concentration p. The sample size 100×50 is used with 300 independent runs; statistical error bars are within or comparable to the size of the symbols.

TABLE I. Exponent relation $\chi+z=(1+\nu)/k$ for smooth and rough substrates at various carrier concentrations p with sample size 100×50; these data are taken from Figs. 1 and 3 and have the same error bars.

	Smooth			Rough		
p	ν	k	$(1+\nu)/k$	ν	k	$(1+\nu)/k$
0.1	0.32	0.66	2.00	0.33	0.63	2.11
0.2	0.33	0.63	2.10	0.31	0.56	2.32
0.3	0.34	0.62	2.17	0.29	0.57	2.25
0.4	0.34	0.62	2.17	0.33	0.58	2.30
0.5	0.36	0.60	2.25	0.31	0.60	2.20
0.6	0.33	0.60	2.22	0.26	0.61	2.09
0.7	0.32	0.60	2.20	0.27	0.64	1.98
0.8	0.30	0.63	2.08	0.25	0.71	1.78

log plot of the width versus time. With the scaling relation (2), $\nu=\chi/z$ and the predicted value, $\chi/z=\frac{1}{3}$. Fluctuations in the magnitude of these effective exponents may be due to long relaxation time (especially at high carrier concentrations). Overall, the dynamical scaling relation (3) for $d=2$, i.e., $\chi+z=(1+\nu)/k\approx2$, seems to be valid (see Table I).

A similar analysis for the interface growth is also carried out on the rough substrate where empty sites attract their neighboring supersaturated particles. Figure 2 shows the variation of the mean front position with time for the whole concentration range. The relaxation time increases with increasing carrier concentration as the substrate becomes rougher; i.e., the viscosity of the medium increases with the concentration. Therefore, one has to be careful in selecting the data points here for evaluating the effective exponent k in the asymptotic regime. Our estimates of k are presented in Fig. 3, which shows a similar nonmonotonic behavior with the concentration p as in the case of the smooth substrate. The interaction between the substrate and the carriers, however, leads to a more pronounced effect here with a minimum value of k $(=0.48\pm0.02)$ around $p\sim0.4$ and a maximum $(=0.71\pm0.01)$ at about $p\sim0.8$. The log-log plot of the interface width versus time, on the other hand, does not show a systematic growth with the concentration; variation of the corresponding exponent ν is presented in Fig. 3. It is hard to estimate the exponent ν at the concentration $p=0.20$ (see Figs. 2 and 3) and, therefore, its magnitude may not be reliable. The relaxation regime expands with increasing carrier concentration p. We have observed a systematic decay in the magnitude of k from 0.48 ± 0.02 (at $t=450$ MCS) to 0.25 ± 0.02 (at $t=2700$ MCS) at a high concentration ($p=0.8$). The magnitude of $\chi+z=(1+\nu)/k$ shows more fluctuation here than that for the smooth substrate; nevertheless, it remains around 2 over the whole concentration regime (see Table I).

In summary, we have studied the growth of the roughness of an irreversible wetting front in two model substrates. We have evaluated the exponent k for the motion of the spreading front and exponent ν for the growth of the interface width. We find that the exponent k depends, nonmonotonically, on the concentration of the carriers of the wetting fluid. The estimate of the exponent k for the spread of the front position ranges from

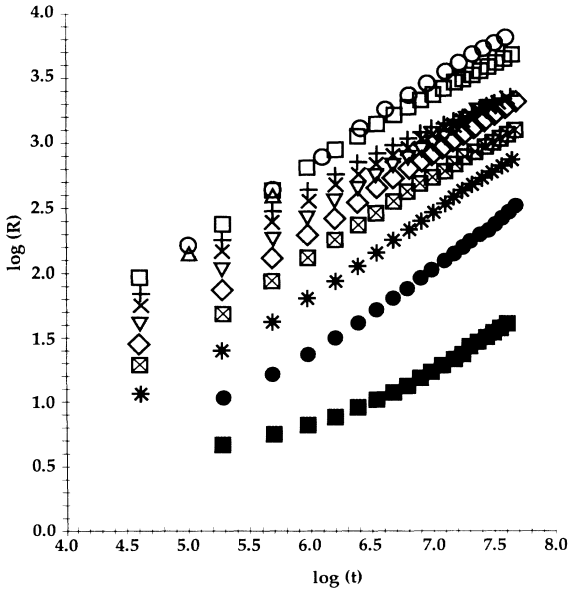

FIG. 2. Logarithm of the mean front position vs logarithm of time for the wetting on a rough substrate. The sample size 100×50 is used with 300 independent runs at carrier concentration $p=0.10$ (○), 0.15 (□), 0.20 (△), 0.25 (+), 0.30 (×), 0.40 (▽), 0.50 (◇), 0.60 (⊡), 0.70 (*), 0.80 (⊙), and 0.90 (■).

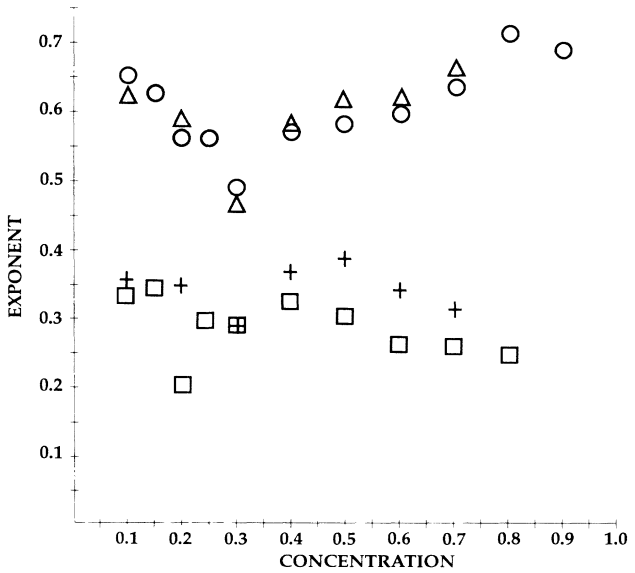

FIG. 3. The exponents for the front motion k with samples 100×50 (○) and 100×100 (△) and for the interface width ν with samples 100×50 (□) and 100×100 (+) on the rough substrate for the same statistics as in Fig. 2.

0.48 ± 0.02 to 0.71 ± 0.02. The interface-width exponent ν, within the fluctuations, is consistent with its superuniversal value $\frac{1}{3}$ for the fluid spread on the smooth substrate, where the dynamical scaling relation $\chi + z \approx 2$ seems valid. This relation (3) is also valid for a rough substrate. The variation of the effective exponents ν and k with carrier concentration suggests that the evolution of the interface in our irreversible fluid spreading may depend on microscopic details (i.e., the nature of the substrate and carrier concentration).

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