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Numerical study of a model for driven interface dynamics

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Abstract. We study a nonlinear Langevin model for interface dynamics where relaxation is controlled by surface diffusion. While the linear part of the model can be solved analytically, a renormalization group analysis on the nonlinear model does not yield a stable fixed point. We have thus solved the model numerically in both two and three spatial dimensions. The dynamical scaling exponents and scaling functions are evaluated. We compare our model to that proposed by Lai and Das Sarma which may be relevant to the long-time, large-distance behaviour of surface growth by molecular beam epitaxy (MBE) processes.

1. Introduction

Thin films are usually grown by deposition of atoms from a vapour onto a substrate. While atomistically smooth and layer-by-layer growth is desired, one often obtains surfaces that are rough. The amount of roughness depends on a variety of physical processes during growth, such as the presence of thermal fluctuations [1, 2], kinetic effects due to uncertainties in intensity of the incoming atomic beam [3], long range screening effects [4, 5], and the presence of quenched impurities [6]. A thorough understanding of the roughening phenomena obviously has great practical importance and has attracted intense theoretical and experimental research over the last few years [7, 8]. On the theoretical side, it is found that growing interfaces often dynamically evolve into self-affine structures so that correlation functions of the interface shape show dynamic scaling [7, 9], enabling one to use ideas commonly used in critical phenomena. As a result it is possible to define universality classes using quantities such as the scaling functions and exponents: models in the same class share the same exponents and functions.

Kinetic roughening has been studied theoretically using two major approaches. The goal being to study the long wavelength and long time behaviour of a growing interface. First, one may use microscopic models to mimic the process of atomic deposition, and this is often achieved using computer simulations. The method usually requires a Hamiltonian which accounts for the essential interactions between the particles and the substrate. Interface growth being a far from equilibrium phenomenon, one normally breaks detailed balance in a simulation by introducing various growth rules which capture certain experimental realities. A typical example is the restricted solid-on-solid model (RSOS) studied by Kim and Kosterlitz [10].

A second approach for studying the kinetic roughening of a growing interface is to write down a stochastic partial differential equation for the evolution of the interface

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shape. This is usually guided by the symmetry of the problem. A representative model is the well known Kardar–Parisi–Zhang (KPZ) equation [11] which describes the time evolution of an interface shape $h(\boldsymbol{x}, t)$

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h + \tfrac{1}{2}\lambda(\nabla h)^2 + \eta(\boldsymbol{x}, t) \tag{1}$$

where $(\boldsymbol{x}, t)$ is the space time point, and $\eta(\boldsymbol{x}, t)$ is a stochastic term which mimics, say, the fluctuation in the incoming atomic beam intensity; η satisfies Gaussian statistics

$$\begin{aligned} &\langle \eta(\boldsymbol{x}, t) \rangle = 0 \\ &\langle \eta(\boldsymbol{x}, t)\eta(\boldsymbol{x}', t') \rangle = 2D\delta(\boldsymbol{x} - \boldsymbol{x}')\delta(t - t') \end{aligned} \tag{2}$$

where ν, λ and D are constants.

Perhaps the simplest quantity which shows interesting dynamic behaviour is the interface width defined as the mean-square-deviation of interface shape: $W(L, t) = [\langle \langle (h(i) - \bar{h})^2 \rangle \rangle]^{1/2}$, where $h(i)$ is the interface height at the position i. For both the RSOS and KPZ models, the width has been found to obey dynamical scaling [9], $W(L, t) = L^{\chi} F(x)$ where $x = t/L^z$, L is the linear system size and t is time. $F(x)$ is the scaling function and χ and z are the scaling exponents. At large times we have $F(\infty) \rightarrow$ constant, thus $W \sim L^{\chi}$. For $\chi > 0$, W increases as L increases thus the interface is rough. At intermediate times and large system size, $F(\boldsymbol{x}) \rightarrow x^{\chi/z}$, or $W \sim t^{\beta}$ with $\beta = \chi/z$. Much theoretical attention is paid to the values of these exponents for different interface models.

The KPZ equation successfully describes many interface growth models such as the RSOS model and various ballistic deposition models [8]. Common to all these microscopic models is the surface relaxation mechanism which is dominated by desorption. In the hydrodynamic limit, desorption is conveniently modelled [3] by the linear (first) term in equation (1). However, if the relaxation mechanism is dominated by surface diffusion, such as in the molecular-beam-epitaxy (MBE) process where the growth temperature is rather high, a generalization of (1) is needed.

Recently, Lai and Das Sarma proposed a hydrodynamic model [12] where the surface relaxation is due to diffusion, i.e. the linear term in the equation is proportional to $\nabla^4 h$. With a choice of a nonlinear term, their nonlinear model can be solved exactly. The exactness of their solution is due to the fact that two of the three parameters in their model are not renormalized so that exponents χ and z can be obtained directly from a scale transformation of the equation [13]. Indeed, these exponents are quite different from those given by the KPZ model [12].

In this paper we propose and study a model for driven interface dynamics where surface relaxation is controlled by diffusion. The nonlinear term in the equation is different from that studied by Lai and Das Sarma and is motivated by microscopic considerations (see below). The deterministic part of our equation is similar to the so called local model for dendritic crystal growth if the Mullins–Sekerka instability is turned off [14, 15]. A renormalization group analysis on the equation does not give a stable infra-red fixed point, we have thus solved the equation numerically in both two and three spatial dimensions. In the physically relevant three dimensions, we obtain $\chi = 0.82 \pm 0.03$ and $\beta = 0.22 \pm 0.01$. In the next section we propose the model; the results will then be presented. Finally we compare our results to those of Lai and Das Sarma [12].

2. The model and results

Surface diffusion implies a conservation of mass: the local growth rate is proportional to the divergence of a current, i.e. $\partial h/\partial t \propto -\nabla \cdot j$. For the problem we are interested in here, the current j is the gradient of the chemical potential [3] $\mu \sim \nabla^2 h$, thus we have $\partial h/\partial t \propto -\nabla^4 h$. Assuming that the surface is growing because there is an external beam of particles striking it, the growth rate should also be proportional to the beam intensity $f = f_0 + \eta$, where f_0 is a constant and η is random which mimics, say, a small fluctuation in the beam intensity. We can then write

$$\frac{\partial h}{\partial t} = -\nu \nabla^4 h + \eta(\boldsymbol{x}, t) \tag{3}$$

where we have rescaled the height variable: $h \rightarrow h + f_0 t$, i.e. h in (3) is now measured from its average. ν and D are constants. We further assume that the noise $\eta(\boldsymbol{x}, t)$ satisfies Gaussian statistics (2). Equation (3) is linear and various height–height correlation functions can be obtained exactly. In particular, the exponents characterizing the scaling form of the interfacial width are obtained, $\chi = (4-d)/2$, $\beta = (4-d)/8$, and $z = 4$, where d is the dimension of the interface ($d+1$ is the spatial dimension).

If we consider the right hand side of (3) as the linear term of a gradient expansion of some general functional of h, such as discussed by Grinstein [16], then various nonlinear terms may contribute to changing the scaling behaviour. While many of the nonlinear terms are irrelevant in the hydrodynamic limit in the sense of renormalization group transformations, some are important and must be included. The KPZ equation is a good example in this regard.

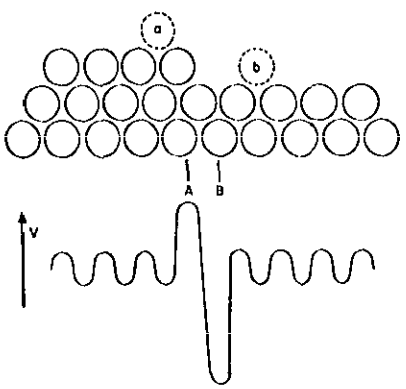

Figure 1. A sketch of an interface step: there is an effective potential barrier near a step (point A). Because of this barrier, it is easier for atoms to flow away from A than to jump over to the lower layer. Atoms deposited on the lower layer may flow to position B since it is a potential valley.

We could get more insight into the physical process in question by considering the following situation. It has been shown both experimentally and from simulations [17, 18], that atoms landing at a kink on the surface prefer to flow on the same layer, rather than to jump over the kink to the lower layer. This is because there is usually an effective potential barrier at the kink [19], as schematically shown in figure 1. While this effect is of little concern when one is considering growth in the hydrodynamic limit, we can nonetheless use it to motivate a choice of a nonlinear term for equation (3). For a kink on the interface, say $h \sim \tanh(x)$, figure 2

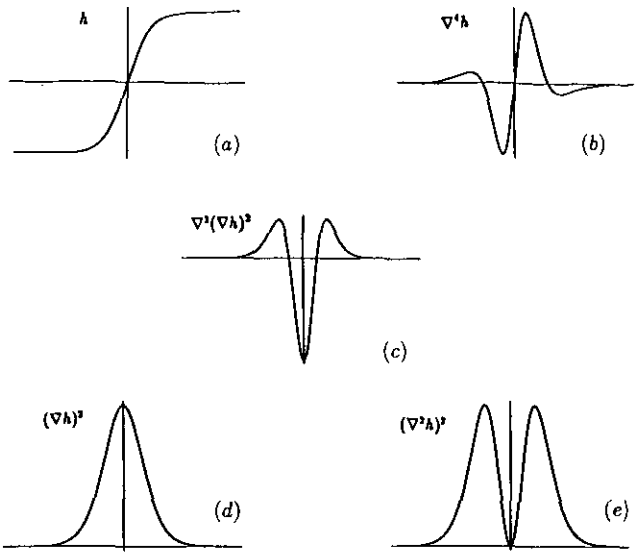

Figure 2. A qualitative description of the local surface shape and its various derivatives. (*a*) $h(x) \sim \tanh(x)$, i.e. a kink on the interface. (*b*)–(*e*) Various derivatives of $h(x)$. (*e*) is included in the interface equation.

shows a number of its derivatives [12]. Since we are interested here in cases where either side of the kink grows but not the places with steep spatial gradients, a term like figure 2(*d*) is ruled out. Furthermore, by power counting there are only a few choices which are relevant in the sense of a renormalization group transformation. In the following we shall study the consequence of adding a nonlinear term like that shown in figure 2(*e*), i.e. $(\nabla^2 h)^2$, to equation (1). The MBE model of Lai and Das Sarma uses the nonlinear term shown in figure 2(*c*), which satisfies the necessary conservation condition required by MBE. However, from the point of view of driven interface dynamics and universality, a study of the nonlinear term of figure 2(*e*) is of as much interests. While the shape of the nonlinear terms are similar, we show below that the scaling exponents are quite different.

A second motivation of choosing figure 2(*e*) as the nonlinear term is the observation that the local curvature of the interface $\kappa \sim \nabla^2 h$, thus (3) gives a local growth rate $v \approx -\nu\nabla^2\kappa + \cdots$. Taking this as an expansion on local curvature and considering only the simplest nonlinear term, we have [15] $v \approx \nu\nabla^2\kappa + \lambda\kappa^2 + \cdots$. The nonlinear term is essentially that given by figure 2(*e*). This growth rate is similar to that of the well known local model for dendritic crystal growth, the only difference being that we have turned off the Mullins–Sekerka instability [14]. Thus a study of this problem may also offer insights into the surface roughening phenomena of a large growing dendrite [15, 20].

In the following we will study the interface growth model described by the nonlinear partial differential equation

$$\frac{\partial h}{\partial t} = -\nu\nabla^4 h + \lambda(\nabla^2 h)^2 + \eta(x,t). \tag{4}$$

A dynamical renormalization group analysis was carried out in order to study the scaling behaviour of the above equation, using the technique of Forster *et al* [13], for

details see [15]. Here we simply quote the main conclusion of that analysis. After a scale transformation $x' \to e^l x$, $t' \to e^{zl} t$, and $h' \to e^{\chi l} h$, the following recursion relations to one-loop order were found

$$\frac{d\nu}{dl} = \nu[z - 4 + \tfrac{1}{4}K_d\bar{\lambda}^2] \tag{5}$$

$$\frac{dD}{dl} = D[z - 2\chi - d + \tfrac{1}{4}K_d\bar{\lambda}^2] \tag{6}$$

$$\frac{d\lambda}{dl} = \lambda[z + \chi - 4 + K_d\bar{\lambda}^2] \tag{7}$$

where $K_d = S_d/(2\pi)^d$ and S_d is the surface area of a d-dimensional unit sphere. From these the recursion relation for the effective coupling constant $\bar{\lambda} = (\lambda^2 D/\nu^3)^{1/2}$

$$\frac{d\bar{\lambda}}{dl} = \bar{\lambda}[(4-d)/2 + \tfrac{3}{4}K_d\bar{\lambda}^2]. \tag{8}$$

Since the second term on the right hand side of (5) is always positive, no stable non-trivial fixed point can be found for $d \leqslant 4$. This is similar to the situation of the KPZ equation in $d = 2$. Furthermore, there is no simple hyperscaling relation between z and χ.

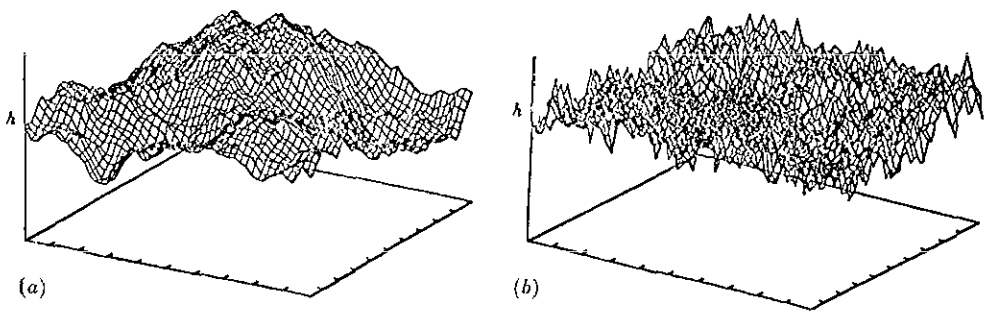

Figure 3. (*a*) A typical shape of a surface generated by our model at time $t = 1000$. Linear system size $L = 100$ and time step $\Delta t = 0.01$; other parameters: $\lambda = 30$, $\nu = 1$, and $2D/\Delta t = 1.0$. (*b*) A typical shape of a surface generated by KPZ equation at $t = 1000$. Other parameters are the same as in (*a*).

We thus integrated (4) numerically in both $d = 1$ and $d = 2$ using the Euler method on a discrete space mesh with $\Delta x = 1$. A typical time step used was $\Delta t = 0.01$. We checked that smaller time steps do not change the results in any important manner†. To obtain reasonable statistics, for each set of system parameters

† We note that for finite mesh sizes a term with a form $\nu_2\nabla^2 h$ may or may not be generated. If it is indeed generated, ν_2 will be very small and can be made arbitrarily small by reducing the mesh sizes, or by increasing the system size L. In any case, we have not detected the presence of such a term in any appreciable fashion for the systems studied.

we typically averaged over 100 runs. For initial conditions we set $h = 0$ at all the sites. Figure 3(*a*) shows the interface shape of our model after at $t = 1000$ for a system of linear size $L = 100$. This is to be compared with the interface shown in figure 3(*b*) generated by the KPZ equation. Obviously the two interface morphologies are quite different. From these figures we clearly see that surface diffusion is not a very efficient relaxation mechanism for smoothing out large wavelength fluctuations, as expected. On the other hand, relaxation by desorption is better at smoothing out these large wavelength fluctuations but the surface remains coarser on small length scales.

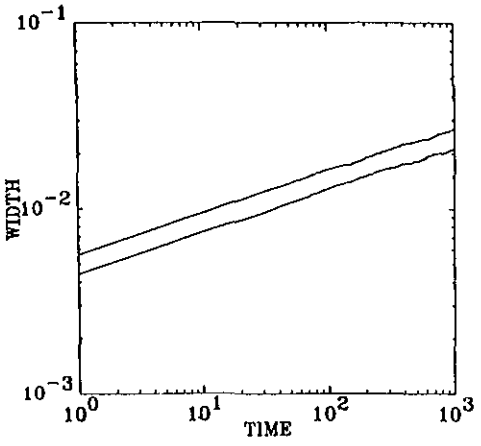

Figure 4. Results in two interface dimensions. Log–log plot of width $W(t)$ as a function of time t. Each curve corresponds to an average of 100 independent runs on systems with linear size $L = 50$. The upper curve used $\lambda = 50$ and the lower one used $\lambda = 30$. Other parameters are the same as those used in figure 3(*a*). The slope gives an estimate of the value of $\beta = 0.22 \pm 0.01$

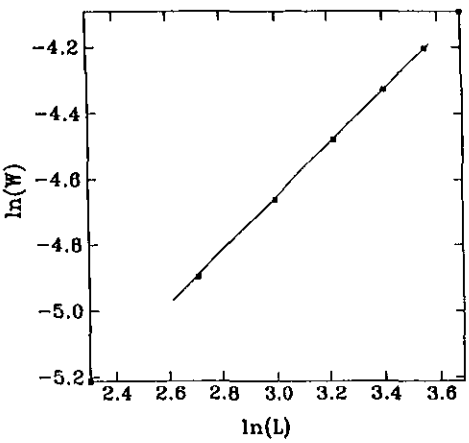

Figure 5. Results in two interface dimensions. Log–log plot of the width W against size L at very large times when W is saturated. The slope gives a value of $\chi = 0.82 \pm 0.03$. System parameters are the same as those used in figure 3(*a*).

The scaling exponents of the interface correlation, β and χ were evaluated from log–log plots of the interface width $W(L,t)$ as a function of t and L, shown in figures 4 and 5. In the physically relevant dimension $d = 2$, we obtained $\chi = 0.82 \pm 0.03$ and $\beta = 0.22 \pm 0.01$. We have checked that these values are stable against changes of system parameters. For example, changing λ from 30 to 50 gives the same result, also shown in figure 4. The exponent β can also be evaluated using the two-point correlation function, $G(t) = \langle (h(x, t+T) - h(x,T))^2 \rangle$, since $G(t) \sim t^{2\beta}$ at intermediate times. The value of β obtained this way is 0.21 ± 0.02 which is consistent to within error bars. These exponents are compared with those obtained using the linear part of (4): $\beta = 0.25$ and $\chi = 1$. We see that the nonlinear term in (4) helps reduce the value of χ from its marginal value of 1. In the model of Lai and Das Sarma [12], where they employed a different nonlinear term, the exponents are: $\beta = 1/5$ and $\chi = 2/3$. Our results are clearly different although β is somewhat close to theirs. We may conclude that our model belongs to a different universality class.

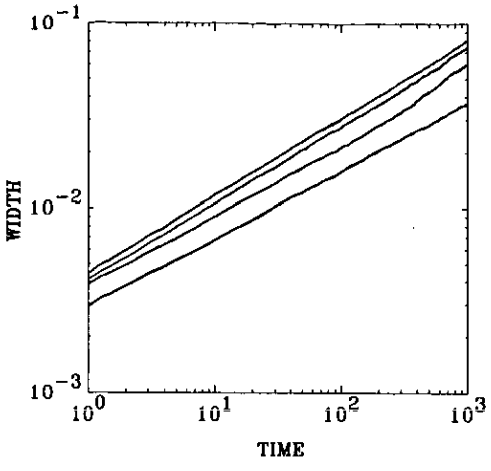

Figure 6. Results in one interface dimension. Log–log plot of width $W(t)$ against t. Each curve corresponds to an average of 100 independent runs on systems with $L = 512$. Lower to higher curves correspond to $\lambda = 10, 25, 40, 50$ respectively. The slope gives the value of $\beta = 0.39 \pm 0.03$ for the two largest values of λ.

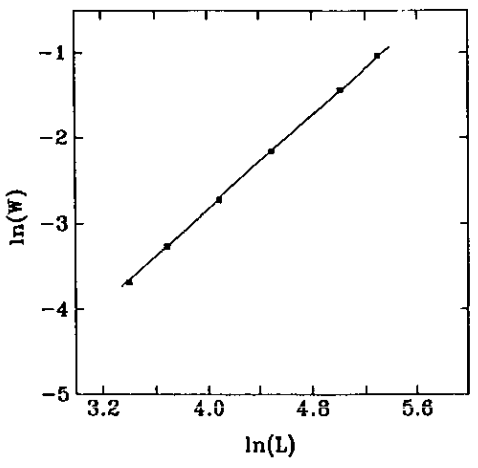

Figure 7. Results in one interface dimension. Log–log plot of width W against size L at very large times. The slope gives a value of $\chi = 1.40 \pm 0.02$.

We have also determined the scaling exponents at the physically less relevant dimension $d = 1$: $\beta = 0.39$ and $\chi = 1.40$. Figures 6 and 7 show log–log plots of the interface width W as a function of time t and system size L which determine the exponents. The two lower curves in figure 6 are for smaller values of the nonlinear coupling strength λ and are still in the crossover regime. While the value of χ is lowered somewhat from that of the linear case where $\chi = 3/2$, it is still higher than the physically marginal value 1. In this case, $W(L, t \to \infty)/L \sim L^{\chi-1}$ diverges when $L \to \infty$, indicating a breakdown of the solid-on-solid condition imposed on the model (4). A similar situation exists in other models where relaxation is controlled by surface diffusion, such as the model of Lai and Das Sarma [12] and lattice models in [21, 22, 23].

3. Summary

In summary, we have proposed and studied a physically meaningful model which is relevant in describing kinetic roughening phenomena, in the hydrodynamic limit, of a growing interface where surface relaxation is controlled by diffusion. In our model the local growth rate is proportional to a gradient expansion of the local curvature and is different from that of Lai and Das Sarma in the nonlinear term. This leads to different dynamic exponents χ and β. These exponents were determined by numerically by solving the interface equation (4). We note that the presence of the nonlinear term reduces the value of roughening exponent χ in both the one and two interface dimensions from that of the corresponding linear model. In particular, in $d = 2$ we found $\chi \approx 0.82$ which is considerablely larger than that of the KPZ model [7, 24]. This indicates that surface diffusion is not strong enough in suppressing kinetic roughening

at large length scales. Finally we note that models with surface diffusion and *non-conserved* noise seem to give rather large values of the roughening exponent χ. On the other hand, for MBE growth one would expect χ to be small. It will be interesting to see what effects will alter this situation [25].

Acknowledgments

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