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LETTER TO THE EDITOR

# Conserved growth in a restricted solid-on-solid model

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**Abstract.** The surface dynamics of conserved growth in a restricted solid-on-solid (RSOS) model is described. A randomly deposited particle is allowed to migrate to the nearest site satisfying the RSOS condition. The surface width, the correlation function and the structure factor measurements are consistent with the Lai and Das Sarma and Villain equation $\partial h/\partial t = -\nu\nabla^4 h + \lambda\nabla^2(\nabla h)^2 + \eta$. The physical origin of the nonlinearity is also discussed.

Over recent years, there have been many studies of the surface structure of various growth models [1]. Among them, the class of models known as solid-on-solid (SOS) models has been extensively studied as simple models of both equilibrium and non-equilibrium properties of surfaces. The characteristic feature of the models within this class is the restriction of fluctuations to exclude all configurations with overhangs and lattice vacancies. An important variation among the SOS models is the restricted SOS (RSOS) model, in which the differences between neighbouring heights of the local columns $|\delta h|$ are usually restricted to zero or unity in magnitude. Even with this restriction, the equilibrium RSOS model still exhibits a roughening transition at three dimensions [2]. Also the non-equilibrium growth in a RSOS model [3] is well described by the Kardar–Parisi–Zhang (KPZ) equation [4]. In fact the RSOS condition suppresses the short wavelength fluctuations and leads to rapid convergence to the asymptotic behaviour. The relation between the RSOS growth models and KPZ equation has been clarified recently by studying the mapping [5] between the growth model and a directed polymer in random potentials [6]. Recently much effort has been given to a 'conserved growth model' which conserves complete particles after they have been deposited [7–13]. There are neither overhangs nor vacancies and the surface currents are conserved in the conserved growth model which is possibly related to the real molecular beam epitaxial (MBE) growth. The tilt-dependent current analysis [14] shows that some discrete growth models belong to the Edwards and Wilkinson (EW) [15] universality class [16]. So far, there is no firm understanding of the relation between discrete growth models and a nonlinear conserved particle equation [13]. Here we will discuss conserved growth in a RSOS model which follows the nonlinear equation.

The interesting quantity of the growth process is the self-affine surface structure. Most studies have concentrated on studying the surface structure, especially on determining the exponents governing surface fluctuations. The surface width $W$ is defined as the standard deviation or the root-mean-square fluctuation of the surface height. The dynamic scaling hypothesis is that in a finite system of lateral size $L$, the width $W$ starting from a flat

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substrate scales as [17]

$$W(t) \sim L^{\alpha} f(t/L^z) \\ \sim t^{\beta} \qquad t \ll L^z \\ \sim L^{\alpha} \qquad t \gg L^z \tag{1}$$

where the scaling function $f(x)$ is $x^{\beta}$ for $x \ll 1$ and is constant for $x \gg 1$. The time $t$ is the average height of the surface. The exponents $\beta$ and $z$ are connected by the relation $z\beta = \alpha$.

Our model is very similar to the simple RSOS growth model [3] except for the constraint of conserved particle growth. The growth algorithm is as follows.

(i) A site $x$ is randomly selected on a $(d-1)$-dimensional lattice.

(ii) If the RSOS condition (RSOSC) on neighbouring heights $|\delta h| = 0, 1, \ldots, N$ is obeyed at $x$ after a particle is deposited, then growth is permitted by increasing the height $h(x) \to h(x) + 1$.

(iii) If the RSOSC is not obeyed at $x$, we scan the neighbouring sites of the $(d-1)$-dimensional lattice and growth of the height by one unit is permitted at the site nearest to $x$ where the RSOSC is satisfied. To be more specific, if the RSOSC is not obeyed at $x$, a site is randomly selected from among the nearest neighbours (NNs) of $x$ which satisfy the RSOSC, allowing growth by increasing $h \to h + 1$ at that NN site. If there is no NN satisfying the RSOSC, then a site is randomly selected from among the next NNs (NNNs) of $x$ satisfying the RSOSC to allow a growth. If no NNN satisfies RSOSC, then among the next NNNs etc.

Without step (iii), our model is exactly the same as the simple RSOS growth model [3]. In the RSOS growth model a particle is dropped at a randomly selected site. If the RSOSC is not satisfied, then the dropped particle is rejected. This rejection rate is around 0.7 in $d = 1 + 1$. However, in our conserved growth model with step (iii) a dropped particle at a randomly selected site wanders around the surface to find the nearest site which satisfies the RSOSC. So the rejection rate is clearly zero and our model faithfully produces a RSOS model with the constraint of conserved particle growth. To find a site satisfying the RSOSC, the dropped particle can migrate both upwards and downwards from the surface. The simple RSOS growth model [3] does not conserve the total deposited particles and produces a KPZ nonlinearity [4]. In our conserved model, since the deposited particle is allowed to migrate both upwards and downwards, there is no surface diffusion term in the EW model [15]. Instead, there may be a conserved nonlinearity due to the RSOS restriction.

Here, we find that our model is very likely to be a discrete SOS model described by the nonlinear MBE growth equation of Lai and Das Sarma [7] and Villain [10].

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

where $h(x,t)$ is the height of the film and $\eta$ is a *non-conserved* Gaussian random noise satisfying

$$\langle \eta(x,t)\eta(x',t')\rangle = 2D\delta(x-x')\delta(t-t'). \tag{3}$$

This equation can be solved by a one-loop renormalization group calculation [7] giving $\alpha = (5-d)/3$ and $z = (7+d)/3$, i.e. $\beta = (5-d)/(7+d)$. In $d = 1+1$, $\beta = 1/3$ is the same as the value of the KPZ exponent, but $z = 3$ is different from $z_{KPZ} = 3/2$. Sun *et al* [18] studied a similar equation with *conserved noise* and found different values: $\beta = 1/11$ and

$z = 11/3$ in $d = 1+1$ [18]. Even though there have been some attempts to understand the continuum equation, there is no clear physical explanation for the nonlinear term $\nabla^2(\nabla h)^2$. Since the values of the exponents, the structure factor and the correlation function measured in our model are consistent with equation (2), we claim that the conserved growth model follows this nonlinear equation. We also discuss the relation between the non-conserved RSOS growth model [3] and our model.

Our simulations are performed in $d = 1+1$ from a flat substrate with periodic boundary conditions in $d-1$ dimensions. Typically for the restriction parameter $N = 1$, but the results, which we have checked by further simulations, are independent of $N$. The time $t$ corresponds to the number of Monte Carlo steps (number of layers). As usual, we monitor the surface width as a function of time, which increases as $t^{\beta}$ for early times and eventually saturates when the parallel correlation $t^{1/z}$ is of the order of the lateral system size $L$.

To determine the growth exponent $\beta$, we measure $W(t)$ as a function of time for a system size $L = 10\,000$ ($d = 1+1$). The minimum value $N = 1$ was used for the restriction parameter. Through the relation $W(t) \sim t^{\beta}$ for early times $t \ll L^z$, and averaging over 60 independent runs, we obtain (figure 1)

$$\beta = 0.32 \pm 0.01 \qquad d = 1+1. \tag{4}$$

The result above is slightly smaller than the expected theoretical value 1/3 from the equation (2). However, there is a small upwards trend of the slope as a function of time in figure 1 so the slope may approach 1/3.

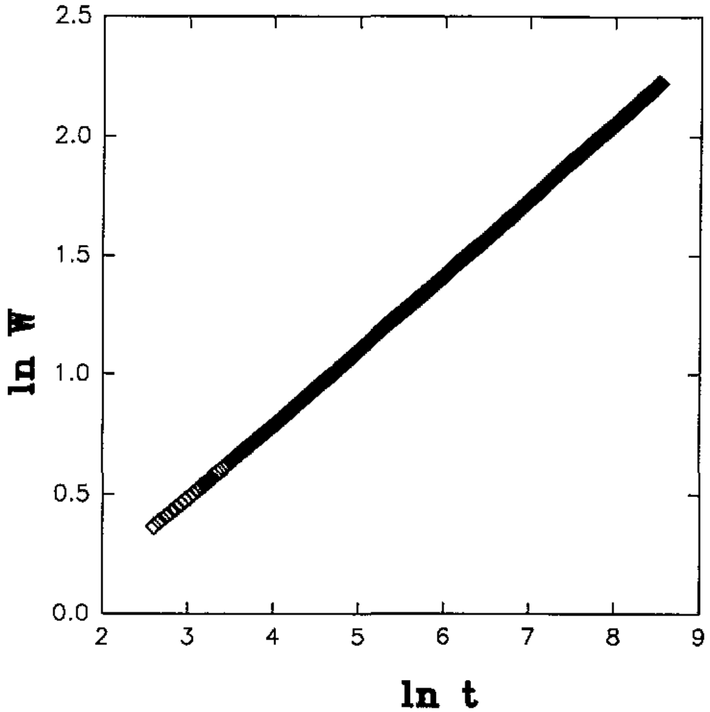


**Figure 1.** Surface width $W$ as a function of time in a log–log plot ($L = 10\,000$).

For the roughness exponent $\alpha$ that describes the saturation of the interface fluctuation, we use the relation $W(t) \simeq L^{\alpha}$ for the system size $L$ in the steady-state regime $t \gg L^{z}$. We have used system sizes of $L = 64, 90, 128, 180, 256$ in $d = 1 + 1$. Since the dynamic critical exponent $z$ is around three, the time required to reach the saturated regime is larger than $L^3$. From the log–log plot of $W(L)$ and size $L$, we get

$$\alpha = 0.95 \pm 0.04 \qquad d = 1 + 1 \tag{5}$$

as shown in figure 2 where as a comparison, the data for the simple RSOS growth model ($\alpha = 1/2$) are also given. Through the relation $z = \alpha/\beta$, we get $z \simeq 0.95/0.32 \simeq 2.97$. These exponents of our model are in very good agreement with $\beta = 1/3$, $\alpha = 1$ and $z = 3$ obtained analytically from equation (2) in [7]. They also satisfy the scaling relations [8, 18, 7]

$$z - 2\alpha - d + 1 = 0 \tag{6}$$

$$z + \alpha = 4 \tag{7}$$

very well. The scaling relation of equation (6) is due to the conserved particle condition that there is no evaporation of the dropped particles.

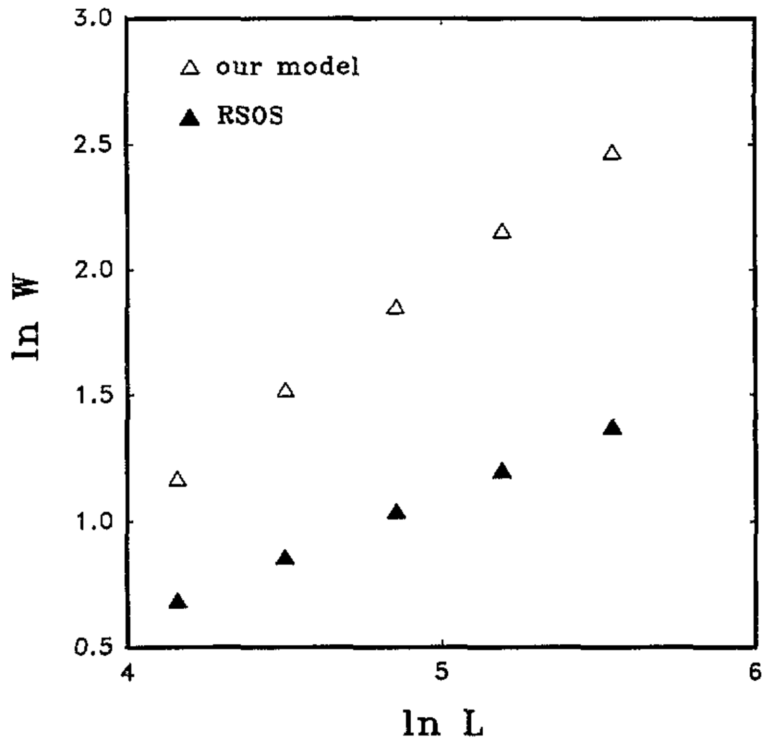


**Figure 2.** Saturated surface width $W$ as a function of $L$ in a log–log plot. For comparison the saturated $W$ of the simple RSOS growth model [3] is shown as well.

Since the above agreement between the values of the exponents may not guarantee that the model belongs to the same universality class as the continuum equation (2), we calculate the structure factor

$$S(L,k,t) = \langle h(k,t)h(-k,t)\rangle$$

for a system of lateral size $L$ where $h(k,t)$ is the Fourier transform of the height $h(x,t)$. As expected from equation (1), figure 3 shows that $S(L,k,t\to\infty)$ follows $1/k^\delta$ for small $k$ with $\delta = 2.99 \pm 0.05$ in $d = 1+1$ being consistent with $\delta = z = 2\alpha + d - 1 = 3$ without showing any $L$ dependence.

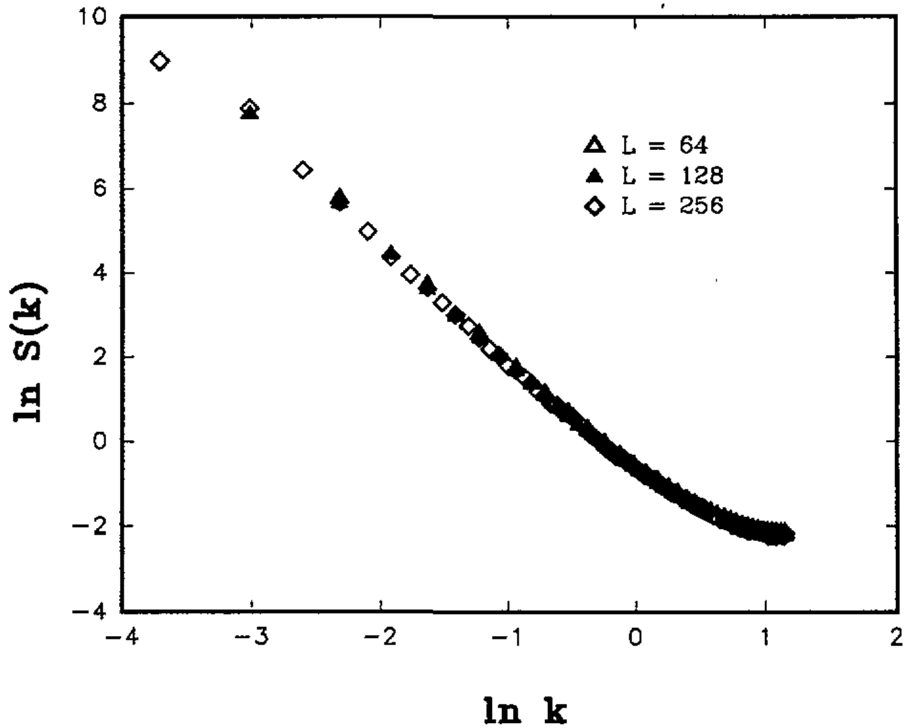


**Figure 3.** Structure factor against $k$ at a saturated regime for $L = 64$, 128 and 256. The negative slope $\delta = 2.99 \pm 0.05$ for small $k$ is consistent with $\delta = 3$ expected from equation (2).

Another interesting quantity is the correlation function $G(r,t) = \langle (h(x+r,t) - h(x,t))^2\rangle$. From the numerical measurement of the correlation function as shown in figure 4, the scaling plot of $G(r,t)/r^{2\alpha}$ against $r/t^{1/z}$ with $\alpha = 1$ and $z = 3$ shows very good data collapse. All these results involving the surface width, structure factor and correlation function support our assertion that our model belongs to the same universality class as equation (2).

Some other conserved growth models [8, 9, 13] also exist. The Das Sarma and Tamborenea (DT) model [9] and the Wolf and Villain (WV) model [8] allow a deposited particle to migrate to maximum bond sites. In realistic MBE growth, Arrhenius hopping may effectively induce a deposited particle to settle into maximally bonded sites. From the measurement of $\alpha$ and $\beta$, these models were believed to follow Mullins' equation ($\lambda = 0$ in equation (2)) [19]. However, the close relation between these models and Mullins' equation has been questioned recently [14, 16, 20]. Specifically, WV model allows only downward jumps so the surface current flows to the lower height sites probably producing the non-zero

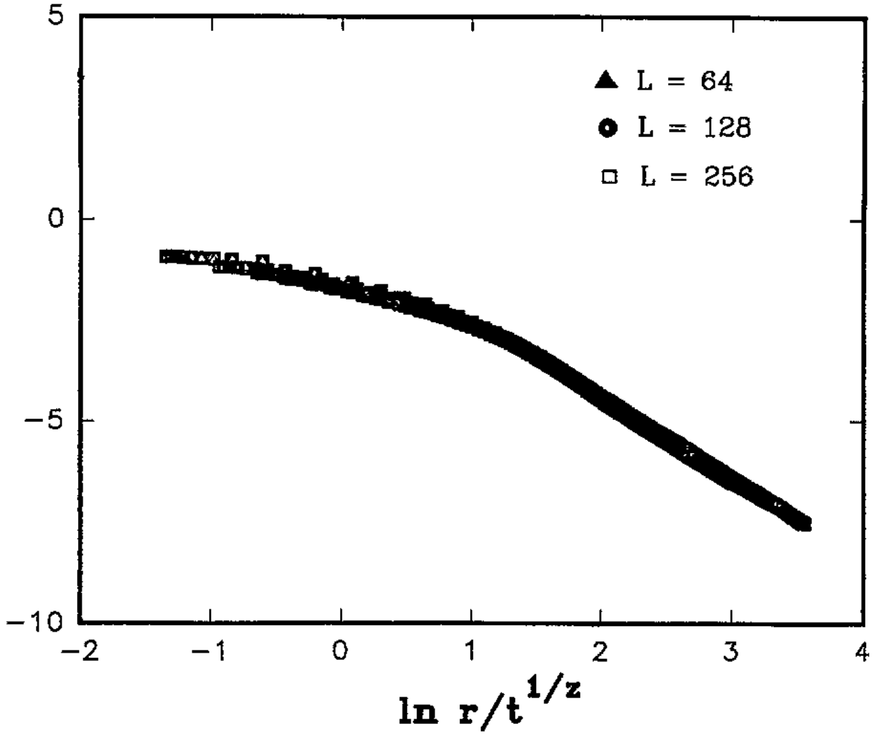


**Figure 4.** The data collapse of the scaled height–height correlation functions $G(r, t)$ for $t = 50, 100, 150, \ldots,$ and 450 with $z = 3$ and $\alpha = 1$. The scaling function $g(x)$ of $G(r, t)$ satisfies $x^{-2}$ for $x \gg 1$ quite well.

diffusion that is characteristic of the EW model, which was supported by the tilt-dependent current measurement of the model [14]. Since a deposited particle is allowed to migrate equally in both up and down directions in our model, we do not expect any EW-type diffusion. So far, there is no clear identification of the microscopic process that generate the nonlinear term. We can rewrite equation (2) as $\partial h/\partial t = \nabla \cdot \nabla[-\nu\nabla^2 h + \lambda(\nabla h)^2] + \eta$ where the surface current is $\nabla[\nu\nabla^2 h - \lambda(\nabla h)^2]$. Since the particle deposited on a slope migrates to a flat area, a surface current is generated from the higher-sloped region to the lower-sloped region. So, we can argue roughly that our model has a positive $\lambda$ in equation (2) [13]. This is the reason why conserved growth with the RSOSC produces a nonlinear effect. It is interesting that the non-conserved RSOS growth model [3] generates the KPZ nonlinearity and the conserved growth model with RSOSC (our model) produces the conserved nonlinearity in equation (2). The sign of $\lambda$ is irrelevant, so it might be interesting to construct a model with a negative $\lambda$ which belongs to the same universality class. There is a different model [11] having the same value for the exponent $\beta$ where Arrhenius hopping is allowed on the SOS model. Since a kink site is more favourable than a single-bond site in the model, it may have a negative $\lambda$ [13]. The different signs for $\lambda$ between our model and [11] is due to the different physical origins [21]. Behaviour similar to that in the KPZ equation is also shown in the finite-temperature RSOS growth model where the KPZ nonlinearity depends on a temperature-like parameter [21]. In fact our model has infinite horizontal diffusion. In realistic growth, the deposited particle may migrate quite a long distance at high temperature to prevent a high step. If the temperature is high enough for the Schwoebel effect to be negligible but low enough to prevent the high steps from forming, the distribution of step height in real crystal growth may satisfy the RSOSC. One can consider step flow on a vicinal surface experimentally. Since $\alpha = 1/2$ in EW model, $\alpha = 1$ in our model and $\alpha = 3/2$ in Mullins' equation, we may classify the MBE growth by measuring the correlation function of the step edges on a vicinal surface.

In summary, we have constructed simple conserved growth in a RSOS model which can be well described by a nonlinear conserved equation. Numerical study of the models shows that the structure factor, the correlation function and the measured values of the exponents are in good agreement with the theoretical results of the continuum equations. Conserved growth with the RSOSC effectively produces the conserved nonlinear term in equation (2). The relation between realistic MBE growth and our model remains to be understood.

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