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LETTER TO THE EDITOR

Phase transition in restricted solid-on-solid models with finite-distance hoppings

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Abstract. Restricted solid-on-solid (RSOS) models with finite-distance hoppings are studied. A randomly dropped particle is allowed to hop to find the nearest site satisfying the RSOS condition within a finite hopping distance l_c. If the particle can find such a site within the distance l_c, then the growth is permitted at that site. If the particle cannot find the site within the distance l_c, the particle is abandoned and the new particle is dropped. It is found that in the substrate dimensions $d_s = 1$ and 2 the universality of such models crosses over from the Kadar–Parisi–Zhang (KPZ) class ($l_c = 0$) to the conserved-KPZ class ($l_c = \infty$) at finite l_c. The tilt-dependent growth velocity and the surface current are also studied to understand the crossover physically.

Recently, there has been much interest in the non-trivial scaling behaviour of the kinetic surface-roughening phenomena [1], because of the possible connection to interface roughening in the growth phenomena. The main quantities of interest in these studies are the exponents α, β, and z which characterize the scaling of the width W. The width W of the system size L is defined as the root mean square of the surface heights and is expected to satisfy the scaling form [1]

$$W(t) = L^{\alpha} f(t/L^{z}) \qquad (1)$$

where $W(t) \sim t^{\beta}$ with $\beta = \alpha/z$ for $t/L^{z} \ll 1$ and where $W(t) \sim L^{\alpha}$ for $t/L^{z} \gg 1$. Since Kadar–Parisi–Zhang (KPZ) [2] suggested a nonlinear continuum equation, which the growth models such as ballistic deposition [3–5] and Eden growth [6–8] follow rather well, many models [1] have been suggested to understand the physics related to the KPZ equation. The restricted solid-on-solid (RSOS) model [9] in which the height difference between the neighbouring columns is usually restricted to zero or 1 is one of the famous models which apparently suppress the corrections to the scaling and lead to the faster convergence to the KPZ behaviour. The common characteristic feature of the models [3–9] which belong to the so-called KPZ universality class is that the models describe *non-conservative* growth processes, i.e. the basic mechanisms for interface roughening need not conserve the number of the dropped particles. More recently, models which are believed to be related to real molecular beam epitaxial (MBE) growth [10–16] have extensively been studied. The characteristic feature of these models is that they describe the *conservative* growth processes in which the number of particles is conserved after being deposited. Recently, we

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have also studied a conservative model with a RSOS condition [17–19]. The essence of this 'conserved RSOS (CRSOS) model' is very similar to the simple RSOS model [9] except that no desorption occurs. To satisfy not only conservation of the number of particles but also the constraint on the difference between the neighbouring heights (or RSOS condition), the dropped particles are permitted to hop (or diffuse) to find a site at which the RSOS condition is satisfied [17, 18]. Extensive studies on various physical properties, such as the surface width and the tilt-dependent surface current of the CRSOS model in the substrate dimension $d_s = 1$ [18] and the scaling properties in $d_s = 1, 2, 3, 4$ [17–19], have shown that the CRSOS model follows the conserved KPZ equation [10, 13]

$$\frac{\partial h(x,t)}{\partial t} = -\nu_4 \nabla^4 h(x,t) + \lambda \nabla^2 (\nabla h)^2 + \eta(x,t) \tag{2}$$

where

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

In the CRSOS model, there may be long distance hopping of a dropped particle to find a site where the RSOS condition is satisfied. If the chance for a particle to hop a long distance (or a distance comparable to the size of a substrate) is high, then our model should have non-local processes. Therefore, we have measured the probability distribution $P(l)$ as a function of l where l is the hopping distance between the dropped site (the selected site) and the deposited site (the nearest site which satisfies the RSOS condition) [18]. If the dropped site satisfies the RSOS condition, the particle does not move and $l = 0$. We have found [18] that in $d_s = 1, 2$ the measured $P(l)$ are fitted well to the exponential distribution $P(l) = A\exp(-l/l_r)$ except at the point $l = 0$. Average hopping distances $\langle l\rangle (\equiv \sum_l l P(l))$ have also been measured and it has been found that $\langle l\rangle = 0.91$ in $d_s = 1$ and $\langle l\rangle = 0.62$ in $d_s = 2$ [18]. Since the measured $P(l)$ satisfy an exponential decay quite well and $\langle l\rangle < 1$, there hardly exist any non-local processes in the CRSOS model.

The simple RSOS model [9] in which no hopping is allowed belongs to the KPZ universality class, whereas the CRSOS model [17, 18] which allows hoppings (but with $\langle l\rangle < 1$) belongs to the conserved KPZ universality class described by equation (2) [10, 13]. Therefore, it is natural that one should ask what universality classes the RSOS models with finite-distance hoppings belong to. The growth rule of the RSOS model with finite-distance hoppings can be defined with the following growth rules: (I) a site $\boldsymbol{x}$ is selected randomly on a d_s-dimensional substrate; (II) if the RSOS condition on the neighbouring columns $|\delta h| \leqslant 1$ is obeyed after a particle is deposited at $\boldsymbol{x}$, then growth is allowed by increasing the height $h(\boldsymbol{x}) \to h(\boldsymbol{x}) + 1$; (III) if the RSOS condition is not obeyed at the position $\boldsymbol{x}$, the dropped particle is allowed to hop to the nearest site to $\boldsymbol{x}$ within a distance l_c from $\boldsymbol{x}$, where the condition is satisfied and growth is allowed at that site; if there is no such site within a cut-off distance l_c, then the particle is abandoned and a new particle is dropped. The model with $l_c = 0$ is then the same as the simple RSOS model [9], and the model with $l_c = \infty$ (or $l_c \simeq substrate\ size$) reproduces the CRSOS model. Hence the model with finite l_c is expected to be described by the continuum equation

$$\frac{\partial h(x,t)}{\partial t} = \nu_2 \nabla^2 h(x,t) + \lambda_K (\nabla h)^2 - \nu_4 \nabla^4 h(x,t) + \lambda \nabla^2 (\nabla h)^2 + \eta(x,t). \tag{4}$$

The model ($l_c = 0$) belongs to the KPZ class and thus follows equation (4) with $\nu_4 = 0$ and $\lambda = 0$ [9], whereas the model ($l_c = \infty$) [17, 18] follows equation (4) with $\nu_2 = 0$ and $\lambda_K = 0$. Since the average hopping distances of the CRSOS model in $d_s = 1, 2$ are less than 1, the universality class of the models with l_c is expected to cross over from the KPZ class to the conserved KPZ class at finite l_c. Recently, Vvedensky *et al* [15] have derived

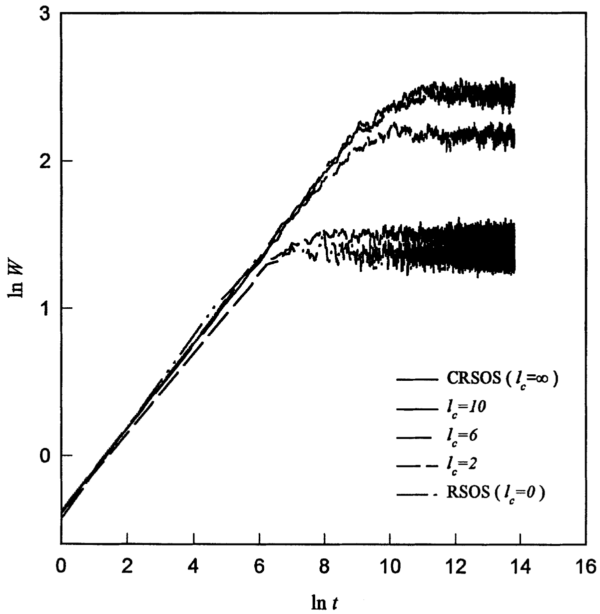

Figure 1. The surface width W of the models with various l_c on the one-dimensional substrate of size $L = 256$ as a function of time on a log–log plot.

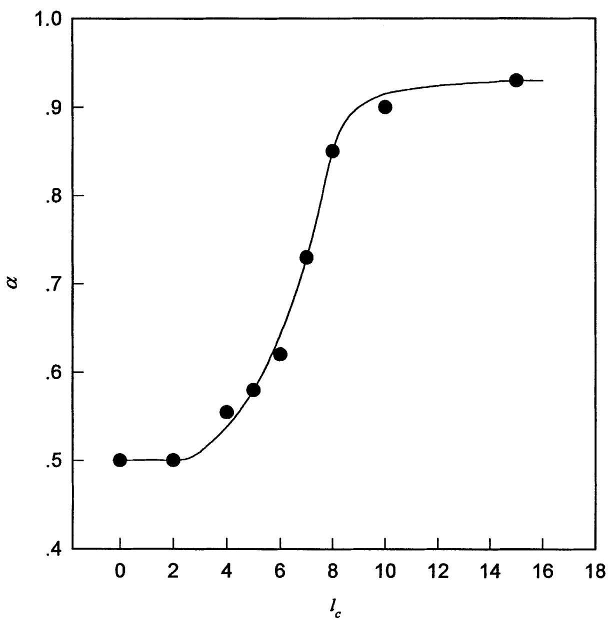

Figure 2. The exponent α in $d_s = 1$ as a function of l_c.

equation (4) analytically for the surface of a single crystal that grows under the typical (or real) epitaxial growth condition. They have taken account of atomic deposition, desorption, and the diffusion (or hopping) on the surface. Vvedensky *et al* [15] have also shown that

$\nu_2 = 0$ and $\lambda_K = 0$ if the desorption and the processes of the downward bias are absent. As we shall see, ν_2 and λ_K, which are apparently non-zero for the model with $l_c = 0$, become rapidly negligible as l_c increases. We believe that our model with finite-distance hoppings should be a nice stochastic model which follows equation (4) and moreover by controlling l_c we can control the coefficients ν_2, ν_4, λ_K, and λ. The first purpose of the present letter is thus to show that the models have a phase transition from the KPZ class to the conserved KPZ class at the finite l_c. The second is to show how the coefficients ν_2, ν_4, λ_K, and λ vary as l_c varies.

The simulation begins with a flat substrate and the periodic condition is used. The simulation results for $W(t)$ for the models with various l_c in $d_s = 1$ are displayed in figures 1 and 2. In figure 1, $W(t)$ on the substrate of size $L = 256$ are displayed. For the early time t ($t \ll L^z$), $W(t)$ of the models with various l_c all satisfy the relation $W(t) \simeq t^\beta$ ($\beta \sim 0.32$) rather well. Since the β values for both the RSOS model [9] and the CRSOS model [17, 18] are close to 1/3, the same early time behaviour for the models with various l_c in figure 1 is the expected result. In contrast, the values of $W(t)$ for various l_c in the steady-state regime (or $t \gg L^z$) are expected to have some values between that for $l_c = 0$ and that for $l_c = \infty$ as one can see from figure 1. We have obtained $W(t)$ in the steady-state regime on the substrates with $L = 64, 128, 256, 360, 512$. By use of the relation $W \simeq L^\alpha$ in the steady-state regime, we have obtained the roughness exponent α for each model with various l_c. The result for α is displayed in figure 2. The α values for the models with $l_c \leqslant 2$ are nearly equal to $1/2$ which is the same as that of the simple RSOS model [9]. For $l_c \geqslant 3, \alpha$ increases as l_c increases and increases abruptly between $l_c = 5$ and $l_c = 6$. For $l_c \geqslant 8, \alpha$ becomes nearly equal to 0.9 which is close to that for the CRSOS model [17, 18]. Considering these results for the exponent α and the effects of the finite size simultaneously, the transition from the KPZ regime to the conserved KPZ regime occurs around $l_c \simeq 5$–6 in $d_s = 1$.

The simulation results in $d_s = 2$ are displayed in figures 3 and 4. In figure 3, the early time dependence of $W(t)$ on the substrate size $L \times L = 256 \times 256$ is displayed. In $d_s = 2, \beta$ for $l_c = 0$ (RSOS model) [9] is close to 1/4 and β for $l_c = \infty$ (CRSOS) model is close to 0.19 [19]. As one can see from figure 3, the time dependence of $W(t)$ for $l_c \geqslant 2$ is almost the same as that for the CRSOS model. In contrast, $W(t)$ for $l_c = 0$ is quite different from that for $l_c \geqslant 2$. This result suggests that in $d_s = 2$ the crossover from the KPZ class to the conserved KPZ class occurs near $l_c = 2$. In figure 4 we have displayed the measured exponents α and β values for the various l_c. Here the exponents α values are obtained from the measured $W(t)$ for the steady-state regime on the substrate sizes with $L = 22$, 32, 45, 64, and the β values are obtained from the data similar to those in figure 4. With increasing l_c, the values of α and β first decrease from the known values for $l_c = 0$ ($\alpha = 2/5$ and $\beta = 1/4$) to 0.3 and 0.15 for $l_c = 1$. In contrast, the values of α and β increase for $l_c \geqslant 2$ and become nearly the same as 0.6 and 0.18 for $l_c \geqslant 3$. 0.6 and 0.18 are very close to the values of α and β for the CRSOS model [19]. The result shown in figure 4 also suggests that the crossover from the KPZ class to the conserved KPZ class occurs at $l_c \simeq 2$–3 in $d_s = 2$. This result in $d_s = 2$ also indicates that even the hoppings of small distance ($l \simeq 2$–3) can make the universality of the surface roughening change drastically in higher dimensions (or $d_s \geqslant 2$).

To understand the crossover phenomena with finite l_c from different points of view, we have measured the coefficient of the KPZ nonlinear term λ_K and the surface tension coefficient ν_2 of equation (4) for the RSOS models with the finite l_c. For the measurement of λ_K we have used the method which was suggested by Krug and Spohn [20] and Kim [21]. If one measures the tilt-dependent growth velocity $v(m)$ on the tilted substrate with the average slope m, then $v(m)$ satisfies the relation

$$v(m) = v(0) + \lambda_K m^2 \tag{5}$$

for small m. We have measured λ_K by using equation (5). The results of the measurements of λ_K in $d_s = 1$ are displayed in figure 5. For the models with $l_c \leqslant 4, \lambda_K$ is negative finite and thus these models should belong to the KPZ class, because the most relevant term in equation (4) is the KPZ nonlinear term $\lambda_K|\nabla h|^2$. However, the absolute value of λ_K abruptly decreases by more than 100 times between $l_c = 5$ and $l_c = 6$. Moreover, the absolute value of λ_K is less than 0.001 for $l_c = 7$. Considering finite-size effects and the results in figure 5 simultaneously, λ_K should become nearly zero for $l_c > 5$. We have also measured ν_2. The method which we have used for the measurement of ν_2 is that suggested by Krug *et al* [22]. To determine the surface tension coefficient ν_2, the surface current $J(m)$ is measured as a function of m. The surface current is measured by counting the number of jumps in between the uphill direction and the downhill direction. If the net current is in the uphill direction, $J(m)$ is positive. ν_2 can be given by $\nu_2 = -\partial J(m = 0)/\partial m$. In the measurement of $J(m)$ we do not consider the length of the jump, instead we just count the number of particles which hop via a downhill (or uphill) jump. The currents are taken for the system size $L = 512$ in $d_s = 1$. It has been found that for models with $l_c \geqslant 1$ $J(m)$ is almost independent of m and the measured values for $|J(m)|$ are very small (or less than 10^{-4}) and similar to those for the CRSOS model [18]. This means that models with $l_c \neq 0$ have no effective surface tension (or $\nu_2 = 0$) or no effective downward bias. From the measurements of λ_K and ν_2 in $d_s = 1$, it is concluded that the transition from the KPZ regime to the conserved KPZ regime occurs at $l_c \simeq 5$ in $d_s = 1$, which is also consistent with the conclusion from the measurement of the exponent α in figure 2.

In $d_s = 2$, we have measured the current J for the models with l_c in the simulations

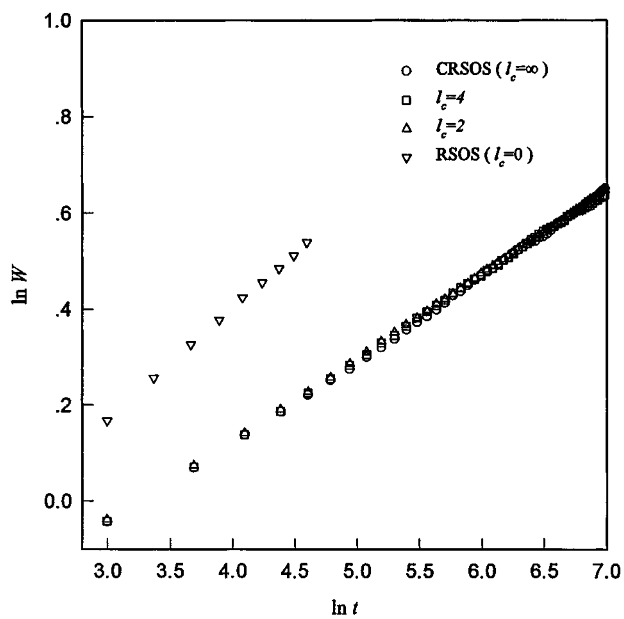

Figure 3. The early time dependence of $W(t)$ of the models with various l_c on the two-dimensional substrate of size $L = 256 \times 256$ as a function of time on a log–log plot.

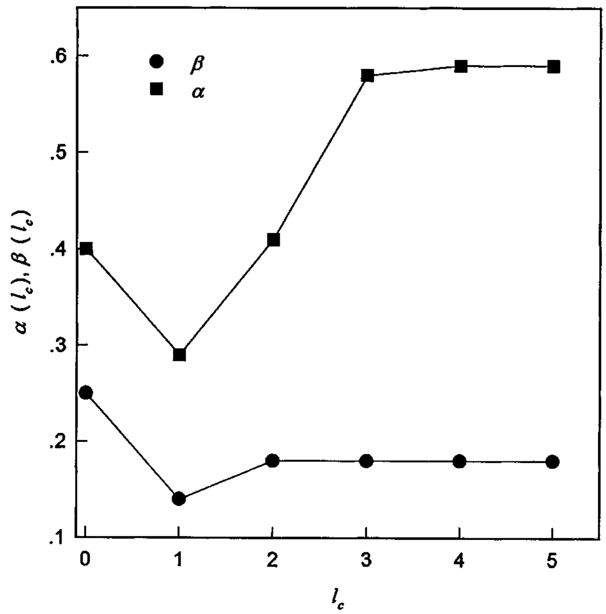

Figure 4. Exponents α and β in $d_s = 2$ as a function of l_c.

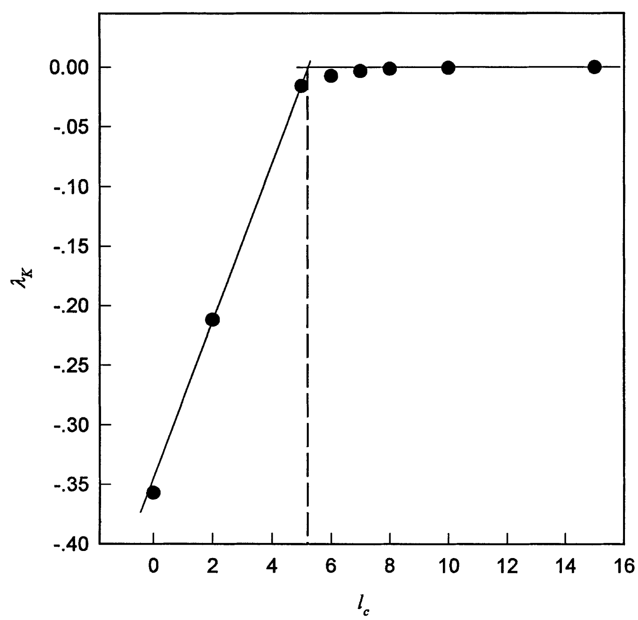

Figure 5. λ_K of the KPZ nonlinear term in $d_s = 1$ as a function of l_c.

beginning with the flat substrate. We have found that in $d_s = 2$ the model with $l_c = 1$ has net negative currents or downward biases in early times ($t \ll L^z$). This result tells us that the effects of the downward bias [15] or the Edward–Wilkinson term ($\nu_2 \nabla^2 h$) [23]

remain for a considerable amount of time in the initial growing stage of the model with $l_c = 1$ and that this effect should make the values of α and β for $l_c = 1$ smaller than the corresponding values for $l_c \neq 1$ (see figure 4). In contrast, we have not found the effects of such downward biases for the models with $l_c \geqslant 2$.

There have been several growth models in which the phase transition occurs [21, 24–26]. In these models the transitions are mainly those from the KPZ class to the Edward–Wilkinson class [23]. In contrast, our model should be one of the models which manifests a phase transition from the KPZ regime to the conserved KPZ regime or to the MBE regime.

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