Nonlocal effects associated with shading in surface growth

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A Monte Carlo simulation of a solid on solid (SOS) model for surface growth that includes nonlocal effects associated with shading is undertaken. The results are analyzed and compared with those resulting from a nonuniform distribution of particles but with no shading. This leads us to suggest that the effects of shading can best be modelled by a spatial and temporal nonuniform flux deposition term, as opposed to the alternative suggestion that shading could be modeled as a correlated noise term. [S1063-651X(99)05903-6]

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I. INTRODUCTION

There is a wide range of mathematical models [1,2] for surface growth but comparatively little work has been carried out on the nonlocal effects [3] associated with shading. These effects can arise in deposition processes as a result of atoms arriving at oblique angles of incidence to the growing surface, as a consequence of which one column can prevent another column from growing because it is being ''shaded'' by it. The surface in the mathematical model is characterized by a height h varying over a d-dimensional substrate of size L. The roughness $w(t,L)=\sqrt{\overline{h^2}-\overline{h}^2}$ can often be represented by a dynamical scaling law,

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

where $f(x)\rightarrow$constant for $x\rightarrow\infty$ and $f(x)\sim x^{\beta}$, $\beta=\alpha/z$ as $x\rightarrow 0$. The exponents α, β, and z determine which universality class the given model belongs to. The models considered in the present paper are derived from the random deposition (RD) model, where a particle is released at a random site above the surface. The height of the column beneath the released particle is increased by one unit. For such a model β is 0.5, α and z are not defined and the surface width climbs monotonically with the time.

II. SIMULATION METHODS

In the model of random deposition with shading (RDS) a particle is released from a random position along a line source (Fig. 1). It moves towards the (two-dimensional) substrate along a path defined by two parameters. These are (random) azimuth and elevation angle. The average elevation angle can be adjusted by the Y and Z offset of the line source. The length of the line source and the size of the substrate can be varied. If the moving particle reaches the surface it sticks to the top of the column it hits. However, if it hits the side of a column it slides down until it reaches the top of the column beneath it (i.e., unlimited vertical motion). Depending on the input parameters of the program various surface relaxation processes can also be included. For example, after the particle reaches the surface it can make a certain number of hops with probabilites determined by the surroundings of the particle. There are two different types of hops: (i) *sliding* this allows the particle to make nearest neighbour hops with given probabilities without changing to a different layer of the growing surface; (ii) *dropping* this gives the particle the capability of dropping with a certain probability from its present layer to a site of lower height (upward motion is not permitted to occur).
Depending on its surroundings (i.e., how many nearest neighbors with lower/equal height), the various possible movements are weighted and the actual movement is selected randomly. After one particle has completed all of its possible movements the next particle is released.

III. RESULTS AND DISCUSSION

Our simulations are usually carried out on a substrate of 35×35 lattice sites and averaged over many simulations with different random numbers. For small angles the described mechanism of releasing the particles by random position and random angle from a line source gives a highly non uniform distribution of particles. In view of this we also considered, just for comparison, a related model called random deposition from a line source (RDL). This model releases particles from a linesource just as in RDS. The position where the particle would hit the substrate is then calculated (ignoring any columns in its ''path'') and the height of that column is increased by one. This excludes shading. Figure 2 shows the distribution of particles along the Y axis. With the Y offset

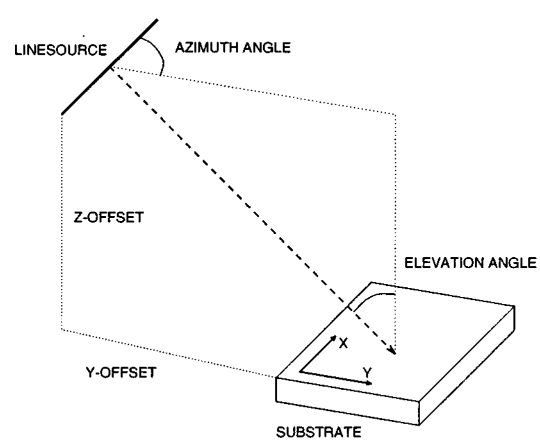

FIG. 1. Macroscopic picture of the model.

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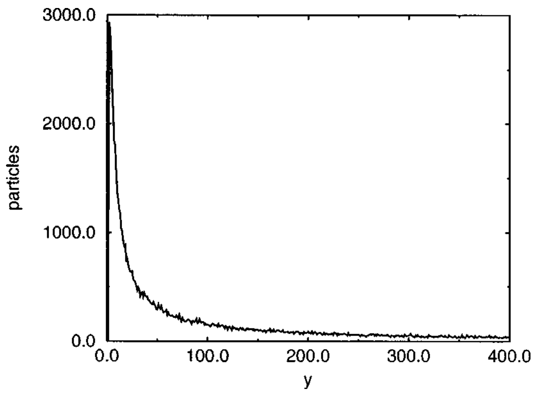

FIG. 2. Distribution of particles along the Y axis.

being one lattice site for a Z offset of 30 000. Figure 3 shows the surface width over time for different average angles of incidence resulting from a higher Y offset for both RDL and RDS.

It is clear that RDL gives a larger surface width than RD, and that RDS gives an even larger width. For RDS, Fig. 4 shows the width over time for different angles of incidence. The fact that RDL gives a series of curves intermediate between pure RD and RDS with a functional form similar to the RDS curves is suggestive of the fact that the latter can be modelled by a term of this type, i.e., a nonuniform flux term.

If we now allow surface relaxation we get different results depending on the number of hops that are permitted to occur. This is shown in Fig. 5. It is an important result and shows that surface relaxation can overcome the effects of shading.

We will now discuss briefly the question of shading and how it can be incorporated into the analysis. To this end we consider first the case of pure RD but with a nonuniform distribution of the particles. In this case the starting equation has the form [1]

$$\frac{\partial h}{\partial t} = F(x) + \eta, \tag{2}$$

where $F(x)$ represents the uneven flux distribution and η is the noise term. Placing

$$h = h' + Ft \tag{3}$$

gives

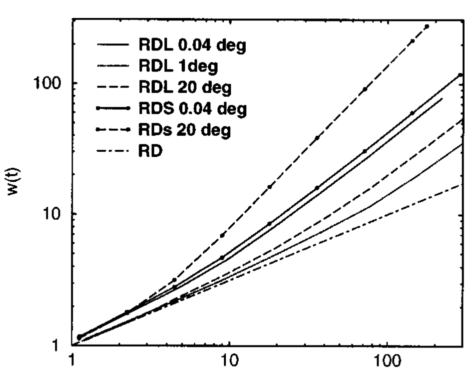

FIG. 3. Random deposition from a linesource (RDL). Elevation angles are given in degrees (deg).

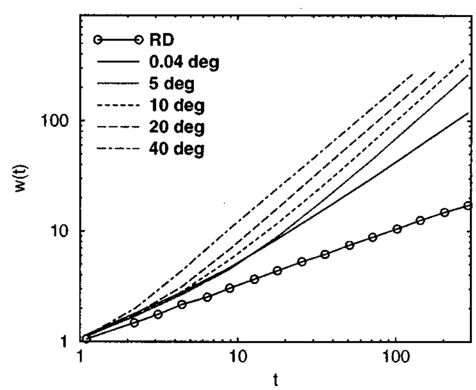

FIG. 4. Different angles of incidence (RDS, no hops), as for Fig. 3.

$$\frac{\partial h'}{\partial t} = \eta. \tag{4}$$

One can then readily solve the equations for the average value of both h and h^2, i.e., $\langle h \rangle$ and $\langle h^2 \rangle$. Assuming that the noise term has the standard correlation function and placing

$$k_1 = \langle F \eta \rangle,$$
$$2k_2 = \langle F^2 \rangle - \langle F \rangle^2$$

shows that the interface width $w(t)$ satisfies

$$w^2(t) = At^2 + Bt, \tag{5}$$

where the second term on the right-hand side comes from the noise term and the parameter A is given by $2(k_1 + k_2)$.

Since RDS at an incoming angle to the normal of the surface of 0.04° is equivalent to a nonuniform distribution of particles, and as the effects of shading at such an angle are anticipated to be small, we would expect RDS at such low angles to satisfy the above equation. As discussed below this is found to be the case.

In order to extend this analysis to incorporate the effects of shading we develop a simple model. This is best appreciated by reference to Fig. 6, which is a schematic representation of an attempt to mimick the effects of shading by means of a time-dependent nonuniform distribution of the incident particles.

The y axis represents the flux and the x axis the length of the substrate. Initially (at $t = 0$) the flux is a constant $(= C_0)$ over the whole of the substrate. (In our earlier mod-

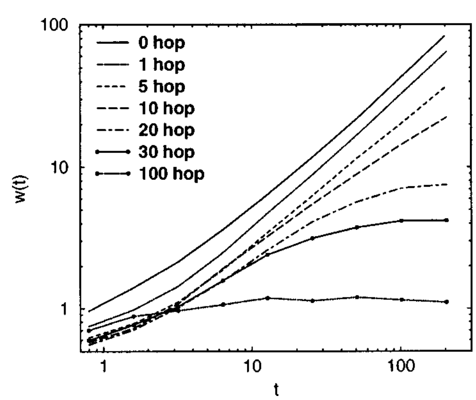

FIG. 5. Different number of hops (RDS, 0.04 deg).

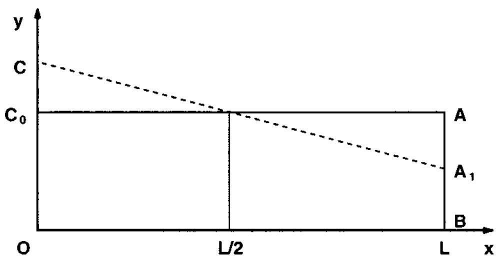

FIG. 6. Model for shading.

els for RDS we know that this is true to a good approximation, once the angle of inclination $\theta > 1°$.) Thus the total number of ''particles'' as represented by the area under the ''curve'' is given by $N = C_0 L$, where L is the ''length'' of the substrate. With increasing time (i.e., $t > 0$) the line $C_0 A$ is 'pivoted' about its mid-point and its ends extended in such a manner that they move along the axis $0y$ (from C_0 to C) or the line AB (from A to A_1). In this manner, as should be clear from the figure, the area under the curve (i.e., CA_1) remains constant at N (i.e., the total incident flux is kept constant throughout the growth process). We will now evaluate the effects of such a time-dependent nonuniform flux distribution.

If we place $C = C_0 + \alpha t^{\gamma}$ then the flux distribution y is related to the position x by

$$y = -mx + C \tag{6}$$

with

$$m = \frac{2}{L}(C - C_0) = \frac{2}{L}\alpha t^{\gamma}. \tag{7}$$

For such a situation the starting equation has the form

$$\frac{\partial h}{\partial t} = F(x,t) + \eta, \tag{8}$$

where

$$F(x,t) = -\frac{2}{L}\alpha t^{\gamma} x + C_0 + \alpha t^{\gamma}. \tag{9}$$

We define an entity $g(x,t)$ such that

$$\frac{\partial g(x,t)}{\partial t} = F(x,t). \tag{10}$$

Hence, by placing $h = h' + g$ we find

$$\frac{\partial h'}{\partial t} = \eta. \tag{11}$$

Note these equations are valid for all points A_1 along the line AB and will hold up to the point $A_1 = B$. The time τ taken to reach this point is given by $\tau = (C_0/\alpha)^{1/\gamma}$. Straightforward solution of the resulting equations for the time interval $0 \leqslant t \leqslant \tau$ lead to the result that

$$w^2(t) = A_1 t^{2(\gamma+1)} + B_1 t, \tag{12}$$

where the second term on the right-hand side comes from the noise term and the parameter A_1 is given by

$$A_1 = \frac{\alpha^2}{3(1+\gamma)^2}. \tag{13}$$

(Note, in relation to a line source, that both α and γ could, in principle, be angle dependent.) A comparison of Eqs. (5) and (12) shows that they are functionally the same, i.e., superficially Eq. (5) looks like a special case of Eq. (12) in which $\gamma = 0$. However, the mathematical conditions governing their validity are not the same, a feature of particular relevance to the values of the prefactors that occur in these equations (e.g., A and A_1). The results in Fig. 4 at angles of 5, 10, 20, and 40 degree all satisfy Eq. (12) with the same value of $\gamma = 0.25$. It is also found that the parameter A_1 is directly proportional to the angle (e.g., within experimental error, the relative values of A_1 are $A_1 = 0.05$, 0.1, 0.2, and 0.4 for 5, 10, 20, and 40 degree angle of incidence, respectively). Consultation of Eq. (13) then shows that the parameter α is proportional to the square root of the angle. This serves to show that the concept of describing the effects of shading (a ''nonlocal'' phenomenon) in terms of a time-dependent nonuniform deposition function appear to be valid.

IV. CONCLUSION

We have shown that the effects of shading on the surface width can be reproduced by introducing a spatial and a temporal nonuniform deposition flux term. Such an approach is to be contrasted with the alternative possibility that shading could be modelled by a correlated noise term.

Our results also show that the interface width shows no sign of saturation unless the number of hops is permitted to be large (as is apparent from Fig. 4 and 5). With an increasing number of such hops we ultimately move to layer by layer type growth (see Fig. 5). These conclusions are in agreement with those reached in an earlier paper, which shows that the very concept of universality classes (e.g., the value of the growth exponent β) is determined by the number of hops that are permitted to occur.

ACKNOWLEDGMENT

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