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Kinetic roughness in the BCSOS model

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Abstract. The surface roughness of a growing crystal is studied by Monte Carlo simulation in a kinetic six-vertex model. Although for equilibrium the results are in good agreement with the exact solution, even a small disequilibrium breaks down the roughening transition. For temperatures below the equilibrium roughening temperature T_R and arbitrary large disequilibrium, as well as for temperatures above T_R but small disequilibrium the surface is logarithmically rough, whereas, for temperatures above T_R and sufficiently large disequilibrium, the surface roughness increases as a power-law of size. A crossover from logarithmic to power-law roughness occurs when the disequilibrium is increased at a fixed temperature above T_R, or the temperature is increased for disequilibrium fixed and sufficiently large.

The dynamics of a growing interface separating two phases has received considerable attention in recent years. A number of growth and deposition models have been proposed and studied (for reviews, see [1]). Much of this interest was motivated by the fact that growth models, apart from their potential practical importance, exhibit new features which are interesting from the point of view of non-equilibrium statistical physics on a fundamental level.

The morphology of the surface can be characterized by roughness. A roughening transition between different phases was originally discovered in connection with non-equilibrium phenomena of crystal growth [2]; theoretically, it was then extensively studied mainly in the case of equilibrium, which is now reasonably well understood [3, 4]. However, its nature in systems which are far from equilibrium is still not sufficiently explored.

An interesting feature of the growth models is non-trivial scaling behaviour. It has emerged from the numerical simulations of simple discrete models of crystal growth that the width of the surface w obeys a scaling law with increasing time t or system size N [5]

$$w(t, N) \approx N^{\zeta} f(t/N^{z}) \tag{1}$$

where $f(x) \to$ constant as $x \to \infty$ and $f(x) \to x^{\zeta/z}$ as $x \to 0$. Thus the steady-state ($t \to \infty$) width diverges as N^{ζ} with a roughness exponent ζ as the size N increases, and the approach to the steady-state is characterized by a dynamical exponent z. In the case of a self-affine structure on a d'-dimensional substrate described by the height variable h, the width w is given by the mean-square height difference

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$w^2 = \langle \overline{h^2} - \overline{h}^2 \rangle$. Here $\langle\ \rangle$ means the statistical average and $\overline{A} = \sum_i A_i/\mathcal{N}$ is the spatial average; i labels substrate sites, and $\mathcal{N} = N^{d'}$ is the total number of sites.

This opens a way to the possibility of classifying the growth models, by analogy with the critical phenomena, into universality classes. Most of the recent effort on growth models have focused on finding the values of the exponents ζ and z, often in connection with the nonlinear Langevin equation proposed by Kardar *et al* [6] (KPZ). These treatments have produced a number of interesting results [7–24], in particular in terms of scaling laws [7, 8, 13–15] and of a possible kinetic roughening transition [16–24]. Many questions, however, are still open. In particular the dimension $d = 3$ ($d' = 2$) appears to be critical for models from the KPZ class, so that it is not clear what the roughening properties will be.

In a recent paper [25] we have introduced a kinetic six-vertex model (model II) as a generalization of the exactly solvable six-vertex model of equilibrium statistical mechanics [26] to a non-equilibrium situation†. van Beijeren's mapping onto the specially symmetric case of the six-vertex model, the so-called F model, allows an exact description of the roughening transition for a surface in thermal equilibrium [28]. Model II was introduced to extend a previously studied growth model (model I [29]) to treat a much richer variety of processes. Both models I and II bear some similarity with, but neither is equivalent to, the hypercube stacking model of Forrest and Tang [18] over which the most accurate simulations in the literature have been performed. Model II contains two parameters: temperature T and disequilibrium (or driving force) $\Delta\mu$, which are used for a parametrization of probability rates for condensation and evaporation of atoms

$$P^{\mathrm{c}} = \frac{\mathrm{e}^{\beta\Delta\mu}}{\mathrm{e}^{\beta\Delta E} + 1} \qquad P^{\mathrm{e}} = \frac{1}{\mathrm{e}^{\beta\Delta E} + 1} \tag{2}$$

where ΔE is a change of the energy of the configuration for a given process and $\beta = 1/k_{\mathrm{B}}T$ is the inverse temperature. Model II appears to be richer in physical content than both model I and the hypercube stacking model. It was found convenient to introduce dimensionless variables T/T_{R} and $\Delta\tilde{\mu} = \Delta\mu/k_{\mathrm{B}}T_{\mathrm{R}}$, using the exactly known roughening temperature T_{R} of the six-vertex model: $k_{\mathrm{B}}T_{\mathrm{R}} = \epsilon/\ln 2$ (where ϵ is vertex energy), for details see [25]. Unlike Amar and Family [17] who employed a Metropolis-like approach we have used (2), which for $\Delta\mu \to 0$ reduces to the Glauber kinetics [30]. We have shown [25] that this model can describe different regimes of crystal growth, i.e. both layer-by-layer and continuous growth, and we have calculated a qualitative curve separating these two modes.

Here we present the results of a further extensive numerical simulation in which we have concentrated on the roughness of the growing surface in the kinetic six-vertex model. We were interested in possible roughening transitions and their relation to different modes of growth. In this work we restrict ourselves to the roughness exponent ζ for which two different behaviours can already be seen for relatively small systems. Measuring the dynamical exponent z is hampered by transient effects, the scaling region is short and very large systems are required to obtain good results.

We used an algorithm employing real time averaging and a special procedure (described elsewhere [25]) for treating the constraint on the height difference between

† A very different application of the six-vertex model to growth problems (in 1+1 dimensions) has been presented very recently in an interesting paper by Gwa and Spohn [27], which exploits more fully the properties of the exact solution.

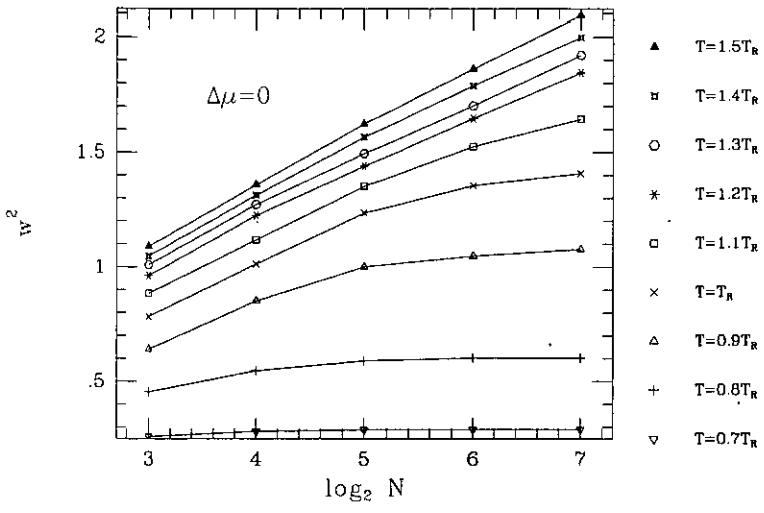


Figure 1. The dependence of the mean-square height difference w on the size N in equilibrium.

the nearest neighbours in the BCSOS model. Using this procedure we were able to perform the calculations for different values of the temperature and chemical potential up to the substrate size of 128×128. We calculated the mean-square height difference for the sizes 8×8, 16×16, 32×32, 64×64 and 128×128. The number of Monte Carlo steps increased with size and the majority of our calculations were done for 3×10^3 steps per site, which turned out to be sufficient for our averaging procedure. Furthermore, the average over at least five independent runs was taken.

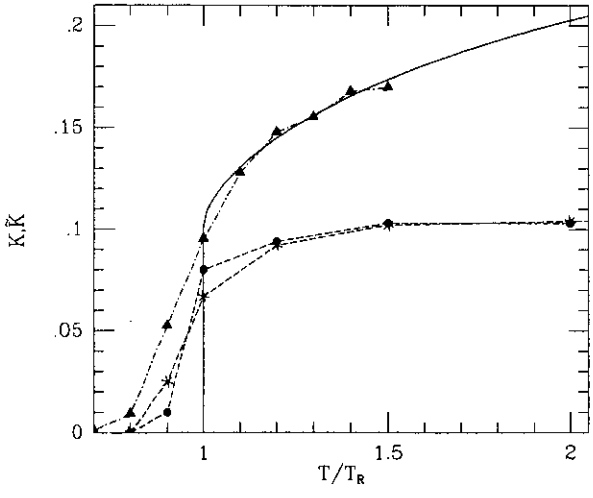


Figure 2. Temperature dependence of coefficients K and $\tilde{K}$: full curve, exact solution for $K(T)$; triangles, $K(T)$ obtained by fitting numerical data; stars, kinetic coefficient $\tilde{K}$; circles, extrapolated kinetic coefficient $\tilde{K}_\infty$.

At first we checked the equilibrium situation and compared our numerical results with the exact solution [26] which is available in this case. The Monte Carlo method

has been used for the study of the thermal roughening transition in the SOS model [31] and also in the BCSOS model [32] for the equilibrium case. Our results for the BCSOS model (figure 1) are very similar to those of [32]. For the thermal roughening transition the relation

$$w^2(N) = \begin{cases} K(T)\ln N & \text{if } T > T_R \\ \text{constant} & \text{if } T < T_R \end{cases} \tag{3}$$

holds. The exact solution of the six-vertex model, in the case of the F-model for $T > T_R$ gives [33]

$$K(T) = \frac{1}{\pi \cos^{-1}\Delta} \tag{4}$$

where $\Delta = 1 - \frac{1}{2}e^{2\beta\epsilon}$. The quantity $K(T)$ obtained by a linear fitting from our data is compared with the exact solution (4) in figure 2: the agreement is good†.

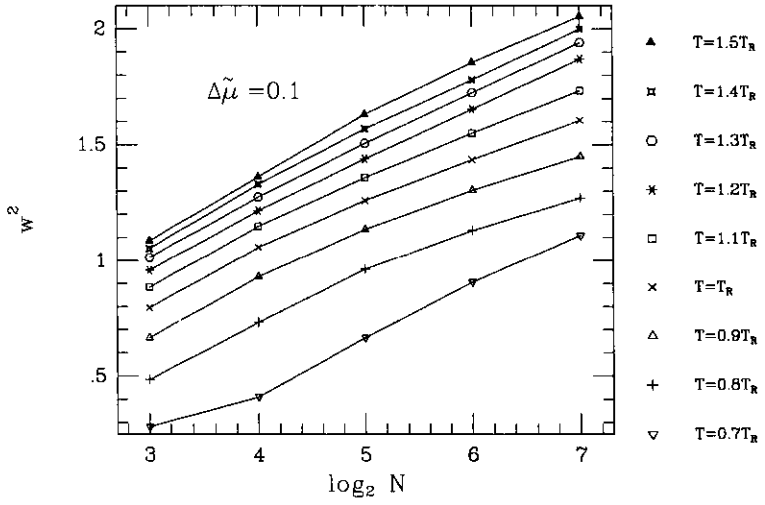


Figure 3. The same as in figure 1 but for very small disequilibrium.

After this check we investigated the influence of a very small disequilibrium on the roughening transition (this problem was investigated theoretically some time ago by Nozières and Gallet [35] and very recently by Hwa *et al* [24]). There is no sign of a transition in the behaviour of the mean-square height difference (figure 3). Our data suggest that even for very small disequilibrium the surface is always rough with roughness still logarithmically increasing with the system size, i.e. with the roughness exponent $\zeta = 0$. This agrees with the recent calculations of Hwa *et al* using the renormalization group [24]. The roughness, even for temperatures below T_R, can be understood because the number of incomplete layers in the sample is increasing with its size even in the layer-by-layer mode.

We also calculated a kinetic growth coefficient (or 'mobility') $\tilde{K} = \lim_{\Delta\mu\to 0} G/\beta\Delta\mu$ where G is the growth rate. It shows a transition in the vicinity of the equilibrium roughening temperature T_R (figure 2) which is connected with

† Notice, however, that there is some controversy in the literature concerning the value of $K(T)$: a different result is given by Bogoliubov *et al* [34].

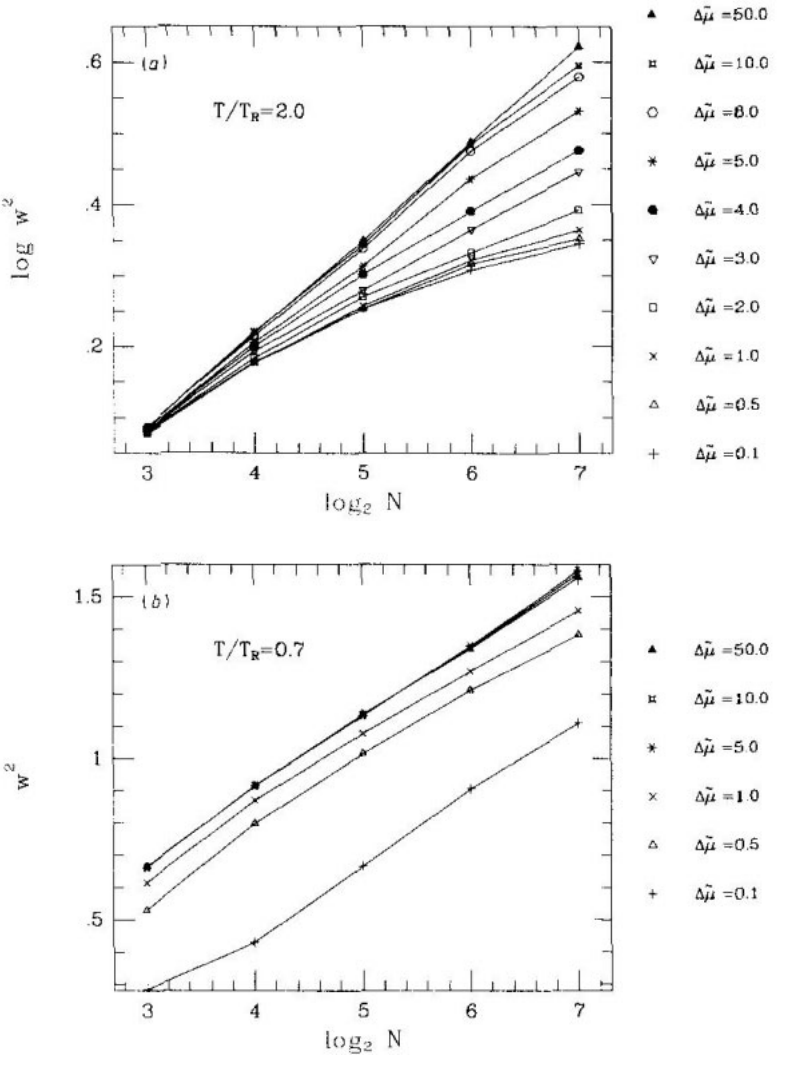


Figure 4. (*a*) The dependence of the mean-square height difference w on the size N for constant temperature $T = 2T_R$ and increasing disequibilibrium. (*b*) The same as in figure 4(*a*), but for $T = 0.7T_R$.

the change of the form of the dependence of the growth rate on β and $\Delta\mu$, i.e. with the change of the mode of growth. These data were obtained from the extrapolation of $G/\beta\Delta\mu$ for small $\beta\Delta\mu$ to $\Delta\mu = 0$ for relatively small system size $N = 32$, and we expect that the transition will become sharper for a larger system. In order to check this point, we performed the calculation for a smaller system ($N = 16$). Supposing $\tilde{K}$ to depend on size as $\tilde{K} = \tilde{K}_\infty + K_1/N$, we can then obtain values for $\tilde{K}_\infty$. The results of this crude estimate are also shown in figure 2. The behaviour of the 'mobility' again agrees with the results of Hwa *et al* [24].

A special limit of our model, in which the rates of the processes are independent of the surroundings (this corresponds to the infinite temperature limit in our parametrization), was studied by Meakin *et al* [7] (only pure growth case, $\Delta\mu \to \infty$ in

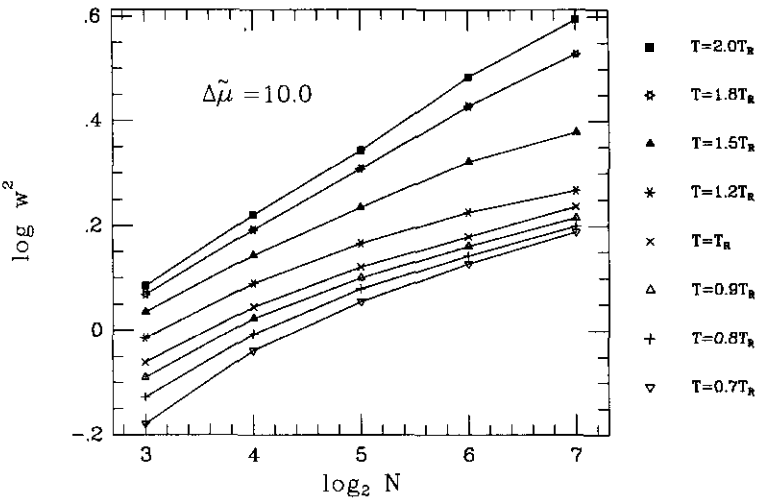
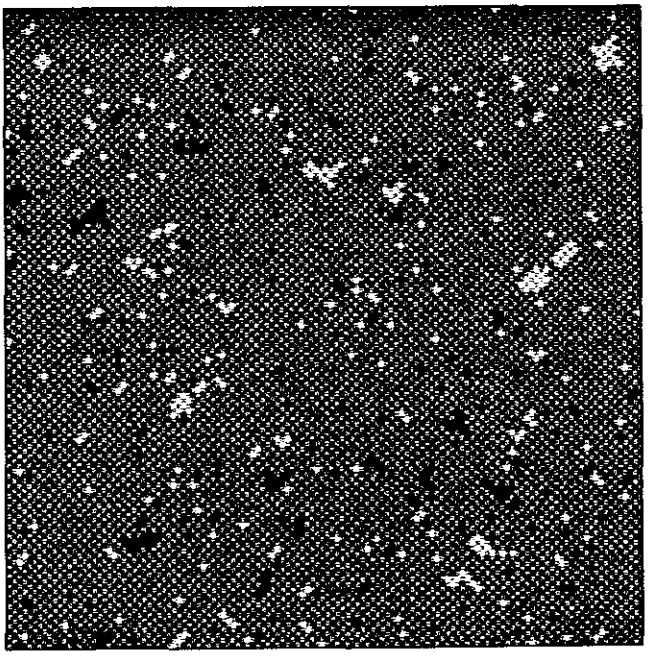


Figure 5. The same as in figure 3, but for large disequilibrium.

our parametrization) and later by Liu and Plischke [36] (two cases: pure growth and equilibrium). They found power-law roughness for T, $\Delta\mu \to \infty$, with the roughness exponent $\zeta = 0.365 \pm 0.005$ [7], $\zeta = 0.375$ [36]. So one can expect a transition from logarithmic to power-law roughness. To check the possibility of a transition we performed calculations for different temperatures and disequilibria. The change of behaviour, however, is very gradual, so that it should be described as a crossover, rather than as a transition. Indeed, crossover behaviour of this kind was considered in the original work of Kardar *et al* [6] and found recently (but in the time dependence) by Guo *et al* [21] and Tang *et al* [37].



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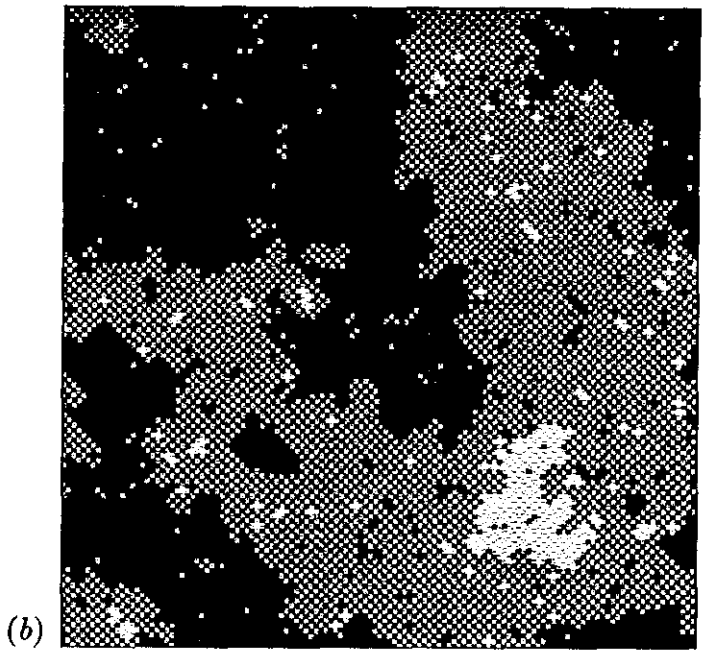

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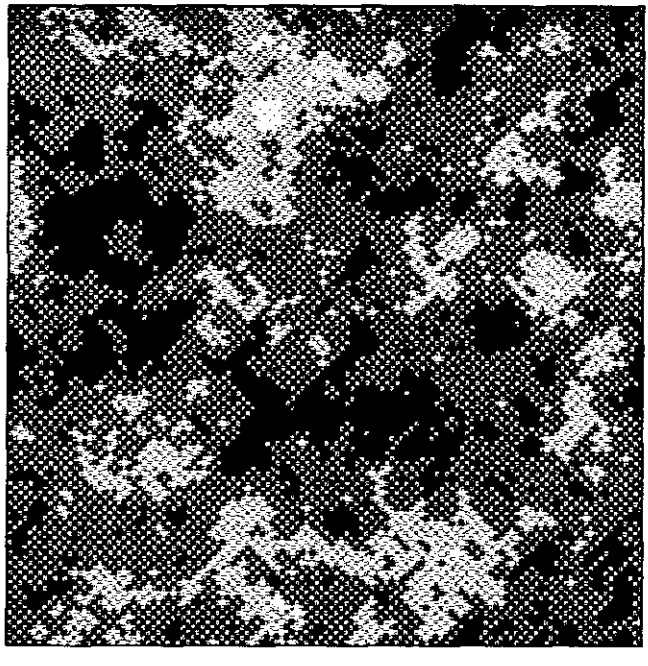


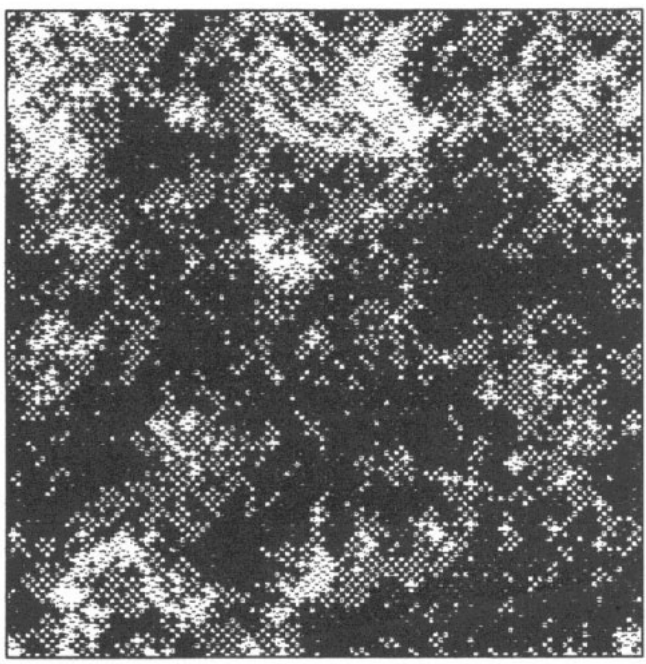
(*c*)

Figure 6. Grey-scale plots profile of the surface at saturation for $N = 128$, $T = 0.7T_R$ and different disequilibria: (*a*) $\Delta\tilde{\mu} = 0$; (*b*) $\Delta\tilde{\mu} = 0.1$; (*c*) $\Delta\tilde{\mu} = 10$. Darker hue indicates higher level. Different profiles contain different numbers of layers: (*a*) 3 layers; (*b*) and (*c*) 5 layers.

The existence of a kinetic roughening transition in $d' = 2$ for models belonging to the KPZ-class is somewhat controversial. Since dimension $d' = 2$ is the marginal dimension, no analytical prediction is known for this case. The results of some numerical simulations of discrete models [22, 19, 20] have been interpreted as evidence of the transition. However, other papers [21, 24, 37] show that there is a crossover rather than a sharp transition; a direct numerical solution of the KPZ equation [38] does not indicate any transition either.

We have observed crossover behaviour in two cases: either with increasing disequilibrium for temperature above the roughening temperature $T = 2T_R$ (figure 4(*a*)) or with increasing temperature for sufficiently large disequilibrium ($\Delta\tilde{\mu} = 10$) (figure 5). In the former case the crossover occurs for $1 < \Delta\tilde{\mu} < 8$ and in the latter for a temperature around $T = 1.5T_R$. A similar crossover with increasing temperature as in figure 5 is also seen for lower constant disequilibrium $\Delta\tilde{\mu} = 5$ (not shown). On the other hand for a temperature below T_R ($T = 0.7T_R$) we do not observe any crossover: the roughness remains logarithmic even for very large disequilibrium (figure 4(*b*)).

For large disequilibrium and at temperatures of the order of T_R, the exponent extracted from our data is lower than that measured by Meakin *et al* [7] and by Liu and Plischke [36]. For example for $T = 2T_R$, $\tilde{\Delta\mu} = 50$ and $N = 128$ we get $\zeta = 0.225$. This value is close to a value $\zeta = 0.25$ obtained by Amar and Family [17] in the case of the restricted SOS model (for the low-temperature phase). To allow a comparison with the results of Meakin *et al* and of Liu and Plischke we also ran our program for the case of probabilities independent of the surroundings (infinite temperature limit) and $\beta\Delta\mu = 25$, i.e. the same $\beta\Delta\mu$ as in the case $T = 2T_R$ and



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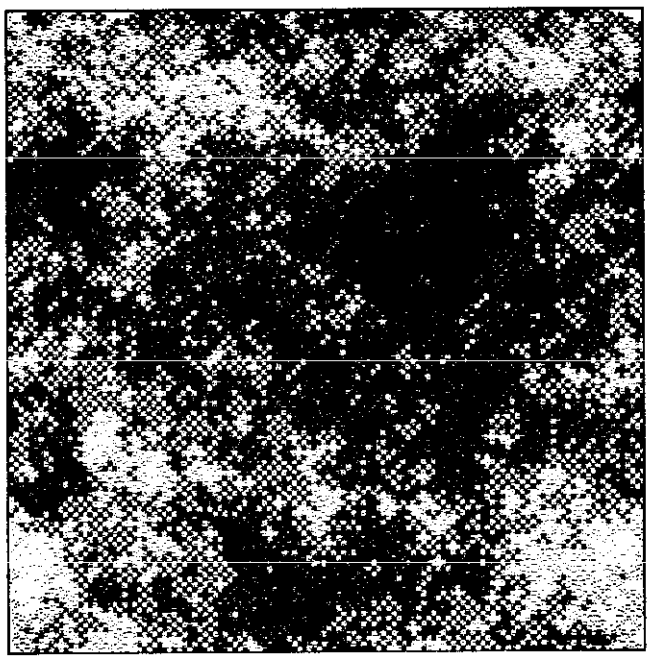

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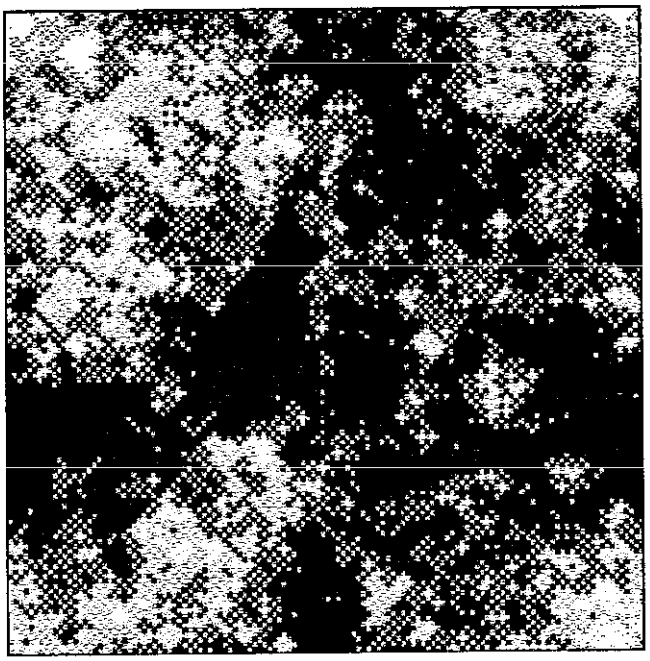

(*c*)

Figure 7. Same as figure 6, but for $T = 1.5T_R$. Different profiles contain different numbers of layers: (*a*) 6 layers; (*b*) and (*c*) 7 layers.

$\tilde{\Delta\mu} = 50$. An estimate of the roughness exponent in this case (again for $N = 128$) is $\zeta \approx 0.35$, in approximate agreement with [7] and [36]. Thus ζ depends on T (see table 1). To save computer time the values of ζ in the table were actually obtained for a smaller size ($N = 32$). In fact ζ depends on N; this dependence, however, is very weak (ζ increases by about 3% when N increases from 32 to 128) and, moreover, is the same for both $T = 2T_R$ and $T = \infty$.

Table 1. Temperature dependence of the roughness exponent for constant $\beta\Delta\mu = 25$.

T	ζ
2	0.218±0.008
3	0.265±0.013
4	0.293±0.015
5	0.307±0.003
6	0.310±0.001
7	0.316±0.006
8	0.315±0.007
9	0.322±0.009
10	0.323±0.011
11	0.321±0.004
12	0.323±0.009
25	0.333±0.011
50	0.335±0.008
∞	0.340±0.009

Our data, in contrast with previous work based on a renormalization-group analysis of stochastic partial differential equations [24], do not indicate a simple correlation between the transition from the layer-by-layer to the continuous mode of growth and the kinetic crossovers in roughness properties. In particular, for small $\Delta\tilde{\mu}$ the roughness is logarithmic for both $T < T_R$ and $T > T_R$ whereas the modes of growth are different [25]. We cannot, however, completely rule out the possibility that such a correlation may appear in a system with a much larger size than our maximal size ($N = 128$).

Figures 6 and 7 show profiles of the surface at saturation (steady growth) for different values of temperature and disequilibrium, illustrating different roughness properties and also different modes of growth.

The main difference between the present work and previous studies, such as e.g. the extensive simulations by Amar and Family [17], is that here we pay special attention to the dependence of the surface roughness on $\Delta\mu$. The model considered by Amar and Family is very similar to ours but is studied in the absence of evaporation ($\Delta\mu \to \infty$). Under these conditions they find power-law roughness except in a narrow range around the equilibrium T_R. Under the same conditions we also find power-law roughness at high T, but not at low T (we ignore the reasons for this latter discrepancy). The important point, however, is that at finite $\Delta\mu$ the power-law behaviour becomes logarithmic for large N, i.e. the (nonlinear) effects giving rise to the power-law behaviour are asymptotically irrelevant. This contrasts with the situation for infinite $\Delta\mu$, as well as with the growth properties of nonlinear stochastic differential equations such as the KPZ equation [6].

Turning to the latter, we are at present studying how to model the present Monte Carlo simulation in terms of stochastic partial differential equations. A preliminary

analysis seems to show that such differential equations do contain nonlinear terms, but are very different from the square gradient occurring in the KPZ equation. A square Laplacian would be a better (although imperfect) representation of the nonlinearities inherent in the simulation. Not surprisingly, a square Laplacian is asymptotically irrelevant. We believe these to be the reasons for some discrepancies between our work and previous work based on stochastic differential equations, such as the studies by Guo *et al* [21, 22] and Hwa *et al* [24].

In summary, studying the roughness in a six-vertex model with Glauber kinetics, we have found two regions with different roughness properties (logarithmic roughness against power-law roughness). More simulation and theoretical work is certainly needed to understand the phase diagram and the nature of the change from one regime to the other, in particular to clarify whether some crossover scaling is fulfilled.

Acknowledgments

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