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Kinetic roughening and phase ordering in the two-component growth model

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Abstract

The interplay between kinetic roughening and phase ordering is studied in a growth SOS model with two kinds of particles and Ising-like interaction by Monte Carlo simulations. We found that, for a sufficiently large coupling, growth is strongly affected by interaction between species. Surface roughness increases rapidly with coupling. Scaling exponents for kinetic roughening are enhanced with respect to the homogeneous situation. Phase ordering which leads to the lamellar structure persisting for a long time is observed. Surface profiles in the strong coupling regime have a saw-tooth form, with a correlation between the positions of local minima and the domain boundaries. © 1998 Elsevier Science B.V. All rights reserved.

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1. Introduction

Growth by vapour deposition is a technologically important process for producing high quality materials. During the last years much progress has been made in understanding growth mechanisms on the microscopic level [1]. However, these results refer mainly to single-component homogeneous growth and growth of binary materials is much less understood. The essential feature in binary systems is phase ordering [2]. Recently, there has been interest in the interplay between phase ordering during growth and kinetic roughening [3–5]. Kinetic roughening is one of the most important aspects of crystal growth. Due to stochastic fluctuations during a deposition process, the growing surface becomes rough and the roughness typically increases with time as a power with an exponent β which allows us to classify different types of growth processes. Kinetic roughening is important from the practical point of view, besides it also attracted a lot of interest in the context of non-equilibrium statistical mechanics [6].

In this paper we discuss the interplay between compositional ordering and kinetic roughening in a simple model for growth of binary alloys which we recently formulated [5].

2. Model

Our model is based on the single-step solid-on-solid geometry. We confine ourselves here to a one-dimensional substrate with coordinate i. The

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surface is described by a single-valued function $h_i(t)$ with the additional constraint $|h_i - h_j| = 1$ for neighbouring sites i and j. A new particle can be added only at a growth site corresponding to a local minimum in the surface height profile. We consider two types of particles, which we distinguish by a variable $\sigma(i, y)$ taking the value $+1$ or -1; here y is a coordinate in the vertical direction. Growth rules are controlled by a change of energy of alloy after deposition of a new particle. The energy is given by the Ising-like interaction. The probability of deposition of a new particle of type σ to a growth site i is proportional to $\exp(-\Delta E(i, \sigma)/k_B T)$, where k_B is Boltzmann's constant and T is temperature. The change of energy is $\Delta E(i, \sigma)/k_B T = -K\sigma[\sigma(i-1, h_{i-1}) + \sigma(i, h_i) + \sigma(i+1, h_{i+1})] - H\sigma$. Here, K is a dimensionless coupling strength and H is an external field. We call this model a two-component single-step (TCSS) model. We consider here only the case of zero external field.

The surface roughness is described by the surface width

$$w(t, L) = \langle \sqrt{h^2 - \bar{h}^2} \rangle,$$

where t is time, L is linear size and the bar denotes a spatial average, $\langle \ldots \rangle$ a statistical average. Ordering is studied by the time evolution of the average domain size along the surface $D(t)$.

3. Results

We performed extensive simulations for various values of K. Evolution of the surface profile is affected by composition of the surface, in particular it depends on composition of the initial flat substrate. We considered three different types: (i) a neutral substrate, i.e. without any interaction with deposited particles; (ii) an alternating substrate, with alternating types of particles; and (iii) a homogeneous substrate composed of one type of particles.

Evolution on the neutral and the alternating substrate is almost the same. In Fig. 1 we can see that the effective exponent ($\beta_{\text{eff}} = 0.45$) is at first larger than the exponent for homogeneous growth,

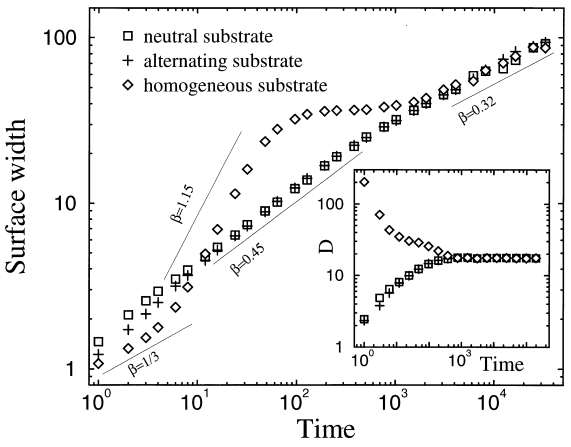


Fig. 1. Surface width w vs. time for coupling strength $K = 1.0$ and three different types of substrate of size $L = 10\,000$. Data are averaged over 30 independent runs. The values of slope, $\beta = 0.45$ and $\beta = 0.32$, were obtained by fit to points for the alternating substrate, the straight line with slope 1/3 is only a guide for the eye.

$\beta = 1/3$, which corresponds to the so-called Kardar–Parisi–Zhang (KPZ) class [7]. However, after a certain time $t_{\text{cross}} \approx 10^3$, the effective exponent crosses over to a value close to 1/3 ($\beta_{\text{eff}} = 0.32$). This behaviour can be explained by evolution of compositional ordering. In the inset to Fig. 1 we present the time dependence of the average domain size for the three substrate types considered. We can see that for all of them the domain size saturates at time close to t_{cross}. Hence, ordering of the surface leads to enhanced increase of the roughness, but when ordering stops the surface roughness increases further with the same exponent as in the one-component, single-step growth model.

In the case of the homogeneous substrate, the behaviour of the surface width changes dramatically (cf. Fig. 1). The general features are the following. At first the width starts to grow with the exponent close to 1/3 (this regime is extended over several decades of deposition time for very strong coupling). It is caused by the fact that practically no domains with minority type of particles are formed because the probability of nucleating these domains is rather small; growth is the same as in the pure single-step model. Then the slope crosses over to a very large value

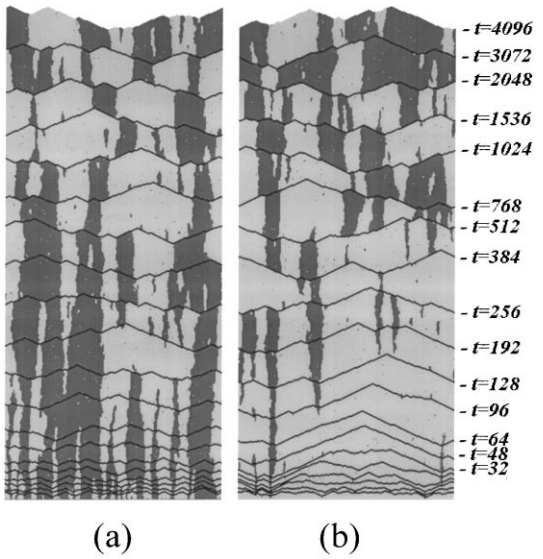


Fig. 2. Examples of evolution of surface profiles for $K=1.0$ and two different substrates: (a) the neutral substrate and (b) the homogeneous substrate. Surface profiles at various times increasing as powers are indicated by black lines, only part of the grown material close to the surface is shown for a given time. Dark and light grey correspond to different types of particles. The system size is $L=250$.

($\beta_{\mathrm{eff}}=1.15$). This unexpected effect is related to the growth of trapezoidal features with length given by the positions of the minority type domains, which start to appear but often quickly disappear again. The rapid increase of roughness ceases when relatively stable minority type domains are nucleated. The further increase of roughness is very slow up to the time when the average domain size saturates and growth continues with the KPZ exponent $\beta=1/3$. We illustrate the difference in evolution on the neutral and on the homogeneous substrate in Fig. 2. We can see that for the homogeneous substrate dark domains appear very slowly.

Let us now turn to the dependence on the coupling K in the case of the neutral substrate. For small K, there is no ordering in the growth direction. Small domains appear and shrink again, but for a larger K a clear lamellar structure exists. We illustrate this in Fig. 3, which shows the evolution of configurations on a substrate with periodic domains imitating the lateral superlattice. We can see that for $K=2$ lamellae persist for a long time. Notice the correlations between the positions of local minima of the surface profile and domain boundaries. We observed that this is a typical case

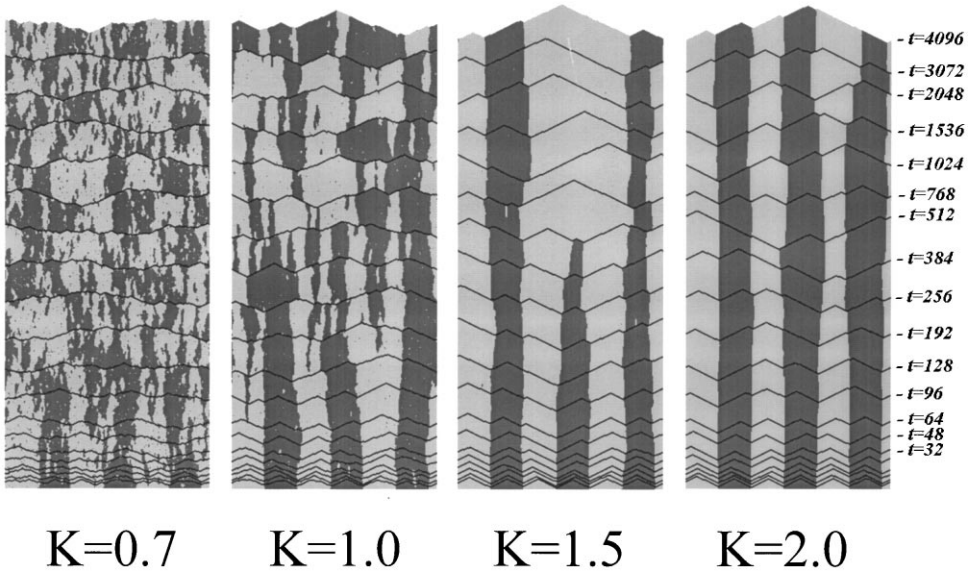


Fig. 3. Examples of evolution of surface profiles on the substrate with alternating domains of different particle types for several coupling strengths K. The meaning of colours and other conditions are the same as in Fig. 2.

for stronger coupling, independent of the type of substrate. We have found that the roughness increases rapidly with coupling. The effective exponent β_{eff} for initial growth increases with K and seems to approach a value of 1/2; for $K=2$ we have found $\beta=0.52\pm0.02$. The crossover time for change of β_{eff} to the KPZ exponent also increases rapidly with K ($t_{\text{cross}}\propto e^{\gamma K}$ with $\gamma\approx3.5$).

4. Conclusion

We demonstrated that phase ordering leads to faster kinetic roughening than in the homogeneous case. However, after some time this behaviour crosses over to the ordinary behaviour for homogeneous growth. But the crossover time increases rapidly with interaction between particles, so practically only the regime with enhanced roughness can be seen for stronger coupling. We also illustrated the strong sensitivity of evolution on the initial composition of the substrate.

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