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Dynamical properties of a growing surface on a random substrate

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The dynamics of the discrete Gaussian model for the surface of a crystal deposited on a disordered substrate is investigated by Monte Carlo simulations. The mobility of the growing surface was studied as a function of a small driving force F and temperature T . A continuous transition is found from a high-temperature phase characterized by linear response to a low-temperature phase with nonlinear, temperature-dependent response. In the simulated regime of driving force the numerical results are in general agreement with recent dynamic renormalization group predictions.

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There has been considerable progress in recent investigations of crystalline surface growth [1–3]. It is known [4,5] that, due to the discreteness and fluctuations (thermal fluctuations and fluctuations in the growth process itself), a crystalline surface undergoes a phase transition between a high-temperature rough phase and a low-temperature smooth phase. The presence of the quenched disorder in the crystal (either in the substrate [6] or in the bulk [7]) changes both the critical temperature and the character of the low-temperature phase. Below critical temperature, T_c , the system develops a glassy phase characterized by the existence of many metastable states to which surface configurations are pinned by disorder. The surface itself remains rough but with very different static and dynamic properties [6,7] compared to the roughness above T_c .

In the present work the dynamic properties of the roughening transition are examined by numerical simulations. The numerical studies of the static properties were reported elsewhere [8]. The simulated system is based on the Hamiltonian of the discrete Gaussian model which was very successful [4,5] in describing the surface on a flat substrate:

$$H = \frac{\kappa}{2} \sum_{\langle i,j \rangle} (h_i - h_j)^2. \quad (1)$$

The sum runs over nearest-neighbor pairs, κ is the surface

tension, and h_i is the height of the surface above the point i on the two-dimensional (2D) basal lattice. In the case of a flat surface h_i takes integer values in the units of lattice spacing a in the direction perpendicular to the surface. To simulate the disordered substrate a random quenched height d_i chosen uniformly (and independently for each site) in the interval $(-a/2, +a/2]$ was first assigned to each site. The height h_i then takes the values $h_i = d_i + n_i a$ where n_i is any positive or negative integer.

In the continuum limit, $h_i \rightarrow \phi(\vec{x})$, $d_i \rightarrow d(\vec{x})$, and near the critical point, Eq. (1) maps to the Hamiltonian of the random phase sine-Gordon model (RSGM) [4]:

$$\mathcal{H} = \int d\vec{x} \left\{ \frac{\kappa\beta}{2} [\nabla \phi(\vec{x})]^2 - g \cos\{2\pi[\phi(\vec{x}) - d(\vec{x})/a]\} \right\}. \quad (2)$$

The periodic cosine term comes from the lattice discreteness and is crucial for the existence of a phase transition. The constant g might be considered as the strength of the periodic pinning potential. The Hamiltonian (2) also describes other disordered systems: two-dimensional vortex-glass with a parallel magnetic field [9], charge density waves, and it is also equivalent to the vortex-free XY model with random field.

If the disorder is absent, the predicted value [1] for the critical temperature of the discrete Gaussian model (1) is of the order $T_R \approx 1.45$, which is close to the results from computer simulations [10]. The behavior of the roughening transition in the presence of an applied force F was studied in detail by Nozières and Gallet (NG) [5]. They found a broadening of the transition due to nonequilibrium conditions with crossover occurring below T_R . In the limit $F \rightarrow 0$, the interface mobility $\mu = v/F$ has a sharp jump at T_R , from a finite value for $T > T_R$ to zero for $T < T_R$. If surface is driven by a small, but finite, driving force it remains rough (with temperature- and force-dependent mobility) even below T_R . The NG theory describing the system in the temperature region close to T_R ("interrupted renormalization" scheme) or well below T_R (homogeneous nucleation) is in quantitative agreement with experiments on (0001) interfaces of hcp ^4He crystals near the roughening transition [11].

The effects of the disordered substrate on the dynamic properties in the vicinity of the phase transition were studied by the dynamic renormalization group (RG) methods [6,12] based on the Langevin dynamics with a small driving force F :

$$\frac{\partial \phi}{\partial t} = -\frac{\delta \mathcal{H}}{\delta \phi} + F + \xi. \quad (3)$$

Here the Gaussian fluctuating noise ξ satisfies $\langle \xi(\vec{x}, t) \xi(\vec{x}', 0) \rangle = 2T \delta(\vec{x} - \vec{x}') \delta(t)$ and the exponentiated random phase $d(\vec{x})$ in Eq. (2) also obeys Gaussian statistics: $\langle \exp\{i2\pi d(\vec{x})/a\} \exp\{-i2\pi d(\vec{x}')/a\} \rangle = a^2 \delta(\vec{x} - \vec{x}')$. The theory predicts that above the critical temperature, $T_c = \kappa/\pi$, the system responds linearly to the applied force, i.e., the mobility μ is finite and independent of F , while below T_c the response is nonlinear, characterized by the temperature-dependent exponent η :

$$\mu \sim \begin{cases} (T/T_c - 1)^\zeta & \text{for } T > T_c, \\ (1 - T/T_c)^\zeta F^\eta & \text{for } T < T_c, \end{cases} \quad (4)$$

where $\zeta \approx 1.78$ is a universal constant and $\eta = \zeta|1 - T/T_c|$. At $T = T_c = \kappa/\pi$ and finite F , Eq. (4) is corrected by a term $\sim |\ln F|^{-\zeta}$ so that mobility does not vanish [6]. Also, for $T < T_c$, Eq. (4) holds only if $F^{-|1 - T/T_c|} \gg 1$. If this condition does not hold, the original Eq. (48) in Ref. [6] has to be used. According to RG analysis, these results are valid close to T_c and in the large L , small g , and small F limit with the crossover regime characterized by two effective lengths: $L_g \sim g_0^{1/2|1 - T/T_c|}$ and $L_F \sim F^{-1/2}$ ($g_0 = \pi g^2/2T^2$ is the bare coupling constant).

Numerical simulations of the model (3) with the Hamiltonian (2) in the limit of small g were recently performed by Batrouni and Hwa [13] in the context of a randomly pinned planar flux array. They found no sign of phase transition in statics but in dynamics they observed a phase transition which is, however, only in qualitative agreement with RG predictions (4). The constant ζ extracted from their data is significantly smaller than that in Eq. (4). On the other hand, the behavior of the surface under the influence of a strong driving force also has many interesting features and it has been the subject of recent investigations [14].

After a brief description of the simulated dynamics we will present our numerical results for the dynamics of the model (1) which maps to the model (2) with coupling constant g of order 1.

Every surface configuration can be completely specified by a collection of column height variables $C = \{h_1, h_2, \dots\}$. The dynamics of the model is determined by the transition rates $W(C \rightarrow C')$ which specify how the system evolves from a given configuration C into a new configuration C' . The probability $P(C, t)$ that the surface has configuration C at time t is determined by the following master equation in terms of these transition rates:

$$\partial_t P(C, t) = \sum_{C'} \{W(C' \rightarrow C)P(C', t) - W(C \rightarrow C')P(C, t)\}. \quad (5)$$

Without driving force, the system evolves to equilibrium and the transition rates satisfy the detailed balance condition: $W(x) = W(-x)e^{-x}$, where $x = \beta \Delta H$, and ΔH is change of energy. The driving force F is included by simply adding a term $\Delta n F$ to ΔH in W , i.e., $W = W(\beta[\Delta H + \Delta n F])$ where Δn is a local change in the height between configurations C and C' . The commonly used choice of W is the Metropolis rate:

$$W(\beta[\Delta H + \Delta n F]) = \min\{1, e^{-\beta(\Delta H + \Delta n F)}\}. \quad (6)$$

The Monte Carlo (MC) simulations presented in this work were performed on the two-dimensional square lattice of linear dimension $L = 64$, and with periodic boundary conditions. The lattice was divided into two sublattices. During the first half of the time step, all heights h_i of one sublattice were simultaneously updated by increasing or decreasing them (independently) by one unit keeping the heights of the other sublattice fixed. The moves are then accepted or rejected according to the Metropolis rule (6) with Hamiltonian (1) and constant $\kappa = 2$. In the second half of the time step, the second sublattice is upgraded keeping the first one fixed.

Starting with the equilibrated configurations saved after measuring the static properties of the system [8], the force was turned on by implementing (6). The velocity of the growing surface averaged over different realizations of the disorder was monitored as a function of MC steps. Typically, up to 10^4 initial MC steps were discarded since the system requires some time to reach its stationary state characterized by a uniform velocity. Measurements were performed over additional MC steps whose lengths depended on the values of F and T . The length of the runs ranged from 5×10^4 (for large F and large T) to 10^6 MC steps (for small F and small T). The average surface heights (in lattice units a) at the end of the MC runs were between several thousand steps for large F and T to several dozen steps for small F and T . For every MC run, the measurements of the surface velocity were grouped into several groups (usually about ten) and the average velocity of these groups with corresponding error bars is presented in Fig. 1 and Fig. 2. A practical problem in these simulations is to measure the response of the system to

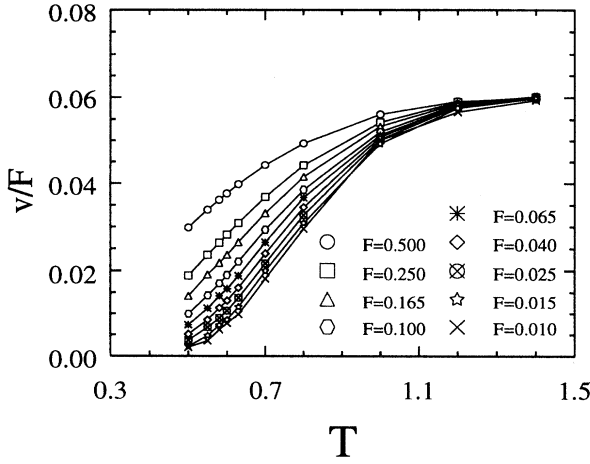


FIG. 1. The dependence of the mobility $\mu = v/F$ as a function of temperature for different F . The system size is $L = 64$ and sample averaging is performed over 50 realizations of disorder. The full curves are guides to the eye.

very small force because very long MC runs are required in order to get reliable statistics. We started with the forces of order 1 and then decreased F gradually toward the lowest value ($F = 0.01$) for which the data analysis still suggests that the surface is moving with uniform velocity although the error bars are much larger compared with the measurements with larger F and T (see Fig. 2). For smaller values of F we could not extract reliable statistics within the computer time available.

Figure 1 shows the behavior of the mobility, $\mu = v/F$, as a function of temperature for different driving forces, F , while Fig. 2 shows the log-log plot of μ versus F for different T . The sample averages were performed over 50 realizations of the disorder. It is clear from the figures that the system has a phase transition from the regime at higher T , where mobility is finite and independent of temperature and

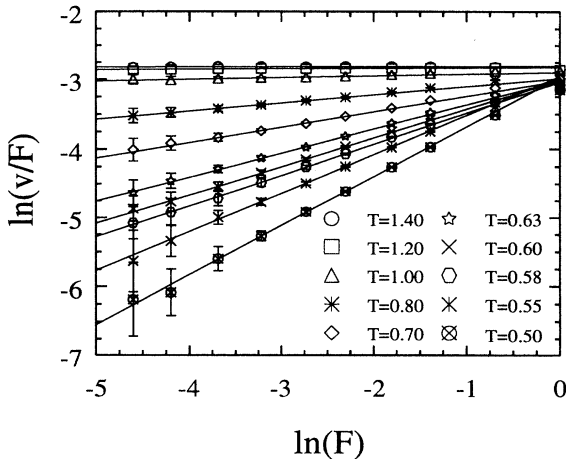


FIG. 2. The log-log plot of the mobility versus driving force. The straight lines are the best fits to $\ln(v/F) = a + b \ln(F)$ including only six the smallest values of F for each T in Fig. 1.

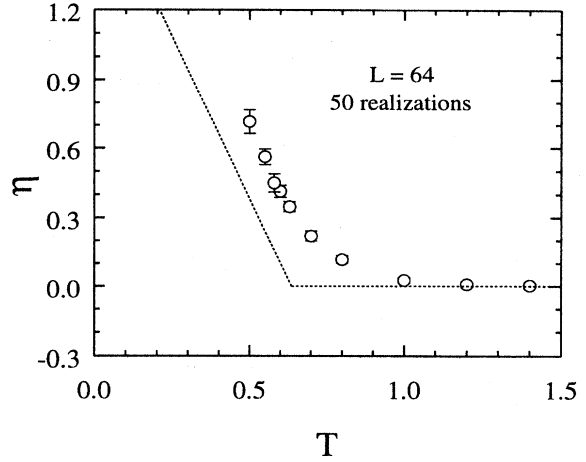


FIG. 3. Plot of the coefficient $b(T)$ (circles) from the fitting equation (see text and Fig. 2). The dotted line is the analytical prediction (4).

force, to the nonlinear regime at lower temperatures where μ depends on F and T . The transition itself is very broad and the position of the critical temperature T_c is not very clear. The straight lines in Fig. 2 are the best fits to the fitting equations $\ln(v/F) = a(T) + b(T) \ln F$. Only the six lowest values of F from Fig. 1 were included in the fit: $F = 0.010, 0.015, 0.025, 0.040, 0.065$, and 0.100 . The slope of the lines, or coefficient b , corresponds to the exponent η in formula (4). Figure 3 shows a comparison of the exponent η plotted according to Eq. (4) (dotted line) and the corresponding values extracted from the data in Fig. 2 (circles). Note that at $T = T_c$ Eq. (4) has to be corrected with the above-mentioned logarithmic contribution due to finiteness of F so that disagreement between the dotted line and the numerical results is expected at and very close to T_c . Generally speaking, there is an agreement between RG methods and the numerical results.

The finite size effects are examined by repeating the simulations for a few temperatures below T_c on the system size $L = 128$ and with sample averages over 25 realizations of the disorder. No significant difference with respect to the $L = 64$ results was noticed. This is expected since, according to RG analysis [6], the size $L = 64$ is already larger than the effective crossover length: $L_F \approx 1/\sqrt{F} = 10$ (which is estimated using the smallest simulated value of F).

To summarize, numerical simulations based on the Metropolis-type dynamics for which the local detailed balance condition is always satisfied were performed and compared with predictions of RG calculations. The broad transition becomes sharper as applied force becomes smaller. The broadening is a consequence of the presence of the spatially varying pinning potential (due to disorder) with the strong coupling constant, the applied uniform external force, and (to a smaller degree) the finite system size.

The comparison of the numerical results and RG predictions suggests that there is a qualitative and to some degree even quantitative agreement between the two, although numerical results suggest that the critical temperature is shifted toward higher values in comparison to the RG result. The

deviation from linear response occurs at temperatures larger than T_c of statics [the numerical value for T_c of statics for model (1) is $T_c = 0.643 \pm 0.006$ [8]]. This is probably due to the strong coupling regime where perturbative RG results are not expected to work. The recent self-consistent, nonperturbative Hartree type calculations for relaxational dynamics show that the critical temperature slowly increases with g if g is larger than some characteristic value below which T_c does not depend on g [15]. It is believed that this discrepancy between critical temperatures in statics and dynamics is

an effect of the existence of many metastable states, and it is also found in other physical systems [16].

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