GLASSY ROUGHNESS OF A CRYSTALLINE SURFACE
UPON A DISORDERED SUBSTRATE

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Abstract

The discrete Gaussian model for the surface of a crystal deposited on a disordered substrate is studied by Monte Carlo simulations. A continuous transition is found from a phase with a thermally-induced roughness to a glassy one in which the roughness is driven by the disorder. The behavior of the height-height correlations is consistent with the one-step replica symmetry broken solution of the variational approximation. The results differ from the renormalization group predictions and from recent simulations of a 2D vortex-glass model which belongs to the same universality class.

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The surface of a crystal formed by the deposition of particles on a flat substrate is undergoing a roughening transition: At temperatures below \( T_r \), the roughening transition temperature, the surface is flat. For \( T > T_r \), the periodic potential due to the discrete and uniform size of the particles is irrelevant and the thermal fluctuations cause the surface to roughen \([1,2]\). The intriguing question of what will be the crystalline surface properties with a disordered substrate has been addressed recently \([3]\). The renormalization group (RG) analysis predicts a low-temperature superrough phase with surprisingly uncommon equilibrium and dynamic \([3,4]\) characteristics. Near the superroughening transition the Hamiltonian of the surface is that of the 2D sine-Gordon model with random phases \([5–7]\). Another system which belongs to the same universality class (and therefore should follow a similar behavior near criticality) is the two dimensional array of flux lines with the magnetic field parallel to the superconducting plane in the presence of random pinning \([8]\). In that context the random sine-Gordon model (RSGM) has been studied by a non-perturbative variational (harmonic) approximation \([4,11]\) which allows replica-symmetry breaking with a low-temperature phase drastically different than that found by the RG approach \([12,13]\). Recent numerical simulations in the weak coupling limit of the RSGM \([14]\) have not observed any signature of a transition in the equilibrium properties. A transition was found, however, in the dynamic response in qualitative agreement with the dynamic RG \([3]\).

In view of these results we present here the study by large scale Monte Carlo (MC) simulations of the disordered-substrate surface model. The main conclusion is the existence of a low-temperature glassy rough phase separated by a continuous transition (at the critical temperature anticipated by the analytic calculations) from the thermally-rough high-temperature phase. Height-height correlations in the glassy phase are consistent with the predictions of the one-step replica symmetry broken solution obtained from the variational approach \([12,13]\). Finite-size scaling for the ratio of moments of a "modified order-parameter" provides a first rough estimate for the correlation length exponent at the transition.

The surface configurations are described in terms of height variables \( h_i \), defined on every
lattice point \( i \) of the 2D basal plane. The Hamiltonian we choose is that of the discrete Gaussian model:

\[
    H = \frac{\kappa}{2} \sum_{<i,j>} (h_i - h_j)^2,
\]

where \( \kappa \) is the surface tension. In the case of a flat surface the \( h_i \) takes integer values in the units of the lattice spacing \( a \) in the direction perpendicular to the surface. To simulate the disordered substrate we first assign a random quenched height \( d_i \), chosen uniformly (and independently for each site), in the interval \((-a/2, +a/2]\). The height \( h_i \) is then forced to take the values \( h_i = d_i + n_i a \) where \( n_i \) is any, positive or negative, integer.

The calculation of the partition function for a given realization of the disorder consists in summing \( \exp \{-\beta H\} \) over all integers \( n_i \). The relation to the RSGM is obtained by using the Poisson summation formula. Introducing continuous fields \( \phi_i \), the partition function may be expressed as:

\[
    Z = \left( \prod_i \int_{-\infty}^{+\infty} d\phi_i \right) \sum_{n_i=-\infty}^{+\infty} \exp \left\{ -\frac{\kappa \beta}{2} \sum_{<i,j>} (\phi_i - \phi_j)^2 + \sum_i 2\pi i (\phi_i - d_i) n_i/a \right\}. \tag{2}
\]

In the continuum limit \( \phi_i \) are then replaced by \( \phi(\vec{x}) \) and the discrete Laplacian by a continuous one. In addition, near the critical point only the first harmonic in the local periodic “potential” for \( \phi \) is relevant \([1]\). When higher (irrelevant) harmonics are discarded the Hamiltonian of the RSGM is obtained:

\[
    Z = \int_{-\infty}^{+\infty} d\phi(\vec{x}) \exp \left\{ -\int d\vec{x} \left[ \frac{\kappa \beta}{2} (\nabla \phi(\vec{x}))^2 - \lambda \cos (2\pi \left[ \phi(\vec{x}) - d(\vec{x}) \right]/a) \right] \right\}. \tag{3}
\]

The equilibrium scaling properties are manifested in the behavior of the height-height correlation function:

\[
    C(\vec{r}) \equiv \left[ \left( \langle h(\vec{r} + \vec{r}_0) - h(\vec{r}_0) \rangle^2 \right)_T \right]_{av}, \tag{4}
\]

where \( \langle \cdots \rangle_T \) denotes a thermal (time) average for a given realization of disorder and \( \langle \cdots \rangle_{av} \) represents the configurational average over different realizations of the disorder. Overbar denotes the averages over all origins of \( \vec{r}_0 \) and all directions.
We briefly recall the major results previously obtained for the $C(r)$: Analytically the
\textit{Renormalization group} \cite{5} and the \textit{variational} \cite{12,13} calculations both predict a transition
at the same critical temperature $T_c = \kappa/\pi$. Both approaches also agree on the properties of
the high temperature phase in which the discrete nature of the particle is irrelevant and the
behavior is that of the simple Gaussian model [without the cosine term in the Hamiltonian
of Eq. (3)]. The behavior of $C(r)$ is therefore given by:

$$C(r) = \frac{T}{\kappa \pi} \ln |r|. \quad (5)$$

As mentioned above the two approaches diverge in their predictions regarding the be-
behavior for $T < T_c$. RG calculations \cite{3,4,6,7} predict a new term with $(\ln |r|)^2$ which will
dominate at large distances. More precisely the first-order calculations yield the following
behavior:

$$C(r) = AC_0(r) + B\tau^2(\ln |r|)^2, \quad (6)$$

where $\tau \equiv 1 - T/T_c$, $C_0(r) = T/(\pi \kappa) \ln |r|$ is the correlation function (5), $A$ is a nonuniversal
constant, and $B = 2/\pi^2 + O(\tau)$ is a universal constant.

The variational approach \cite{12,13}, on the other hand, predicts the same scaling in $\ln |r|
as for $T > T_c$. The prefactor, however, becomes $T$-independent and sticks to its value at $T_c
for the whole $T < T_c$ phase:

$$C(r) = \frac{T_c}{\pi \kappa} \ln |r|. \quad (7)$$

The MC calculations were performed using the Metropolis algorithm for the discrete
Gaussian Hamiltonian Eq. (1) on a square lattice with periodic boundary conditions. The
simulations were carried on the CM computers of the Thinking Machines Corporation. At
every time step all the variables $h_i$ of one sublattice were simultaneously updated by in-
creasing or decreasing them (independently) by one unit. The moves are then accepted or
rejected according to the Metropolis rules.

Following the approach introduced by Young in spin-glass MC \cite{15,16}, for every real-
ization of disorder two replicas of the system were simulated. They had random initial
conditions (realized by adding random integer heights on top of the random substrate) and each had its own independent time evolution. In addition to the information extracted from their overlap (see below) the two-replica approach allows close monitoring of the approach to equilibrium. After equilibration was established, the measurements were taken over a time interval which was one or several equilibration times long. Depending on the lattice size and the length of the MC runs, the disorder averaging were performed using 100 to several thousands realizations of the disorder.

The Monte-Carlo simulations of the static height-height correlation function of the pure discrete Gaussian model were performed by W. Shugard et al \[17\]. They confirmed the existence of the phase transition between a high-temperature rough phase characterized by a logarithmic behavior of $C(r)$ and a flat low-temperature phase. We reproduced their results as a special case of our model without disorder. However, introducing the disorder drastically changes the character of the low-temperature phase.

Fig. 1 shows on a semilog plot the behavior of $C(r)$ around the critical temperature $T_c = \kappa/\pi = 0.6366$ for our choice of $\kappa = 2$. The simulations were performed with maximum lattice size of $L = 64$. For each temperature, measurements were repeated, with a new set of 100 realizations of the disorder, five to ten times. The average values of these measurements with corresponding error bars are shown in Fig. 1.

We compare our results with both the renormalization group predictions Eq. (6) and with the results derived by the variational analysis with one-step symmetry breaking scheme Eq. (7). In both cases the theoretical results refer to the large $|r|$ behavior of $C(r)$ while numerical results are always limited by the lattice size $L$ and by finite-size effects.

According to the RG (6), for $T$ near $T_c$ and for large $|r|$ the effect of the second term, $B\tau^2(\ln|r|)^2$, should dominate. To compare with Eq. (6) we need to be close to $T_c$ but not too close (since the coefficient is proportional to $\tau^2$ and the distance $|r|$ at which this term will dominate will be beyond the size of the system). We therefore choose $T = 0.5$ for the comparison. The broken line shows Eq. (6) for that temperature and $A = 1$. It can be seen clearly that the upper bending trend of the broken line is inconsistent with the MC data.
The down bending of the MC points for every temperature (which was also observed in the data taken for the pure system) are due to the finite-size effects. The replica variational approach predicts (see Eq. (7)) $C(r)$ to remain logarithmic for all $T$ with a $T$-independent coefficient for $T \leq T_c$. The data shown in Fig. 1 is consistent with this behavior. In our fit we used the values of the $C(r)$ for $|r|$ between 4 and 14 lattice spacings. We neglected the higher values of $C(r)$ because of the presence of the finite size effects as well as of strong sample to sample fluctuations. The full straight lines in Fig. 1 are the best fit curves. In Fig. 2 we show the temperature dependence of the slopes for nine values of $T$ between 0.45 and 0.9 including those in Fig. 1. The vertical dotted line $T = \kappa/\pi$ is the analytic result for $T_c$. While in high-$T$ phase the slope of $C(r)$ changes linearly with $T$, for the low-$T$ phase it saturates around the value $1/\pi^2$ as is predicted by Eq. (7).

To gain more insight in the transition and the properties of the low-temperature phase, a glassy order-parameter, its correlations, and/or probability distribution, should be invoked. We tried to look at the local autocorrelation function:

$$q^{\alpha\beta}_i(t) = \left\{ \left[ h^\alpha_i(t_0 + t) - \overline{h^\alpha_i(t_0 + t)} \right] \left[ h^\beta_i(t_0 + \epsilon_{\alpha\beta}t) - \overline{h^\beta_i(t_0 + \epsilon_{\alpha\beta}t)} \right] \right\}, \tag{8}$$

where $t_0$ is an initial time (larger than the time required to equilibrate the system) and overbar means average over lattice sites. The replica indices $\alpha, \beta = 1$ or 2 and $\epsilon_{\alpha\beta} = 0$ if $\alpha = \beta$ or 1 if $\alpha \neq \beta$. This local quantity is first averaged over all sites:

$$q_{\alpha\beta}(t) = \frac{1}{N} \sum_{i=1}^{N} q^{\alpha\beta}_i(t), \tag{9}$$

$N = L \times L$. This order-parameter definition includes the equal time overlap between different replicas as well as the auto-overlap of the same replica at different times. In the limit of infinite time separation in the latter the probability distribution for both should coincide. It is Gaussian for $T > T_c$ but is expected to deviate from it for $T < T_c$. One can then look for the phase transition by calculating the ratio of the moments

$$g(T, L) = \frac{1}{2} \left\{ 3 - \frac{[q^{2}_{\alpha\beta}]_\text{av}}{[q^{\alpha\beta}_i(T)]_\text{av}} \right\}, \tag{10}$$
after thermal equilibrium has been reached. If the transition is of the second order the expected finite size scaling of this quantity is $g(T, L) \sim \tilde{g}(L^{1/\nu}(T - T_c))$ where $\nu$ is the correlation length exponent, $\xi \sim |T - T_c|^{-\nu}$.

Trying to evaluate $q_{\alpha\beta}$ and $g$ we could not reach enough accuracy to extract reliable results within the computer time available. A similar problem has been observed in simulations of the 3D Ising spin glass \cite{16} and the 3D gauge glass \cite{18}. One possible approach is to look for a quantity with similar scaling but for which the statistical errors are smaller. The problem we have to overcome is that the deviations from the Gaussian distribution occur first (for $T$ just below $T_c$) at very small values of $q$ compared with its rms. To accentuate the contribution from these small values we tried to evaluate the “renormalized” quantity $\tilde{q}_{\alpha\beta}(t)$:

$$\tilde{q}_{\alpha\beta}(t) = \frac{\sum_{i=1}^{N} q_{i\alpha\beta}^\ast(t)}{\sum_{i=1}^{N} |q_{i\alpha\beta}^\ast(t)|}.$$  \hspace{1cm} (11)

The distribution $P(\tilde{q})$ (see, e.g., Ref. \cite{16} for its definition) indeed exhibits a transition from a distribution with one maximum at $\tilde{q} = 0$ to a distribution with two maxima symmetric with respect to $\tilde{q} = 0$ (which becomes a local minimum). The figures of $P(\tilde{q})$ will be exhibited in a future publication \cite{19}. Here we only depict in Fig. 3 the result of the quantity $g$ defined in Eq. (10) but with $\tilde{q}$ replacing $q$. Equilibration was confirmed by the convergence of $\tilde{q}_{\alpha\alpha}$ and $\tilde{q}_{\alpha\beta}$. Depending on the temperature and the size of the simulated system, the MC runs for equilibration were between $2^{15}$ to $2^{19}$ MC steps. For smaller system size the average over disorder is performed using over 1000 samples. However, for large system size, $L = 64$, the equilibration time for temperatures below $T_c$ is long, and we worked with a hundred samples. As in the calculation of $C(r)$, for each temperature the measurements were repeated several times. Again, the average values of these measurements with corresponding error bars are shown in Fig. 3. Clearly, Fig. 3 strongly suggests existence of the phase transition somewhere in the temperature range 0.63-0.66. A finite size scaling plot of $g$ is shown in inset of Fig. 3. The best fit is obtained with $T_c = 0.643 \pm 0.006$ and $\nu = 1.23 \pm 0.10$. The value of $T_c$ is in good agreement with the analytic predictions discussed above.
We would like to emphasize that the main purpose in presenting the data for $g$ is to provide an independent confirmation for the existence of the transition. We believe that replacing $\tilde{q}$ by $q$ will not change the critical temperature. In addition, usually the same exponent $\nu$ controls the finite-size effects for all thermodynamic quantities, so the value found here may be a first rough estimate for this critical exponent. There is no analytic prediction for $\nu$ within the variational approach [the RG approach \[4\] predicts $\xi \sim \exp(A/\tau^2)$ and is, again, in disagreement with our data]. Our plots of $P(\tilde{q})$ do not exhibit replica symmetry breaking but they are not accurate enough to rule it out. Simulations of larger systems should resolve this issue.

Finally, we comment on the only other numerical work \[14\], in which no transition was found in the equilibrium $C(r)$: These simulations were performed in the weak coupling regime $\lambda \ll 1$ of the DSGM. In contrast the ones presented here are in the strong coupling regime with all harmonics having coefficients $O(1)$. This raises the possibility that these cases belong to distinct universality classes. Whether such a scenario may be reconciled with the phase transition in the dynamics found in the same weak-coupling simulations \[14\], remains to be seen.

To summarize, numerical evidence has been presented, from both the height-height correlations and the overlap distribution, for the existence of a phase transition in the scaling properties of a surface upon a disordered substrate. The low-temperature phase has glassy characteristics. The behavior of $C(r)$ is consistent with that predicted from the one-step replica symmetry breaking solution although no direct evidence for (or against) such a breaking was found. Is this symmetry broken? Why there is such a discrepancy between the numerical results and these of the RG approach which was so successful in explaining the behavior of the pure (flat-substrate) surface? These are two among essential unanswered questions. More studies will be needed to reach a fuller understanding of the disordered-substrate surface, the flux-lines array in 2D type-II superconductors, and other physical systems related to the random-phase sine-Gordon model.

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FIGURES

FIG. 1. Semilog plot of $C(r)$ for $L = 64$. The straight lines are the best fits to $C(r) = a(T) + b(T) \ln |r|$. The broken line is the RG prediction Eq. (3) at $T = 0.5$ with $A = 1$.

FIG. 2. Plot of the coefficient $b(T)$ from the fitting equation $C(r) = a(T) + b(T) \ln |r|$. The vertical dashed line is the analytic $T_c$. The horizontal line is the slope predicted by the Eq. (4) for all $T \leq T_c$.

FIG. 3. Plot of $g(T, L)$ vs temperature $T$ for different lattice sizes. The critical temperature is indicated by the crossing of the curves. The full line is the guide to the eye. The inset shows the finite size scaling plot with the indicated values of $T_c$ and $\nu$ (see text).
Figure 1.
$T = \frac{k}{p}$

$b = \frac{1}{p}$

Figure 2.
Figure 3.

\[ T_c = 0.64 \]
\[ n = 1.23 \]