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Dynamics of the preroughening transition

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Abstract. We use the renormalization-group method to study the dynamics of the solid-on-solid model proposed by den Nijs for the preroughening transition. The implications of our results for the spatial and temporal behaviour of crystal–vapour interfaces are discussed.

The interface between crystals and vacuums or between solids and fluids has been thoroughly studied in recent years (for a recent review see [1]). In low-enough temperatures, the atoms in the solid–vacuum interface arrange themselves to form a thermodynamically stable ordered structure which has either a different order from the bulk or the same order as the bulk. When the interfacial structure has a different order, the interfacial structure is called a reconstructed structure, while when the interfacial structure has the same order, it is called an ordered flat structure. As the temperature is raised, the surface structures may lose their order, and exhibit an equilibrium order–disorder phase transition, called the reconstruction transition [2, 3]. The disordered interface above the reconstruction transition may still have finite interfacial thickness. Thus it is called the disordered flat interface. Upon further heating, another surface phase transition can occur from the disordered flat interface to the rough interface. This transition is called the roughening transition (for a recent review see [4]). Above this roughening transition temperature, the interfacial thickness diverges, and specific crystal facets no longer exist.

The characteristics of the reconstruction and roughening transitions have been much studied separately, and have been found to be distinct from those of the bulk phase transition. For example, the interface of opposite-sign domains of the Ising model undergoes the roughening transition at a lower temperature than that of the bulk phase transition, the Curie temperature, and belongs to a different universality class, the Kosterlitz–Thouless transition [5]. On the other hand, the reconstruction transition can often be found in the [110] surfaces of FCC noble-metal single crystals [2], and has been studied separately from the roughening transition. Recently, phenomenological models to understand both the reconstruction and roughening transitions simultaneously have been proposed [7, 8]. Among them, the restricted solid-on-solid (RSOS) model proposed by den Nijs generates complicated surface phase structure which contains the ordered flat, the reconstructed, the disordered flat, and the rough surface structures [3]. The complicated surface structure results from the competing effects of the ferromagnetic interactions of the nearest neighbours and antiferromagnetic interactions of further nearest neigbours [3, 9].

In the phase diagram proposed by den Nijs [3], the disordered flat phase is an intermediate phase of the reconstructed and rough surface phases or of the ordered flat and rough surface phases. In this phase, the surface contains an array of steps with positional disorder and long-range up–down–up–down order as shown in figure 1. Accordingly the average height is shifted by a half from that of the ordered flat interface. The transition

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from the ordered flat to the disordered flat phase is called *the preroughening transition*. The preroughening transition includes many interesting physical features and has been studied using the renormalization group (RG) method, and low-temperature series expansion [3,9]. The RG method is based on the continuum sine–Gordon Hamiltonian, which is an extension of the one for the roughening transition. The Hamiltonian of the sine–Gordon model for the preroughening transition can be written as

$$\mathcal{H} = \int d^2r[\tfrac{1}{2}\gamma(\nabla\phi(r))^2 - V_1\cos(2\pi\phi(r)) - V_2\cos(4\pi\phi(r))] \tag{1}$$

where $\phi(x)$ represents the height of the interface at the position r on the substrate. When $V_2 = 0$, the above Hamiltonian reduces to that for the roughening transition.

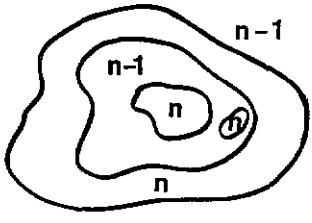

Figure 1. A surface configuration of the disordered flat structure.

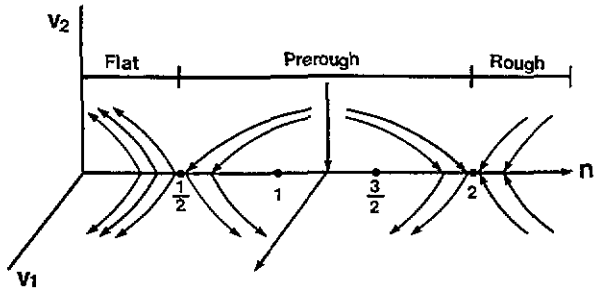

Figure 2. RG flow diagram of the roughening and preroughening transitions with $n = \pi T/\gamma$.

RG analysis of the static Hamiltonian equation (1) has been performed [3,9]. The essential features of the RG analysis may be understood by examination of the flow diagram shown in figure 2; depending on the choice of initial conditions on the critical surface, one finds that two, one or none of the fugacities flow to zero. If both do so, then one has no restraining potential for the surface, and it becomes rough. Conversely, if only one of the fugacities is finite, the phase is prerough, and if both of the fugacities are finite, the phase is flat.

However, the dynamics of the preroughening transition has not yet been studied, which is the purpose of this paper. Here we shall perform dynamic RG analysis for the preroughening transition. In general, the dynamic equation for reaching a stable equilibrium state can be derived from the static Hamiltonian via the Langevin equation [10],

$$\eta\frac{\partial\phi(r,t)}{\partial t} = -\frac{\Gamma}{kT}\frac{\delta\mathcal{H}}{\delta\phi(r,t)} + R(r,t) \tag{2}$$

with thermal noise $R(\boldsymbol{r}, t)$ and friction coefficient η. Thus the dynamic equation for the preroughening transition after redefining the coefficients is

$$\eta \frac{\partial \phi(\boldsymbol{r}, t)}{\partial t} = \gamma \nabla^2 \phi - 2\pi V_1 \sin(2\pi\phi) - 4\pi V_2 \sin(4\pi\phi) + R(\boldsymbol{r}, t) \tag{3}$$

where R is a random noise force with a white spectrum

$$\langle R_k(t) R_k(t') \rangle = G_k \delta(t - t'). \tag{4}$$

In this paper, we will use the perturbative RG method introduced by Nozières and Gallet to perform the dynamic RG analysis [11]. Originally the method was applied to the problem of the dynamics of the roughening transition [12], and detailed calculations have been presented [11]. Since the calculations for the preroughening are similar to those for the roughening transition, we will only present the essential steps of calculations for the dynamic RG transformations here. First, we split the random force R into two parts, $R = \bar{R} + \delta R$, which are statistically independent. Here we may regard δR as the effect of the short-wavelength, rapidly varying degrees of freedom left out of the coarse-grained description. Thus we shall take an average over δR. For comparison, the standard RG transformation is carried out by integrating out the field $\phi(k)$ in $\Lambda/b < k < \Lambda$, while the current method uses the random force $R(k)$ for integrating out. Accordingly the noise spectrum is readily divided into $G_k = \bar{G}_k + \delta G_k$, contributed by $\bar{R}$ and δR respectively. Moreover we obtain the averaged height $\bar{\phi} = \langle \phi(\bar{R} + \delta R) \rangle_{\delta R}$ by performing a partial average over δR, and define $\delta\phi \equiv \phi - \bar{\phi}$.

Then the dynamic equations of $\bar{\phi}$ and $\delta\phi$ are

$$\eta \frac{\partial \bar{\phi}}{\partial t} = \gamma \nabla^2 \bar{\phi} - 2\pi V_1 \langle \sin(2\pi\bar{\phi} + 2\pi\delta\phi) \rangle - 4\pi V_2 \langle \sin(4\pi\bar{\phi} + 4\pi\delta\phi) \rangle + \bar{R} \tag{5a}$$

$$\begin{aligned} \eta \frac{\partial \delta\phi}{\partial t} = {} & \gamma \nabla^2 \delta\phi - 2\pi V_1 [\sin(2\pi\bar{\phi} + 2\pi\delta\phi) - \langle \sin(2\pi\bar{\phi} + 2\pi\delta\phi) \rangle] \\ & - 4\pi V_2 [\sin(4\pi\bar{\phi} + 4\pi\delta\phi) - \langle \sin(4\pi\bar{\phi} + 4\pi\delta\phi) \rangle] + \delta R. \end{aligned} \tag{5b}$$

We first solve for $\delta\phi$ by iterating and expanding in powers of V_1 and V_2. In the zeroth order,

$$\delta\phi^{(0)}(r, t) = \int \mathrm{d}^2 r' \, \mathrm{d}t' \, \chi_0(r - r', t - t') \delta R(r', t') \tag{6}$$

where χ_0 is the solution of the equation for the case of $V_1 = 0$, $V_2 = 0$, and $R = 0$ in equation (3), that is $\eta \partial\phi/\partial t = \gamma \nabla^2 \phi$. Explicitly, the solution is

$$\chi_0(r, t) = \frac{1}{4\pi\gamma t} \exp(-\eta r^2 / 4\gamma t). \tag{7}$$

In the first order,

$$\begin{aligned} \delta\phi^{(1)} = - \int \mathrm{d}^2 r' \, \mathrm{d}t' \, \chi_0(r - r', t - t') [& 2\pi V_1 \{\sin(2\pi\bar{\phi} + 2\pi\delta\phi) - \langle \sin(2\pi\bar{\phi} + 2\pi\delta\phi) \rangle\} \\ & + 4\pi V_2 \{\sin(4\pi\bar{\phi} + 4\pi\delta\phi) - \langle \sin(4\pi\bar{\phi} + 4\pi\delta\phi) \rangle\}]. \end{aligned} \tag{8}$$

Next combining the results, equations (6) and (8), and inserting $\delta\phi = \delta\phi^{(0)} + \delta\phi^{(1)}$ into equation (5*a*), we obtain the following equation, up to the order $\mathcal{O}(V_1^2, V_1V_2, V_2^2)$,

$$\eta\frac{\partial\bar{\phi}}{\partial t} = \gamma\nabla^2\bar{\phi} - 2\pi\bar{V}_1\sin(2\pi\bar{\phi}) - 4\pi\bar{V}_2\sin(4\pi\bar{\phi}) + \bar{R}$$
$$+ 8\pi^3\bar{V}_1^2\int d^2r'\,dt'\,\chi_0(r-r', t-t')[\sin(2\pi\bar{\phi}(r)+2\pi\bar{\phi}(r'))(e^{-2n\delta g(\rho,\tau)}-1)$$
$$- \sin(2\pi\bar{\phi}(r)-2\pi\bar{\phi}(r'))(e^{2n\delta g(\rho,\tau)}-1)]$$
$$+ 16\pi^3\bar{V}_1\bar{V}_2\int d^2r'\,dt'\,\chi_0(r-r', t-t')[\sin(2\pi\bar{\phi}(r)+4\pi\bar{\phi}(r'))(e^{-4n\delta g(\rho,\tau)}-1)$$
$$- \sin(2\pi\bar{\phi}(r)-4\pi\bar{\phi}(r'))(e^{4n\delta g(\rho,\tau)}-1)]$$
$$+ 32\pi^3\bar{V}_1\bar{V}_2\int d^2r'\,dt'\,\chi_0(r-r', t-t')[\sin(4\pi\bar{\phi}(r)+2\pi\bar{\phi}(r'))(e^{-4n\delta g(\rho,\tau)}-1)$$
$$- \sin(4\pi\bar{\phi}(r)-2\pi\bar{\phi}(r'))(e^{4n\delta g(\rho,\tau)}-1)]$$
$$+ 64\pi^3\bar{V}_2^2\int d^2r'\,dt'\,\chi_0(r-r', t-t')[\sin(4\pi\bar{\phi}(r)+4\pi\bar{\phi}(r'))(e^{-8n\delta g(\rho,\tau)}-1)$$
$$- \sin(4\pi\bar{\phi}(r)-4\pi\bar{\phi}(r'))(e^{8n\delta g(\rho,\tau)}-1)] \tag{9}$$

where $\bar{V}_1 = V_1e^{-n\delta g(0,0)}$, $\bar{V}_2 = V_2e^{-4n\delta g(0,0)}$, with $n = \pi T/\gamma$, and

$$\delta g(\rho,\tau) \equiv (2\pi\gamma/T)\langle\delta\phi^{(0)}(r,t)\delta\phi^{(0)}(r',t')\rangle \tag{10}$$

with $\rho = r - r'$ and $\tau = t - t'$. In order to obtain the renormalized corrections of γ and η, we make the following replacement,

$$\begin{aligned}\sin\{2\pi\phi(r) - 2\pi\phi(r')\} &\to 2\pi(\phi-\phi')\langle\cos 2\pi(\phi-\phi')\rangle \\ &\equiv 2\pi(\phi-\phi')e^{-2nh(\rho,\tau)}\end{aligned} \tag{11}$$

where

$$h(\rho,\tau) = \int_0^1 dk\,\frac{1}{k}[1 - J_0(k\rho)e^{-\gamma k^2\tau/\eta}] \tag{12}$$

under the assumption of the sharp cut-off, $\theta(1-x)$. The function, $h(\rho,\tau)$, can also be obtained by using Kadanoff's operator algebra formalism [13]. The Taylor expansion of $\phi - \phi'$ generates $\nabla^2\phi$ and $\partial\phi/\partial t$ terms, which contribute to the renormalizations of γ and η respectively. In equation (9), we discarded the irrelevant harmonic terms contributing to higher harmonics. After rescaling, $\tilde{\rho} = \rho(1-\epsilon)$ and $\tilde{k} = k/(1-\epsilon)$, we obtain the following RG recursion relations,

$$dV_1/d\epsilon = (2-n)V_1 \tag{13}$$

$$dV_2/d\epsilon = (2-4n)V_2 \tag{14}$$

$$d\gamma/d\epsilon = (2\pi^4V_1^2/\gamma)A(n) + (32\pi^4V_2^2/\gamma)A(4n) \tag{15}$$

$$d\eta/d\epsilon = (8\pi^4V_1^2\eta/\gamma^2)B(n) + (128\pi^4V_2^2\eta/\gamma^2)B(4n). \tag{16}$$

In the above equations, $A(n)$ and $B(n)$ are defined as

$$A(n) \equiv n \int \tilde{\rho}^3 \, \mathrm{d}\tilde{\rho} \int_0^\infty \mathrm{d}x \, \frac{1}{x} \exp\left(-\frac{1}{4x} - 2nH\right) \frac{\mathrm{d}\delta\, g(\tilde{\rho}, x)}{\mathrm{d}\epsilon} \tag{17}$$

and

$$B(n) \equiv n \int \tilde{\rho}^3 \mathrm{d}\tilde{\rho} \int_0^\infty \mathrm{d}x \, \exp\left(-\frac{1}{4x} - 2nH\right) \frac{\mathrm{d}\delta\, g(\tilde{\rho}, x)}{\mathrm{d}\epsilon} \tag{18}$$

where we have set $x = \gamma\tau/\eta\rho^2$, and

$$\frac{\mathrm{d}\delta\, g(\tilde{\rho}, x)}{\mathrm{d}\epsilon} = J_0(\tilde{\rho})\mathrm{e}^{-\tilde{\rho}^2 x} \tag{19}$$

$$H(\tilde{\rho}, x) = \int_0^1 \mathrm{d}k \, \frac{1}{k}[1 - J_0(k\tilde{\rho})\mathrm{e}^{-k^2\tilde{\rho}^2 x}]. \tag{20}$$

The numerical behaviour of the functions $A(n)$ and $B(n)$ was described [11], and the values at the fixed point are $A(2) = 0.398$ and $B(2) = 0.234$.

The recursion relations for the preroughening transition are very similar to those for the roughening transition, but including a higher harmonic term. That is, when $V_2 = 0$, the above recursion relations reduce to those for the roughening transition exactly. The flow diagram for the parameters V_1 and V_2 is depicted in figure 2. Depending on the choice of initial conditions on the critical surface, two, one or none of the fugacities flow to zero. If both do so, then there is no restraining potential for the surface, so that the the surface is unpinned, which means the surface is rough. While if $V_1 = 0$ and $V_2 \neq 0$, then a pinning–unpinning transition partially occurs. Thus the surface is prerough. If both parameters are non-zero, then the surface is flat. Therefore the roughening transition occurs at $n = 2$ and the preroughening transition occurs at $n = \frac{1}{2}$.

In the disordered flat phase, where $\frac{1}{2} < n < 2$, V_2 decreases under RG transformations, so that the fugacity V_2 is irrelevant. Thus within the RG scheme, the study of the dynamics in the disordered flat phase is very similar to the one obtained for the roughening transition below the roughening temperature. On the other hand, the fugacity V_1 blows up under infinite RG transformations, so that the expansion in powers of V_1 in the RG analysis might be meaningless. But in this case, the *stop*-RG transformation must be applied. The RG transformation must stop at finite iterations when the length scale is comparable to the correlation length ξ which is known to be finite below the roughening temperature. For this case, V_1 and V_2 remain finite, and they are still small. We checked numerically that, even in the presence of V_2, γ/η will behave similarly under RG transformations to the case of $V_2 = 0$. Since the fugacities remain small enough, we may adapt the well known result for the height–height correlation above the roughening transition that $w^2 \equiv \langle(\phi(r, t) - \phi(0, t))^2\rangle$ scales as $\ln r$. In fact, w^2 is equivalent to the function $H(r, t)$ in equation (20). At an early stage, the growth of the interface is driven by nucleation of small seeds. The length r corresponds to the typical size of seeds, which increases as $\sim \sqrt{t}$. Hence the height–height fluctuation w^2 scales as $\sim \ln t$. This behaviour stops at the characteristic time $t^* \sim \xi^2$. A similar result was obtained by stochastic numerical simulations by Devillard [14], where the correlation length ξ is replaced by the system size L, because $\xi > L$.

Beyond the characteristic time t^*, the separation between isolated seeds becomes closer, and coalescence may occur. In this regime, it was shown by numerical simulation [14] that

the fluctuation w^2 decreases, and it saturates to a size-independent constant value. However, beyond the characteristic time t^*, RG analysis breaks down, because V_1 becomes so large that expansion in powers of V_1 does not make sense. However, in the long-time limit, it is obvious that the fluctuation w^2 converges to a constant value, because the interface is flat below the roughening temperature. Since the value of the fluctuation at t^* increases with system size, and the saturated value is independent of system size, we may expect that the fluctuation will decrease after a characteristic time, and it will then be saturated. Next when an external force is applied, we might say by using the result for the roughening transition [11] that $\Delta\mu < \gamma/L^2$, the surface grows as if the force were zero, and for $\Delta\mu > \gamma/L^2$, the renormalization of γ and η stops, and the interface is rough.

In conclusion, we have studied the dynaimcs of the disordered-flat structure by applying the dynamic renormalization group to the Langevin-type equation derived from the sine–Gordon Hamiltonian. We found that the roughening transition occurs at $n \equiv \pi T/\gamma = 2$, and the preroughening transition at $n = \frac{1}{2}$. The preroughening transition is driven by the second harmonic term of the lattice pinning potentials. The renormalized parameters of surface tension and friction due to the second harmonics are described by the same functions $A(n)$ and $B(n)$ as those used in the roughening transition. The second fugacity converges to zero under infinite RG transformations. Since the first fugacity blows up under RG transformations, we must apply the stop-RG transformation. In this case, the first and the second fugacities remain finite. Even in the presence of the second fugacity, the nature of the RG transformation does not change from the case of the absence of V_2. Thus we have found that the height–height correlation function grows as $\ln t$ for $t < L^2$, and it saturates to its equilibrium value in the long-time limit. For the applied force, $\Delta\mu < \gamma/L^2$ the surface grows as if the force were zero.

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