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DYNAMIC SCALING OF GROWING SURFACES WITH GROWTH INHOMOGENEITIES OF SCREENED COULOMBIC FUNCTION*

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The dynamic scaling properties of growing surfaces with growth inhomogeneities are studied by applying a dynamic renormalization-group analysis to the generalized Kardar-Parisi-Zhang(hereafter abbreviated to KPZ) equation, which contains an additional term of growth inhomogeneities. In a practical crystal growth process, these growth inhomogeneities can be induced by surface impurities and defects and are modeled by a screened Coulomb function in this paper. Our results show that the existence of the growth inhomogeneities can significantly change the dynamic scaling properties of a growing surface and can lead to a rougher surface.

Keywords: surface growth, dynamic renormalization-group theory, growth inhomogeneity
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I. INTRODUCTION

The dynamics of surface growth under nonequilibrium conditions has undergone an enormous activity during the last decade. Considerable theoretical and experimental efforts have been devoted to this field.[1−14]

Surface growth is generally governed by stochastic process involving nonequilibrium many-body effects. These complexities preclude the application of standard analytical approaches to this problem. As a result, the development of the scaling theory for describing the dynamics of growing surfaces was prompted. In the dynamic scaling theory, a central quantity of interest is the global width $W(L,t)$, which obeys the dynamic scaling law[15]

$$W(L,t) = L^{\chi} f(t/L^{z}). \tag{1}$$

The scaling function f has asymptotic properties: $W(L,t) \sim t^{\chi/z}$ for $t << L^{z}$ and $W(L,t) \sim L^{\chi}$ for $t >> L^{z}$, where χ and z are the roughness and dynamic exponents of a growth process and are usually taken to identify the universality class which the growth process considered belongs to. $W(L,t)$ is defined by

$$W(L,t) = \frac{1}{\sqrt{L}} <_r \sum_{\boldsymbol{r}} [h(\boldsymbol{r},t) - \overline{h}_L(t)]^2 >^{1/2}, \tag{2}$$

where the height variable $h(\boldsymbol{r},t)$ gives the location of the surface at the position $\boldsymbol{r}(\boldsymbol{r} \in R^d)$ and time t, $\overline{h}_L = \frac{1}{L}\sum_{\boldsymbol{r}} h(\boldsymbol{r},t)$ is the mean value of $h(\boldsymbol{r},t)$, and the angular brackets stand for a noise average. The scaling of $W(L,t)$ provides a clear physical interpretation of the surface roughness and can be readily measured in both theoretical and experimental studies of surfaces. In many seemingly unrelated growth processes, the large-scale properties of the surface width are observed to be scale invariant and universal.

Kardar, Parisi and Zhang[3] proposed that the following nonlinear Langevin equation:

$$\frac{\partial h(\boldsymbol{r},t)}{\partial t} = v\nabla^2 h + \frac{\lambda}{2}(\nabla h)^2 + \eta \tag{3}$$

governs the macroscopic dynamics of a stochastically growing surface. The first term on the right hand side of Eq.(3) represents the surface tension, which prefers a smooth surface. The second term is a nonlinear term that describes lateral growth. The last term is a Langevin noise to mimic the stochastic nature of any growth process. In Eq.(3), the average growth velocity has been subtracted so that the noise has zero mean, i.e., $<\eta(\boldsymbol{r},t)>=0$. In the simplest case, the stochasticality is then described by an unrelated Gaussian noise with the second moment

$$<\eta(\boldsymbol{r},t)\eta(\boldsymbol{r}',t')>=2D\delta^d(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t'), \tag{4}$$

where D characterizes the noise amplitude.

It is widely believed that the KPZ equation provides a valid hydrodynamic description of a broad

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class of surface models involving the local growth.[3−5] Examples include Eden model[16] and restricted solid-on-solid (RSOS) model.[17] In addition, this equation is also closely related to a large variety of other nonlinear problems.[2] The applicability of the KPZ equation seems to encompass length scales from an atomic level to macroscopic phenomena of everyday life.

The standard analytical tool now used in the analysis of the scaling properties of nonlinear Langevin equations of the type in Eq.(3) is the dynamic renormalization-group analysis (DRG), which was developed by Forster *et al.*[18] in the study of the stochastic version of the Burgers equation, and was used to the analysis of the KPZ equation by Kardar *et al.*[3,4] Thereafter, much important and interesting results have been achieved in this field.[5−8]

In a practical crystal growth process, since surface impurities and defects have an external, position-dependent contribution to the local growth, so the growth process exhibits an inhomogeneous growth in the substrate plane. The effect of the inhomogeneities can be described by a dynamic equation with a term of growth inhomogeneity $U(\boldsymbol{r})$.[19] In the simple case of single defect, $U(\boldsymbol{r})$ is localized in a small spatial region and can be modelled, in the continuum limit, by a delta-function: $U(\boldsymbol{r}) = U_0\delta(\boldsymbol{r})$. We have studied its scaling properties by DRG method.[20] As a theoretical generalization, in this paper we model the growth inhomogeneity by a screened Coulombic function and apply a DRG approach to the generalized KPZ equation with this inhomogeneity term. Obviously, it is more realistic than the delta-function model. It is noted that the "single defect" here can actually represent the situation where the surface has a low impurity and defect density. Our results of DRG analysis show that the surface impurities and defects, by inducing inhomogeneous growth on surfaces, can significantly change the scaling properties of the growing surfaces and can lead to rougher surfaces.

II. THEORETICAL MODEL AND DYNAMIC RENORMALIZATION ANALYSIS

The growth inhomogeneity in our dynamic equation is expressed in the form

$$U(r) = \frac{A}{r}\mathrm{e}^{-q_m r}, \tag{5}$$

where A characterizes the strength of inhomogeneity and $1/q_m$ characterizes its Debye screening length. The generalization of the KPZ equation has the following form:

$$\frac{\partial h(\boldsymbol{r},t)}{\partial t} = v\nabla^2 h + \frac{\lambda}{2}(\nabla h)^2 + \eta + U(\boldsymbol{r}). \tag{6}$$

Following the procedure and scheme adopted in Refs.[3,4,18], we next apply a DRG approach to Eq. (6).

At first, we make a dimensional analysis: A change of scale $r \to br$ is accompanied by $t \to b^z t$, $h \to b^\chi h$. After this rescaling, Eq.(6) transforms to

$$\begin{aligned} b^{\chi-z}\frac{\partial h}{\partial t} =& vb^{\chi-2}\nabla^2 h + \frac{\lambda}{2}b^{2\chi-2}(\nabla h)^2 \\ &+ b^{-(d+z)/2}\eta + b^{-1}U(\boldsymbol{r}), \end{aligned} \tag{7}$$

where Eq. (4) is used to determine the scaling of noise $\eta(\boldsymbol{r},t)$. Under this transform the parameters change to

$$\begin{aligned} &v \to b^{z-2}v, D \to b^{-d-2\chi+z}D, \\ &\lambda \to b^{\chi+z-2}\lambda, A \to b^{z-\chi-1}A. \end{aligned} \tag{8}$$

After a Fourier transformation, we have

$$h(\boldsymbol{r},t) = \int_{-\infty}^{+\infty}\int_{k<\Lambda} \mathrm{d}\omega\mathrm{d}^d k \frac{1}{(2\pi)^{d+1}} h(\boldsymbol{k},\omega)\mathrm{e}^{\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)}. \tag{9}$$

Equation (6) becomes

$$\begin{aligned} -\mathrm{i}\omega h(\boldsymbol{k},\omega) =& -vk^2 h(\boldsymbol{k},\omega) - \frac{\lambda}{2}\int\int \mathrm{d}\Omega\mathrm{d}^d q \\ &\cdot \frac{1}{(2\pi)^{d+1}}\boldsymbol{q}\cdot(\boldsymbol{k}-\boldsymbol{q})h(\boldsymbol{q},\Omega)h(\boldsymbol{k}-\boldsymbol{q},\omega-\Omega) \\ &+ \eta(\boldsymbol{k},\omega) + U(\boldsymbol{k}). \end{aligned} \tag{10}$$

Note that the momentum integrals are performed in the transverse d-dimensional space subject to an upper cutoff Λ. $U(\boldsymbol{k})$ is the Fourier transform of $U(\boldsymbol{r})$ in d-dimensional space.

$$U(\boldsymbol{k}) = \frac{A_d}{(q_m^2 + k^2)^{(d-1)/2}}, \tag{11}$$

where A_d is an integral constant related to both the strength A and the dimensionality d. The noise $\eta(\boldsymbol{k},\omega)$ satisfies

$$< \eta(\boldsymbol{k},\omega) >= 0 \tag{12a}$$

and

$$< \eta(\boldsymbol{k},\omega)\eta(\boldsymbol{k}',\omega') >= 2D\delta^d(\boldsymbol{k}+\boldsymbol{k}')\delta(\omega+\omega'). \tag{12b}$$

From Eq. (10), we have

$$\begin{aligned} h(\boldsymbol{k},\omega) =& G_0(\boldsymbol{k},\omega)[U(k) + \eta(\boldsymbol{k},\omega)] \\ &- \frac{\lambda}{2}G_0(\boldsymbol{k},\omega)\int\int \mathrm{d}\Omega\mathrm{d}^d q \frac{1}{(2\pi)^{d+1}}\boldsymbol{q}\cdot(\boldsymbol{k}-\boldsymbol{q}) \\ &\cdot h(\boldsymbol{q},\Omega)h(\boldsymbol{k}-\boldsymbol{q},\omega-\Omega), \end{aligned} \tag{13}$$

with a bare propagator $G_0(\boldsymbol{k},\omega)=\dfrac{1}{vk^2-\mathrm{i}\omega}$.

Equation (13) is a convenient starting point for a perturbative calculation of $h(\boldsymbol{k},\omega)$ in powers of the nonlinear coupling constant λ. If defining an effective response function $G(\boldsymbol{k},\omega)$ by $h(\boldsymbol{k},\omega)=G(\boldsymbol{k},\omega)[2\pi U(k)\delta(\omega)+\eta(\boldsymbol{k},\omega)]$, we can represent Eq.(13) diagrammatically by Fig.1 with and indicating the bare propagator $G_0(\boldsymbol{k},\omega)$ and the effective response function $G(\boldsymbol{k},\omega)$, $\times$ and Δ depicting the noise $\eta(\boldsymbol{k},\omega)$ and the growth rate inhomogeneity $2\pi U(k)\delta(\omega)$, respectively.

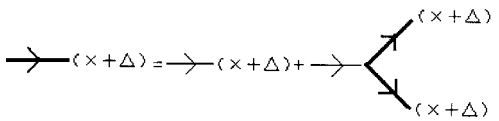


Fig.1. Diagrammatic representation of Eq. (13).

Due to the stochastic property of surface growth, we only need to consider, in the perturbation series of Fig.1, the contributions of the diagrams with the noise($\times$). These diagrams, we find, can be represented equivalently by a new effective response function $G'(\boldsymbol{k},\omega)$ and an effective bare propagator $G_0'(\boldsymbol{k},\omega)$ with and , respectively, as indicated in Fig.2. As a matter of fact, Fig.2 includes all the scaling information we concerned in Fig.1 .

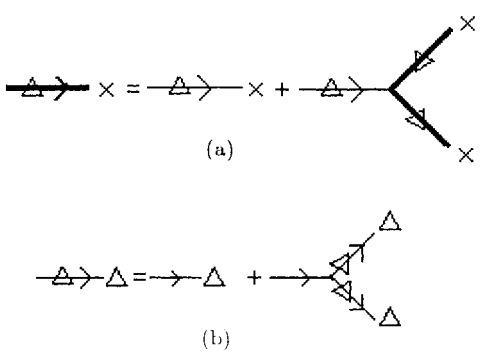


Fig.2. The diagrammatic representation of $G'(\vec{k},\omega)$ (a) and $G_0'(\vec{k},\omega)$ (b).

It can be seen that the effective bare propagator $G_0'(\boldsymbol{k},\omega)$ includes only the response of $G_0(\boldsymbol{k},\omega)$ to the inhomogeneity $U(\boldsymbol{k})(\Delta)$. If we only reserve the leading-order response in the graphic expansion of $G_0'(\boldsymbol{k},\omega)$, as shown in Fig.3, we have

$$\begin{aligned}G_0'(\boldsymbol{k},\omega)=&G_0(\boldsymbol{k},\omega)+2(-\frac{\lambda}{2})G_0(\boldsymbol{k},\omega)\\&\cdot\int\int \mathrm{d}\Omega\mathrm{d}^dq\,\frac{\boldsymbol{q}\cdot(\boldsymbol{k}-\boldsymbol{q})}{(2\pi)^{d+1}}G_0(\boldsymbol{q},\Omega)\\&\cdot G_0(\boldsymbol{k}-\boldsymbol{q},\omega-\Omega)(2\pi)U(q)\delta(\Omega).\end{aligned}\tag{14}$$

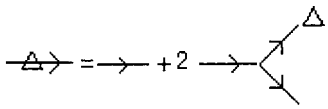


Fig.3. An approximate representation of $G_0'(\vec{k},\omega)$.

We are only interested in the properties of $G_0'(\boldsymbol{k},\omega)$ in the static and long-wavelength-limit $(\boldsymbol{k},\omega)\to 0$, which completely determine the behaviors of the system in the hydrodynamic regime of interest. The $\omega\to 0$ limit can be taken away. So we only need to calculate $G_0'(\boldsymbol{k},0)$ and to reserve the zero-order term of k in the integral calculation of $G_0'(\boldsymbol{k},0)$. In this situation, $G_0'(\boldsymbol{k},0)$ can be given approximately by

$$\begin{aligned}G_0'(\boldsymbol{k},0)=&G_0(\boldsymbol{k},0)\Big[1+2\Big(-\frac{\lambda}{2}\Big)\frac{A_d}{v^2(2\pi)^d}\int \mathrm{d}^dq\\&\cdot\frac{\boldsymbol{q}\cdot(\boldsymbol{k}-\boldsymbol{q})}{q^2(\boldsymbol{k}-\boldsymbol{q})^2}\frac{1}{(q_m^2+q^2)^{(d-1)/2}}\Big].\end{aligned}\tag{15}$$

Performing the integral in Eq. (15) in spherical coordinates and taking the corresponding approximation, we obtain

$$G_0'(\boldsymbol{k},0)=G_0(\boldsymbol{k},0)\left[1+C_d\frac{\lambda A}{v^2q_m}\right],\tag{16}$$

where C_d is an integral constant only relevant to substrate dimension d. Assuming $G_0'(\boldsymbol{k},0)$ in the form of $G_0'(\boldsymbol{k},0)=\dfrac{1}{v'k^2}$, we have

$$\frac{1}{v'}=\frac{1}{v}+C_d\frac{\lambda A}{v^3q_m},\tag{17}$$

where v' is known as the effective surface tension.

It can be seen from our discussion and calculation above that the effect of the growth rate inhomogeneities on growing surfaces can be attributed to the fact that it results in a new effective surface tension v', which generally has a very complex scaling be havior. In fact, the existence of surface impurities and defects can change the surface tension. Physically, this result is understandable. Considering a limiting situation where the value $|A|$ is large enough so that the first term of Eq. (17) can be neglected, we may have

$$v'=\frac{q_mv^3}{C_d\lambda A}.\tag{18}$$

In order to guarantee $v'>0$, A and λ must take the same positive or negative sign. In fact, only in this situation, the defects and impurities can affect the large-scale surface morphology.[19]

Substituting the scale transformation in Eq.(8) and $q_m \to b^{-1}q_m$ into Eq.(18), the scaling behavior of v' in the limiting case can be given by

$$v' \to b^{z-4}v'. \tag{19}$$

In the following, we will focus our attention to this simple case.

In terms of the new effective surface tension v', the dynamic equation corresponding to Fig.2 (a) can be expressed as

$$\frac{\partial h(\boldsymbol{r},t)}{\partial t} = v'\nabla^2 h + \frac{\lambda}{2}(\nabla h^2) + \eta. \tag{20}$$

Equations (20) and (3) have the same form. By applying a standard DRG approach to Eq. (20) as in Refs.[3,4] and [18], and considering the scaling behavior of v' expressed in Eq.(19), we can arrive at the following set of differential recursion relations for the parameters v', D and λ:

$$\begin{aligned}
\frac{\mathrm{d}v'}{\mathrm{d}l} &= \Big(z - 4 - K_d\frac{\lambda^2 D}{v'^3}\frac{(d-2)}{4d}\Big)v', \\
\frac{\mathrm{d}D}{\mathrm{d}l} &= \Big(z - 2\chi - d + K_d\frac{\lambda^2 D}{v'^3}\frac{1}{4}\Big)D, \\
\frac{\mathrm{d}\lambda}{\mathrm{d}l} &= (\chi + z - 2)\lambda,
\end{aligned} \tag{21}$$

where $K_d = \dfrac{S_d}{(2\pi)^d} = \dfrac{S_{d-1}}{(2\pi)^d}\int_0^\pi \mathrm{d}\theta \sin^{d-2}\theta$, S_d is the surface area of a unit sphere in d-dimensional space. From Eq. (21), we can solve for the DRG fixed points of Eq.(20). As a result, we find that the fixed-point values of χ and z below the critical dimension are

$$\begin{aligned}
\chi &= -\frac{4 + d(d-2)}{2(2d-3)}, \\
z &= \frac{8(d-1) + d(d-2)}{2(2d-3)}.
\end{aligned} \tag{22}$$

It can be seen that χ and z here still satisfy the exponent identity $\chi + z = 2$. In fact, this identity is a consequence of the Galilean invariance of Eq.(20).[16] The χ and z of the standard KPZ equation given in Refs.[3] and [4] are expressed as

$$\begin{aligned}
\chi &= \frac{(2-d)(d-2)}{2(2d-3)}, \\
z &= 2 + \frac{(d-2)^2}{2(2d-3)}.
\end{aligned} \tag{23}$$

The roughness χ as a function of the surface dimension d given by Eqs.(22) and (23) are shown in Fig.4. The divergence at $d = 3/2$ turns out to be an artifact of the one-loop approximation.[10]

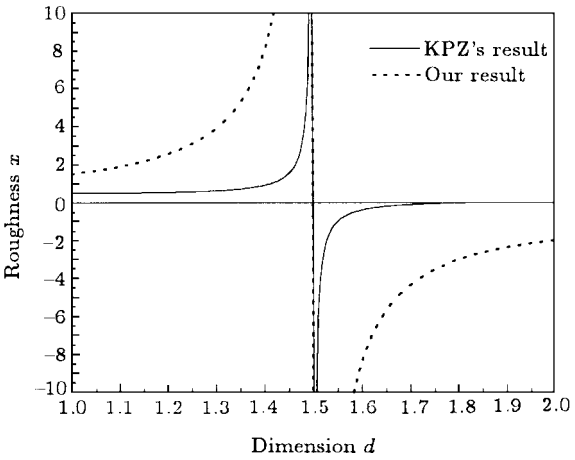


Fig.4. Roughness exponent χ as a function of the surface dimension d. The solid and the dashed lines show the results given by Eqs. (22) and (23), respectively.

At d=1, Eqs. (22) and (23) give the values of χ=1.5, z=0.5, and χ=0.5, z=1.5, respectively. These results imply that the existence of the growth inhomogeneities induced by defects can significantly change the scaling behaviors of the growing surface s in crystal growth and tend to lead to rougher surfaces and shorter dynamic relaxation processes to steady-growth state.

Ⅲ. DISCUSSION AND CONCLUSIONS

In this paper, we have studied the dynamic scaling properties of growing surfaces with growth inhomogeneities induced by defects and impurities. The growth inhomogeneity is modelled by a screened Coulombic function, and the generalized KPZ equation is analysed by the DRG method. Our results show that this kind of inhomogeneity can significantly change the scaling behaviors. They can lead to a larger roughness exponent and a smaller dynamic exponent than those of the standard KPZ equation, implying that the existence of surface impurities and defects, by inducing a spatially inhomogeneous growth, tend to roughening the growing surfaces and shorten its dynamic relaxation process to the steady-state. Similar results are also gained in the delta-function model of growth inhomogeneities.[20] Physically, these results can be understood. Defects and impurities are always existing in a practical growing surface, so our discussion is certainly helpful to understand the behaviors of practical growth processes.

The key step in our calculation is to introduce an effective bare propagator $G_0'(\boldsymbol{k},\omega)$, through which we can attribute the effect of the growth inhomogeneities

to a new effective surface tension v', which generally has a complex scaling behavior and implies that a practical growing surface with impurities and defects will exhibit complicated scaling behaviors. In our work here, only the limiting case of strong potential is addressed. In the case of a weak defect potential ($|A| \to 0$), the behavior of the KPZ can be obtained.

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