Dynamic Scaling in Epitaxial Growth

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I. OUTLINE

In this article I provide a brief theoretical perspective on our current understanding of the dynamic scaling phenomena in nonequilibrium epitaxial growth with the emphasis on the extensively studied ultrahigh vacuum thin film deposition growth, such as MBE growth, where the main growth front smoothening mechanism competing against the surface kinetic roughening induced by inherent shot noise fluctuations in the random deposition process is the adatom mobility associated with surface diffusion at the growth front. The Introduction sets the tone, and in subsequent sections I expand upon the key themes arising in the Introduction. In particular, the issues of universality, continuum growth equations, atomistic growth models, and unstable growth as in smooth growth and mound formation are discussed in the four sections following the Introduction.

II. INTRODUCTION

Epitaxy is usually thought of as an extremely smooth growth process leading to atomically sharp surfaces/interfaces with little (∼ one atomic monolayer) interface roughness. In particular, layer by layer epitaxial growth on a singular surface takes place via two dimensional island formation where the surface roughness oscillates between zero and one monolayer as each new atomic layer is formed by the deposited atoms from the incident flux with no more than a few (∼ 1) incomplete atomic monolayers being active at the growth front. The reason for this extremely smooth epitaxial growth morphology is the high adatom mobility at the growth front enabling the incident atoms to be “quickly” (i.e. before the arrival of the next incident atom in its neighborhood) incorporated at epitaxial growth sites.
on the surface resulting in the atomically flat growth morphology. The somewhat loosely defined “epitaxial growth temperature” ($T_e$) is, in fact, thought to be the temperature which is high enough for fast adatom diffusion to cause layer by layer (step flow) growth on a singular (vicinal) surface, but low enough for atomic desorption from the growth front to be unimportant. This scenario for epitaxial growth is well established in the literature through in situ RHEED analysis (and other similar experimental techniques) of the growth front and through extensive computer kinetic growth simulations.

It turns out that this well-accepted paradigm for morphologically smooth epitaxial growth is conceptually flawed from a statistical mechanical perspective — the smooth epitaxial growth mode is actually unstable. The layer by layer growth mode on a singular surface (or the step flow growth mode on a vicinal surface) is, in fact, always an initial transient which asymptotically must lead to kinetically rough growth at long times and large distances. The random fluctuations (i.e. the shot noise) inherent in the incident beam dominate the adatom surface diffusion at long times (i.e. after the initial layer by layer growth transient), and the interface roughness (as measured, for example, by the root mean square fluctuation in the interface width, or equivalently, by the number of incomplete layers dynamically active at the growth front) always increases monotonically (until it reaches saturation at a steady state determined by the substrate size) as a function of time after the initial transient (during the initial transient the interface roughness oscillates between zero and one monolayer indicating smooth epitaxial growth with an essentially flat atomically sharp growth morphology). It is indeed true that for fast enough adatom diffusion the (unstable) layer by layer growth transient may last for many deposited layers, and for many practical purposes this may suffice. Also, for fast diffusion (i.e. high temperatures) and small enough substrate sizes, the steady state saturated roughness may be small producing a smooth surface.

In addition to unstable layer by layer and asymptotically “stable” kinetically rough growth modes, there has been much recent interest in a third surface growth scenario where mounds or pyramids dominate the growth morphology, and these mounds/pyramids may
coarsen or steepen with time. Such a surface growth process via mound formation is thought to arise from the so-called Ehrlich-Schwoebel (ES) barrier existing at surface step edges which hinders the downward adatom motion by introducing an additional step-edge diffusion bias. The additional step-edge diffusion bias makes it less likely for an adatom to attach to a down-step than to an up-step, and therefore gives rise to characteristic “wedding-cake” structures on the growing surface as adatoms on upper terraces are prevented by the Ehrlich-Schwobel barrier from coming down. The net result is a rough morphology (albeit of a particular type involving mounds/pyramids or similar “wedding-cake” structures) with the roughness increasing monotonically in time as growth progresses.

The kinetic surface roughening phenomenon is experimentally well established. Layer by layer epitaxial growth on a flat singular surface manifests itself in RHEED intensity oscillations from the growing surface — each oscillation corresponds to the completion of a single layer. The RHEED intensity oscillation phenomenon associated with the layer by layer growth process is so well-established that it is routinely used as a characterization tool in MBE growth monitoring the number of grown layers. Experimentally it is known that at low temperatures growth is kinetically rough or three-dimensional (because the mobility of the incident atoms is low) as indicated by there being no RHEED intensity oscillations (the intensity drops monotonically with time indicating progressively rougher growth) whereas at high temperatures (when the adatoms are “sufficiently” mobile) growth occurs via the two dimensional layer by layer mechanism as indicated by the existence of pronounced RHEED intensity oscillations. The important conceptual point is, however, the generic observation that these pronounced RHEED intensity oscillations always decay and eventually disappear, indicating that the high-temperature smooth two-dimensional layer by layer growth is an unstable transient, which eventually turns into kinetically rough three dimensional growth. How long the transient layer by layer growth mode persists depends on the adatom mobility (which in turn depends exponentially on the growth temperature), and at high enough temperatures it may be possible to grow many layers without appreciable kinetic roughening. It should be noted, however, that the growth temperature cannot be
arbitrarily high so as to avoid desorption from the growth front. In practice, the growth temperature should be as high as possible (within the restriction of avoiding significant desorption) to obtain the best layer by layer epitaxial growth. (I should mention here that most real surfaces being necessarily slightly vicinal, RHEED intensity oscillations actually disappear at high temperatures as the diffusion length becomes comparable to the terrace size and two-dimensional layer by layer growth mode gives way to the step flow growth mode — in a truly high symmetry singular surface this would not happen and the high temperature limit then is set by the no-desorption constraint.)

One of the key recent developments in epitaxial growth phenomena has been the realization that the coarse-grained kinetically rough growth morphology follows a rather general dynamical scaling behavior. In particular, the root mean square fluctuation \( W \) in the evolving surface height, \( h(r, t) \) where \( h \) is the height of the interface at time \( t \) for the substrate position \( r \), obeys the following dynamic scaling law (a similar dynamic scaling law holds for the height-height correlation function as well [1–4]):

\[
W(L, t) \sim L^\alpha f(L/\xi(t)),
\]

(2.1)

where

\[
W^2 = \langle (h(r, t) - \langle h \rangle)^2 \rangle,
\]

(2.2)

is the mean squared interface width (\( \langle h \rangle \) being the average film thickness, \( \langle h \rangle = F t \) where \( F \) is the average growth rate), \( L \) is the substrate width, and the correlation length \( \xi(t) \) grows with time as

\[
\xi(t) \sim t^{1/z},
\]

(2.3)

with \( z \) being the dynamical exponent (which describes how correlations spread laterally along the substrate over time), and \( \alpha \) the roughness exponent. At long times, when \( \xi \sim t^{1/z} \gg L \), lateral correlations have essentially spread over the whole substrate, and the system reaches a saturated steady state, indicating that the scaling function \( f(x) \) must have the long-time asymptotic form:
\[ f(x \gg 1) \sim 1. \] (2.4)

In the short-time situation \((\xi(t) \ll L)\), however, the surface roughness \(W\) should be independent of the lateral system size \(L\) because lateral correlations have not yet spread over the whole substrate, and therefore the short-time asymptotic form for the scaling function \(f(x)\) must be:

\[ f(x \gg 1) \sim x^{-\alpha}. \] (2.5)

Combining the above equations one obtains the following limiting behavior of the dynamical surface roughness \(W(L, t)\):

\[
W(L, t) \sim t^\beta \text{ for } t \ll L^z \\
\sim L^\alpha \text{ for } t \gg L^z,
\] (2.6)

where \(\beta = \alpha/z\) is the growth exponent.

The physical picture underlying the dynamic scaling description is the following. The shot noise associated with the random deposition of the incident beam produces kinetic roughness in the evolving growth morphology which leads to monotonic increase in the interface width (roughness) \(W\) as a function of time. In the limit of very large substrates \((L \to \infty)\) there is no natural limiting length scale in the problem and therefore the kinetic roughness \(W \sim t^\beta\) increases forever. This increase follows a power law, \(W \sim t^\beta\), because there is no natural time scale in the problem other than that defined by the growth rate which defines the unit of time. Note that the average thickness of the growing film is, by definition, proportional to the growth time, \(<h> \propto Ft\), and therefore in all these scaling relations one could replace \(t\) by \(<h>\). For a finite substrate, a steady state is reached when the lateral correlations spread over the whole system \((\xi \geq L)\) and the interface width saturates to a steady state value, \(W(L, t \gg L^z) = W_0 \sim L^{\beta z} \equiv L^\alpha\), which naturally scales as a power of the system size. The key point is the existence of a lateral (dynamical) correlation length, \(\xi(t) \sim t^{1/z}\), which scales with time according to the dynamical exponent \(z\). This is, of course, the standard scenario for dynamic scaling in physical phenomena. Note that the
kinetically rough surface morphology is a self-affine fractal object which exhibits anisotropic generic scale invariance where the anisotropy arises from the inequivalence between growth and substrate directions [1–4].

It should be noted that there exists no rigorous proof that a dynamic scaling scenario must, in general, apply to the epitaxial growth morphology. But there is a great deal of empirical evidence, based on both theoretical and simulational work as well as rapidly accumulating experimental support, for the applicability of dynamic scaling to epitaxial growth. The essential idea underlying the dynamic scaling hypothesis is that there being no characteristic length and time scales in the problem, dynamic scaling must hold at large length scales and long times. I note that in all real epitaxial growth processes there obviously are several characteristic length scales (e.g., the lattice size, the diffusion length, etc.) which determine the “critical regime”, i.e. the asymptotic dynamic scaling sets in at distances (and times) much longer than the characteristic lengths (and times) naturally appearing in the problem. (Calculation of these “short” distance cutoffs, e.g., the diffusion length in MBE growth, could be quite tricky for specific experimental situations.) Below these “short” distance (time) cutoffs dynamic scaling does not occur, and (non-universal) transient behavior dominates. One example of such “small-scale” transient behavior is the smooth layer by layer growth regime with oscillatory surface roughness occurring at length scales smaller than $\tilde{\ell}$, where $\tilde{\ell}$ (determined by the adatom diffusion length) is the appropriate “coherence length” [9] for epitaxial growth. (Equivalently one could define a coherence time [9].)

The usual scale invariant dynamical scaling behavior is the stable long distance (time) asymptotic behavior of the system at large scales. It should be emphasized that in many practical situations the characteristic “short” distance or time cutoff (e.g., the coherence length or the coherence time for layer by layer growth) may be so large that the stable asymptotic behavior is not of particular experimental or practical relevance, and the transient unstable growth regime completely dominates the experimental observations. For the layer by layer growth transient the “short distance” cutoff grows exponentially (or faster)
with temperature, for example, the diffusion length and therefore the coherence length for the smooth layer by layer growth regime increases exponentially with temperature making it possible to grow very smooth large area thin films without any appreciable kinetic surface roughness. It is to be noted, however, that the layer by layer growth regime is always a finite size (time) phenomenon with kinetic surface roughening dominating at large scales.

III. UNIVERSALITY IN KINETIC SURFACE ROUGHENING

The set of exponents $\alpha, \beta, z = \alpha/\beta$ for a particular growth process defines a dynamic universality class which characterizes the long wavelength asymptotic properties of kinetic surface roughening associated with that particular growth process. Motivated by the central role played by the concept of universality in our understanding of equilibrium critical phenomena, one naturally asks whether a few universality classes determined by symmetry, conservation laws, and other factors controlling growth dynamics could describe seemingly many different surface growth processes. In particular, the important question is whether there are only a few possible independent sets of exponents $(\alpha, \beta, z)$ describing epitaxial growth in different materials and under different growth conditions. We would of course also want to know what fundamental aspects of a growth process uniquely determine its universality class. A great deal of attention has recently been focused on the issue of the possible universality class(es) of epitaxial growth (in particular, MBE type growth). Although the subject is very much in flux and no firm conclusion has yet been reached, some consensus has emerged in the last few years. I summarize below the currently existing consensus about the four different possible dynamic universality classes for kinetic surface roughening in epitaxial growth, and discuss the continuum equations appropriate for each of these four universality classes in the next section.

1. **KPZ universality** If the growth process is nonconserved (i.e. if desorption and/or formation of surface overhang and bulk vacancies is dynamically significant at the growth front), then the asymptotic universality class of the growth process is thought to
belong to the Kardar-Parisi-Zhang (KPZ) universality class \[^{[10]}\] whose exact exponents are known only in one substrate dimension \((d = 1 + 1)\) with \(\alpha = 1/2, \beta = 1/3, z = 3/2\) in \(d = 1 + 1\). The KPZ exponents for the actual surface growth problem, where the substrate dimension is two \((d = 2 + 1)\), are known only approximately (from extensive numerical simulations) to be \(\alpha \simeq 0.39, \beta \simeq 0.24, z \simeq 1.61\). I note that as a matter of principle all epitaxial growth processes must be nonconserved at the largest scales of length and time because some desorption as well as some overhang/vacancy formation is unavoidable in any real growth problem. Thus, the current consensus is that the KPZ universality class is, in fact, the \textit{generic} growth universality class which must apply to all growth problems at long enough scales of lengths and times. On the other hand, the KPZ exponents are almost never found in any real epitaxial surface growth experiments where the measured roughness \((\alpha)\) and dynamical \((z)\) exponents tend to be much larger than the KPZ values \((\alpha \simeq 0.39; z \simeq 1.61)\). The KPZ universality class therefore has this dubious dichotomy of being theoretically generic for the large scale asymptotic growth behavior and, at the same time, being empirically inapplicable to almost all of the currently existing experimental data on surface growth. Part of the reason for this dichotomy obviously lies in the fact that in most epitaxial growth situations, desorption from the growth front as well as vacancy/overhang formation during growth are dynamically insignificant in the experimental time and length scales, and therefore the asymptotic generic universality simply does not manifest itself. After all, in epitaxial growth experiments, eg. MBE growth, one takes great care in avoiding evaporation and vacancy/overhang formation during growth, and it is therefore perhaps not surprising that the KPZ exponents are never seen in epitaxial growth experiments. Although numerical simulations of MBE growth allowing for defect (eg. overhangs and vacancies) formation rather clearly demonstrate \[^{[11–13]}\] the expected asymptotic crossover to the KPZ universality, one of the most serious open issues in this subject has been the persistent lack \[^{[14]}\] of clear and convincing experimental support for the existence of the generic KPZ universality.
in real epitaxial growth.

2. **EW universality** For conserved (i.e. no desorption or vacancy/overhang formation) solid-on-solid (SOS) type growth processes the KPZ universality is inapplicable, and at least three different possible conserved SOS growth universality classes have extensively been discussed in the literature during the last five years. The most obvious one is the so-called Edwards-Wilkinson (EW) growth universality class \[ \text{[15]} \] which applies whenever the growth process involves some “downward funneling” type relaxation mechanism which pushes the growth front atoms down to the local height minima \([16]\). Any tendency (however small) for the atoms to preferentially attach to down-steps at terrace edges rather than to up-steps during growth automatically leads to the EW universality class. (Note that this tendency of preferential attachment to down-steps over up-steps is precisely opposite to what happens for growth under an Ehrlich-Schwoebel step-edge diffusion bias where atoms preferentially attach to up-steps rather than down-steps — this explains why one occasionally encounters in the literature statements to the effect that a “negative” Ehrlich-Schwoebel barrier leads to EW universality.) The EW growth universality class is characterized by the exactly known critical exponents \( \alpha = 0(1/2), \beta = 0(1/4), z = 2(2) \) in \( d = 2 + 1(1 + 1) \) dimensions. (The EW critical exponents for kinetic roughening are exactly known in arbitrary dimensions.) An important point is that EW universality predicts “smooth” growth \( (\alpha = \beta = 0) \) in the physical \( 2 + 1 \)-dimensional kinetic surface roughening process, implying only logarithmic increase in the kinetic roughness with time and system size. (Note that vanishing critical exponents implies logarithmic increase in kinetic roughening and *not* vanishing roughening as one may naively assume.) Of all the theoretically possible growth universality classes, the EW universality class has the smoothest evolving growth morphology because it has the smallest possible values of the growth \( (\beta) \) and the roughness \( (\alpha) \) exponents in any dimension. This is significant from a technological perspective because large area smooth thin films
and surfaces are required for most electronic materials applications. Understanding growth techniques and physical mechanisms which may induce EW universality in epitaxial growth would be immensely valuable technologically. It has recently been suggested [17] that surfactants induce smooth epitaxial growth by causing preferential attachment of deposited adatoms at down-steps and thereby introducing the EW universality behavior \((\alpha = \beta = 0)\) in a natural manner. A systematic experimental search for various techniques which induce EW growth could be quite useful.

3. **MH universality** In conserved SOS growth situations where “surface diffusion” is dynamically significant in the absence of any EW relaxation process (i.e. no downward funneling or preferential attachment to down-steps), the growth process may belong to the linear surface diffusion (the so-called Mullins-Herring, MH) universality class [18,19]. The critical exponents for the MH growth universality class are exactly known theoretically: \(\alpha = 1(3/2), \beta = 1/4(3/8), z = 4(4)\) in \(d = 2 + 1(1 + 1)\) dimensions. Although several experimental claims in the literature report measurements of kinetic surface roughening exponents, \(\beta \approx 0.25\) and \(\alpha \approx 0.9 - 1\), consistent with the MH universality predictions, it is unclear at the present time whether the MH universality could ever be a true asymptotic universality class (at long times and distances) rather than being a short distance/time crossover phenomenon with the asymptotic universality being given by the EW universality defined in (2) above or the MBE universality defined in (4) below. The current theoretical consensus is that the MH universality can only be a crossover and not an asymptotic universality class. I note that the MH universality (sometimes also referred to as the “linear surface diffusion” universality) has the largest critical exponents \(\alpha\) and \(\beta\) among the four epitaxially relevant universality classes being discussed here, implying that MH universality produces the maximum large-scale kinetic surface roughness in the evolving growth morphology. Note that \(\alpha = 1\) for the MH universality in the surface growth problem, which means that the saturated steady state interface width is proportional to the substrate
size, \(W(L, t \to \infty) \propto L\) in \(d = 2 + 1\). In one dimension (\(d = 1 + 1\)), the roughness exponent, \(\alpha = 1.5\), exceeds unity, which is a manifestly peculiar situation implying that the large scale steady state morphology of the growing surface is not self-affine in \(d = 1 + 1\) because \(W(L, t \to \infty)/L\) actually diverges as \(\sqrt{L}\) in the thermodynamic limit. This extreme pathological roughness in the evolving growth morphology of the MH universality class effectively rules it out as a true asymptotic description for a physical surface growth problem even though it may very well dominate the short-time (non-asymptotic) kinetic surface roughening in many experimental situations where surface diffusion plays an important role. I mention that the dynamic exponent, \(z = 4\), is very large for the MH universality class, making the evolution of lateral correlations extremely slow, \(\xi(t) \sim t^{1/4}\), and this slow evolution of correlations considerably complicates studying crossover properties as well as steady state behavior in the MH universality problem.

4. **MBE universality** The most relevant universality class in the context of conserved epitaxial growth is the molecular beam epitaxy (MBE) universality, which somewhat confusingly goes by several other names in the literature as well: conserved epitaxial growth, conserved KPZ, nonlilnear surface diffusion, and Villain-Lai-Das Sarma (VLD) or equivalently Lai-Das Sarma-Villain (LDV) universality. All describe this same universality I refer to as the MBE universality in this article. This universality class is believed by many to be the correct large scale asymptotic description for the kinetic surface roughening properties of epitaxial growth morphology (which explains my nomenclature for this universality) provided that the growth process is conserved SOS (no desorption and overhang/vacancy formation) and that the “downward fun-neling” type EW relaxation processes are absent or are dynamically unimportant. The critical exponents for the MBE universality class are calculated to be \(\alpha = 2/3(1), \beta = 1/5(1/3), z = 10/3(3)\) in \(d = 2 + 1(1 + 1)\) dimensions. These calculated exponents were thought to be exact until very recently when some questions have
been raised about their exactness. Any corrections (if there are any, the issue is by no means settled) to these exponent values are, however, estimated \cite{21,22} to be well below 1%, and are therefore of no practical significance. There are many reports in the literature of measuring critical exponents $\beta \approx 0.2 - 0.3$ and $\alpha \approx 0.6 - 0.9$ in surface growth experiments, which support the applicability of the MBE universality class to real epitaxial growth morphology. Existing realistic MBE growth simulations based on kinetic Monte Carlo studies \cite{4,23} also lead to critical exponents consistent with the MBE universality class exponents. It should be noted that often these experimentally measured or numerically simulated exponents appear to be somewhat larger than the MBE universality exponents ($\beta = 0.2$, $\alpha = 0.67$), indicating that real epitaxial growth morphology may actually be exhibiting a crossover from the MH universality ($\beta = 0.25$, $\alpha = 1.0$) to the MBE universality. One definitive way of distinguishing between these two universality classes would be a measurement of the surface skewness $s$

\begin{equation}
    s = \frac{\langle (h - < h >)^3 \rangle}{\langle (h - < h >)^2 \rangle^{3/2}},
\end{equation}

associated with the growth morphology. Both the EW and the MH universality (being linear universality classes) predict a vanishing value of $s$ whereas the MBE universality class \cite{4} predicts $s \neq 0$ in the steady state saturated morphology (as well as in the pre-asymptotic transient regime). There have recently been reports \cite{24} of non-zero surface skewness measurements in epitaxial growth morphology, again supporting the viewpoint that the MBE universality class indeed provides the appropriate dynamic scaling description of epitaxial growth. (In the context of surface skewness, I point out that the non-conserved KPZ universality also has a nonzero value of $s$ in the preasymptotic transient regime in both $d = 1 + 1$ and $2 + 1$ dimensions, but in the asymptotic steady state situation the skewness magically vanishes, $s = 0$, in $d = 1 + 1$ dimensions by virtue of the validity of a fluctuation-dissipation theorem which is also responsible for producing the exact values of KPZ exponents in one substrate.
Theoretical understanding of dynamic scaling in kinetic surface roughening has been exclusively based on stochastic partial differential equations describing the time evolution of the coarse-grained surface height variable $h(r,t)$ ever since the pioneering work [10] of Kardar, Parisi and Zhang (more than ten years ago) who showed that the well-known (in the context of fluid dynamics) noisy Burgers equation is the appropriate long wavelength asymptotic dynamical description for nonconserved generic growth under non-SOS ballistic deposition conditions (which allow the formation of overhangs and vacancies at the growth front). In this section I will briefly discuss the continuum growth equations which define the four universality classes described in the last section.

It is notationally more convenient to write the dynamical equations in terms of the height fluctuation, $h(r,t) - \langle h \rangle$, which is equivalent to a transformation to a moving frame of reference which takes the average interface height $\langle h \rangle = Ft$ as the reference position rather than the original substrate $\langle h \rangle = 0$. This eliminates the trivial constant term, given by the average growth rate $F$, explicitly from the equation. From now on $h$ implies the height fluctuation (around the average) rather than the height variable itself. The celebrated KPZ equation [10] is then the deceptively simple-looking nonlinear stochastic equation

$$\frac{\partial h}{\partial t} = \nu_2 \nabla^2 h + \lambda_2 (\nabla h)^2 + \eta,$$

where the spatial derivative $\nabla \equiv \frac{\partial}{\partial r}$ is in the substrate plane, and $\eta$ is the stochastic shot noise associated with the random fluctuations in the incident beam. Usually $\eta(r,t)$ is taken to be a Gaussian white noise of zero mean $\langle \eta \rangle$ with the noise correlator

$$\langle \eta(r_1,t_1)\eta(r_2,t_2) \rangle = D \delta(r_1 - r_2)\delta(t_1 - t_2)$$

where $D$ is the strength of the bare noise.
I do not discuss here the KPZ equation at all because, as stated in the last section, it is not particularly relevant for understanding epitaxial growth morphology in experimental length and time scales. (Several excellent reviews [1,2,23] of the KPZ equation exist in the literature.) Two particular features of Eq. 4.1 should be noted: (a) It is the lowest order growth equation consistent with the symmetries of the problem, and (b) the nonlinear $(\nabla h)^2$ term in the equation, a manifestly nonequilibrium growth term as it breaks the up-down symmetry in the problem, is a nonconserved term associated with vacancy/overhang formation (or desorption) at the growth front.

Before proceeding any further I write down below the three continuum growth equations which correspond respectively to the three other universality classes introduced in the last section:

\[ \text{EW : } \frac{\partial h}{\partial t} = \nu_2 \nabla^2 h + \eta, \]  

\[ \text{MH : } \frac{\partial h}{\partial t} = -\nu_4 \nabla^4 h + \eta, \]  

\[ \text{MBE : } \frac{\partial h}{\partial t} = -\nu_4 \nabla^4 h + \lambda_{22} \nabla^2 (\nabla h)^2 + \eta, \]

Several features of these four growth equations, Eqs. 4.1-4.4, corresponding to the universality classes 1-4 respectively in section II, should be noted: the EW and the MH equations are linear and are therefore very simple; the KPZ (MBE) equation is simply the nonlinear version of the EW (MH) equation with the appropriate 2nd (4th) order nonlinearity being included in the equation; the MBE equation is effectively a conserved KPZ equation with a nonconserved external noise rather than a conserved noise \[ \frac{\partial h}{\partial t} = -\nu_4 \nabla^4 h + \lambda_{22} \nabla^2 (\nabla h)^2 + \eta = \nabla^2 (-\nu_4 \nabla^2 h + \lambda_{22} (\nabla h)^2) + \eta; \] EW and KPZ equations are 2nd order equations while MH and MBE equations are fourth order and therefore a growth equation containing all of these terms will be dominated by the KPZ nonlinearity (if it is non-zero) or by the EW term (if $\lambda_2 = 0$) with the $\nu_4 \nabla^4 h$ and the $\lambda_{22} \nabla^2 (\nabla h)^2$ terms being irrelevant in the renormalization group sense. I emphasize, however, that even in such a
situation the $\nabla^4 h$ and the $\nabla^2(\nabla h)^2$ terms could significantly affect crossover properties and dominate the critical properties at “short” length and time scales.

Restricting to epitaxially relevant conserved SOS growth (with the nonconserved noise arising from external beam fluctuations) it is easy to see \cite{3,20} that the coarse-grained continuum growth equation must obey a continuity equation consistent with the conservation of the surface current in the problem:

$$\frac{\partial h}{\partial t} + \nabla \cdot j = \eta, \quad (4.5)$$

which follows simply from the mass and volume conservation in epitaxy associated with the no overhang/vacancy/desorption hypothesis. Thus the growth equation must have the form $\frac{\partial h}{\partial t} = -\nabla \cdot j + \eta$ where the surface current density $j$ can only be of a form which is consistent with the symmetries in the growth problem. (It should be noted that the KPZ equation, Eq. 4.1, is explicitly ruled out because the KPZ nonlinearity, $(\nabla h)^2$, cannot be expressed as the divergence of a current.) The only general symmetries in the epitaxial growth problem are the translational invariance along the growth direction (i.e. it does not matter where the substrate is placed) and the rotational invariance in the substrate $r$-plane. Taking into account these general symmetries and the conserved current constraint, the conserved epitaxial growth equation could be written as \cite{20}

$$\frac{\partial h}{\partial t} = \nu_2 \nabla^2 h - \nu_4 \nabla^4 h + \lambda_{22} \nabla^2(\nabla h)^2 + \lambda_{13} \nabla(\nabla h)^3 + \eta, \quad (4.6)$$

keeping terms only up to the fourth order. This is the most general possible low order conserved epitaxial continuum growth equation. The conserved universality classes discussed in the last section are all special limiting cases of Eq. 4.6, as is obvious by comparing Eq. 4.6 with Eqs. 4.2-4.

A simple power counting analysis shows that in Eq. 4.6 the most relevant long wavelength term is the EW $\nabla^2 h$ term, followed respectively by the $\nabla(\nabla h)^3$ term, the $\nabla^2(\nabla h)^2$ term, and the $\nabla^4 h$ term in order of most relevant to the least relevant growth processes at the largest scales.
Since asymptotic critical exponents are always determined by fluctuations at the largest scales, one concludes that the EW universality, if present (i.e. if $\nu_2 \neq 0$), is the most relevant universality in the problem. The other terms may still be quite important in determining the effective exponents at shorter scales (and thus affect crossover behavior), but the asymptotic universality class is always EW if $\nu_2 \neq 0$ in Eq. 4.6. An additional notable point is that the most relevant fourth order term, the $\lambda_{13} \nabla(\nabla h)^3$ term, originally introduced in ref. [20] through symmetry considerations and recently rediscovered [27] in the context of unstable growth under an ES barrier, generates the EW $\nabla^2 h$ term upon renormalization [28] and therefore also leads to EW universality although it is formally a higher order term. Thus even if $\nu_2 = 0$, but $\lambda_{13} \neq 0$ in Eq. 4.6, the growth universality class is still EW! (I note that the most relevant conserved term in each order, namely the $\nabla(\nabla h)^{2n+1}$ term with $2n = 2, 4, 6, \text{etc.}$, always generates EW universality upon renormalization — it is, however, difficult to imagine physical processes which could lead to $\nu_2 = 0$ but these nonlinear terms non-zero.)

The fourth order linear (Eq. 4.3) or nonlinear (Eq. 4.4) continuum growth equations become applicable to conserved epitaxial growth only in the absence of all EW relaxation processes (i.e. when $\nu_2 = \lambda_{13} = 0$), or as crossover effects at short distance/time scales before the EW growth terms in Eq. 4.6 become dynamically significant. As mentioned in section III, there is a large body of experimental data [1,2,4,7] on the surface kinetic roughening in epitaxial growth reporting a roughness exponent $\alpha \sim 0.6 - 0.9$ and a growth exponent $\beta \sim 0.2 - 0.3$, which are totally inconsistent with the EW exponents ($\alpha = \beta = 0$), but are consistent with the MH growth equation ($\alpha = 1.0, \beta = 0.25$) and the MBE growth equation ($\alpha = 0.67, \beta = 0.2$). Empirically, therefore, it seems that epitaxial growth belongs to the MBE universality class as defined by Eq. 4.4 (which incorporates as a special case the MH equation, Eq. 4.3, in the special situation of the vanishing nonlinearity $\lambda_{22} = 0$).

Obtaining the critical exponents from the continuum growth equation is simple and straightforward for the linear equations (Eqs. 4.2 and 4.3) because the linear equations can be directly solved via Fourier transformation. The nonlinear MBE growth equation, Eq.
4.4, is thoroughly nontrivial, however, and has been analyzed using the dynamical renormalization group technique \[20\] and the direct numerical integration technique \[28,29,22\]. I summarize below the theoretical exponent values for Eqs. 4.2-4:

\[
\text{EW} : \ \alpha = (3 - d)/2, \ \beta = (3 - d)/4, \ z = 2, \quad (4.7)
\]

\[
\text{MH} : \ \alpha = (5 - d)/2, \ \beta = (5 - d)/4, \ z = 4, \quad (4.8)
\]

\[
\text{MBE} : \ \alpha = (5 - d)/3, \ \beta = (5 - d)/(7 + d), \ z = (7 + d)/3. \quad (4.9)
\]

In Eqs. 4.7-9, \(d\) is the total spatial dimension, and obviously the physically relevant dimension for kinetic surface roughening in epitaxial growth is \(d = 2 + 1 = 3\). The one dimensional substrate problem, \(d = 1 + 1\), is, in fact, extensively studied theoretically (mainly because of convenience and ease in numerical simulations), and may have considerable potential experimental relevance in terms of kinetic roughening of step edges \[14\] on vicinal surfaces. While the above results (Eqs. 4.7 and 8) for the linear EW and MH universality classes are obviously exact, the MBE universality results given in Eq. 4.9 are obtained from a one-loop dynamical renormalization group analysis which is leading order in the \(\epsilon\)-expansion where \(\epsilon = 5 - d\). Given that the expansion parameters \(\epsilon = 2(3)\) in \(d = 3(2)\) are obviously not small, one may legitimately question \[21\] the validity of the calculated exponents in Eq. 4.9. Direct numerical integration of Eq. 4.4, however, gives \[28,29,22\] the same (within the numerical accuracy \(\sim 1-2\%)\) exponents in \(d = 2\) and 3 dimensions as those of Eq. 4.9, providing support to the one-loop dynamical renormalization group result \[20\]. It is possible that the exponents of Eq. 4.9 are, in fact, exact for the MBE universality class due to some hidden symmetry in the problem \[20,20\], but the issue has to be considered open at this time \[21\].

Combining the current conservation condition with the general conserved SOS growth equation (Eq. 4.6) one gets the following expression for the surface current in epitaxial growth
\[ j = - (\nabla h) \{ \nu_2 + \lambda_{13} (\nabla h)^2 + \cdots \} + \nabla \{ \nu_4 (\nabla^2 h) - \lambda_{22} (\nabla h)^2 + \cdots \}, \tag{4.10} \]

where the first term, a nonequilibrium surface current \( j_{\text{NE}} \), is proportional to the surface slope \( \nabla h \) and the second term can be thought of \[3\] as the contribution from a generalized chemical potential \( \mu \), where \( \mu = \mu_0 + \mu_{\text{NE}} \) with \( \mu_0 \propto \nabla^2 h \) is the standard “equilibrium” chemical potential leading to the Mullins-Herring equation \[30\] and the so-called nonequilibrium chemical potential \( \mu_{\text{NE}} \) is given by \( \mu_{\text{NE}} \propto \lambda_{22} (\nabla h)^2 + O((\nabla h)^4) + \cdots \). Thus, Eq. 4.10 can be rewritten \[31\] as \( j = j_{\text{NE}} + \nabla \mu \) where \( j_{\text{NE}} \propto (\nabla h) \). Note that the chemical potential contribution to the current \( j \) does not explicitly depend on \( \nabla h \) whereas the nonequilibrium current contribution, \( j_{\text{NE}} \), which leads to the EW universality is proportional to \( \nabla h \). This provides \[31\] a simple and effective technique of detecting the possible existence of the EW universality in a particular growth model. If there is a net inclination dependent surface current on a tilted substrate in a growth model, then \( j_{\text{NE}} \neq 0 \), indicating the presence of the EW universality in the model (this is true only if the current is downward and therefore stabilizing — if the inclination dependent current is upward then that indicates the existence of an ES barrier in the problem with the associated growth instability). On the other hand, if the measured inclination dependent current vanishes on a tilted substrate, then obviously the EW universality is absent in the model. This simple technique of measuring the inclination dependent surface current on a tilted substrate has turned out to be a powerful tool for detecting the presence or absence of the EW universality in various growth models, and is operationally very effective in determining the EW universality long before the measured critical exponents show a crossover to EW behavior \[2,31\]. Application of this technique of measuring inclination dependent surface current on tilted substrates enables one to effectively distinguish among unstable ES barrier growth (upward current), EW universality (downward current), and the fourth order MBE growth universality (vanishing inclination dependent current) in various discrete epitaxial growth models (some of which are discussed in the next section).

I conclude this section by mentioning that the actual values of the coefficients \( \nu_2, \nu_4, \)
\[ \lambda_{22}, \lambda_{13}, \text{etc.} \] entering the continuum growth equations are not important in determining the respective asymptotic universality classes except in the trivial sense that a particular coefficient must be non-zero for that particular universality class to show up. The explicit values of these coefficients are, however, important in determining the crossover behavior in the growth problem, for example, if only the (most relevant) \( \nu_2 \) and the (most irrelevant) \( \nu_4 \) terms are non-zero in Eq. 4.6 then the growth universality class is obviously EW since \( \nu_2 \nabla^2 h \) is more relevant than \( \nu_4 \nabla^4 h \), but a simple dimensional analysis shows that the EW universality can show up only for lateral length scales larger than \( (|\nu_4|/|\nu_2|)^{1/2} \) or equivalently for time scales larger than \( (|\nu_4|/|\nu_2|)^{2} \), and therefore in a real finite size/time experiment the EW universality may simply not manifest itself, leading to effective MH universality exponents. This is a situation where an inclination dependent current measurement on a tilted substrate may lead to the “correct” (i.e. EW) asymptotic universality even though the “effective” exponents are still in the MH crossover regime. Finally, I point out that the coefficients \( \nu_2, \lambda_{13}, \) and \( \lambda_{22} \) are expected to be proportional to the external flux rate \( F \) in the leading order because these terms are manifestly nonequilibrium contributions (\( \nu_2 \) and \( \lambda_{13} \) to \( j_{\text{NE}} \), and \( \lambda_{22} \) to \( \mu_{\text{NE}} \)) to the growth process, and therefore should vanish in the absence of the external flux. The \( \nu_4 \) term, on the other hand, is the usual equilibrium surface diffusion contribution [30] and its presence in the nonequilibrium growth problem is still somewhat mysterious [3, 19, 2].

**V. ATOMISTIC GROWTH MODELS**

All real epitaxial growth takes place in discrete systems with atoms and lattices whereas the coarse-grained long wavelength theory discussed in the last section is, by definition, a continuum theory. A question naturally arises about whether such a coarse-graining procedure leading to a continuum dynamical growth equation which describes the long wavelength asymptotic dynamic scaling properties of the growth problem is, in general, allowed for all discrete epitaxial growth phenomena. The answer to this question is not known, and only in
a few problems a rigorous connection between a discrete growth model and its coarse-grained continuum description has been established. One hopes, with considerable physical justification, that such a coarse-graining prescription leading from a discrete problem to a continuum description should, in fact, be possible at “sufficiently long” wavelengths. (Whether real experimental growth studies are always carried out in this “sufficiently long” wavelength regime or not is, of course, a totally different issue which is extremely difficult to answer.) Recently, some subtle and serious questions have been raised \[32\]-\[34\] by several different groups regarding the validity of the continuum descriptions for discrete growth problems, particularly in cases involving nonlinear (eg. KPZ, MBE, etc.) growth terms. Although the details of these doubts vary considerably from case to case, it is fair to say that one of the tentative conclusions emerging from these analyses \[32\]-\[34\] is that in some situations involving nonlinear growth processes discrete growth problems and their coarse-grained continuum descriptions may belong to different universality classes. (Not surprisingly no such problem arises in linear growth problems, eg., EW universality.) There is thus sufficient reason to be critical and skeptical about blindly applying continuum theoretical results to discrete growth problems.

The most effective technique to study atomistic epitaxial growth is via the direct numerical simulation of the discrete growth process. There have been numerous such studies using a variety of techniques and models in the context of dynamic scaling in epitaxy — see, for example, refs. \[4,5,11-13,16,18,19,22,23,34\] and the review articles in refs. \[1-3\]. In the context of epitaxy, where adatom mobility at the growth front is the dominant smoothening mechanism and the shot noise fluctuations inherent in the deposition beam is the roughening mechanism, the kinetic (or, the stochastic) Monte Carlo simulation \[4,5,11-13,23\] has been the most realistic direct numerical technique for studying MBE growth. In this technique both deposition and diffusion are taken to be stochastic processes simulated by various random number generators (and hence the name, Monte Carlo simulation) with the atomic diffusion at the growth front taken to be an Arrhenius activated hopping process with the activation energy (consistent with the principle of detailed balance) determined by the na-
ture of local bonding for the hopping atom. Depending on the local bonding of the diffusing atom, several different activation energies (and consequently several different diffusion rates) participate in the hopping process, leading to the possibility of rather strong finite size and crossover effects in the simulation. Thus, the full activated diffusion stochastic Monte Carlo simulation of epitaxial growth, while being reasonably realistic in capturing the evolving surface morphology, is not always the ideal method for obtaining the asymptotic growth exponents.

Purely nonequilibrium zero temperature growth models, with instantaneous relaxation of the deposited adatoms according to some physically \[18,19\] or mathematically \[16,22\] motivated local rules, have been very popular and extremely successful in characterizing the asymptotic growth universality class and the dynamic scaling behavior of epitaxy. I will discuss one such conserved SOS nonequilibrium growth model (called the DT model by Krug \[2\]), introduced in ref. \[19\] and extensively studied in refs. \[4,5,35–37\]. Before discussing the model I mention two significant salient features of the model which make it particularly relevant for studying dynamic scaling in epitaxial growth: (1) the scaling exponents \(\alpha, \beta\) calculated for this simple nonequilibrium model agree quantitatively with the corresponding exponents for the full activated diffusion stochastic Monte Carlo simulation results in both \(d = 1 + \frac{1}{2}\) and \(d = 2 + \frac{1}{3}\) dimensions \[4,37\]; (2) due to a simple symmetry \[2\] in the growth rules of this model, the inclination dependent surface current vanishes exactly for tilted substrates, implying that this model most certainly does not have the most relevant EW term in its continuum description (i.e. \(\nu_2, \lambda_{13} = 0\) in this growth model) — this particular feature makes this model unique among the existing nonequilibrium SOS growth models, the other two such models introduced in ref. \[16\] and in ref. \[18\] are known to belong asymptotically to the EW universality class.

In the growth model of ref. \[19\], atoms are deposited randomly and sequentially (i.e. one at a time at a randomly chosen spatial position on the surface) on a cubic substrate according to an average rate and within the SOS constraint, after deposition each atom could relax within a lateral diffusion length (which is most commonly taken to be just one lateral lattice
spacing) subject to the following conditions: only deposited atoms with no lateral bonds to
other surface atoms are allowed to move, and the atom moves (within the lateral diffusion
length) only to increase its local coordination number (i.e. lateral bonding) — otherwise it
does not move and the next atom is deposited. Note that these local diffusion rules allow
only downward relaxation of the adatoms (to kink and trap sites, but not necessarily to
height minima [16] or to sites of maximum local bonding [18]), and in case of ties (i.e. more
than one final site satisfying the relaxation condition) the atom moves randomly with an
equal probability to any of the allowed final sites. Each deposited atom is allowed to relax
only once immediately following deposition, but more elaborate local relaxation rules have
also been considered [38] with concommitant increase in the dynamic scaling possibilities.
Note that the particularly simple local relaxation rules of this manifestly nonequilibrium
growth model are motivated by the actual atomistic hopping processes at the MBE growth
front in the low to intermediate growth temperatures. The idea is that only singly bonded
atoms (to their neighbors underneath them, an essential ingredient of conserved SOS growth)
have appreciable surface mobility at low growth temperatures, the hopping probability of
adatoms with higher coordinations being suppressed exponentially. The nonequilibrium
growth model of ref. [19] is a typical example of limited mobility diffusion models which
have been successful in modeling epitaxial growth.

Extensive computer simulations (using up to $10^{12}$ deposited atoms) of this nonequilibrium
growth model in $d = 2 + 1$ dimensions show [37] a clear crossover in the growth exponent
$\beta$ from $\beta \approx 0.25$ at short time scales to $\beta \approx 0.20$ at longer times (the estimated roughness
exponent $\alpha \approx 0.6 \pm 0.1$), indicating that this model truly belongs to the MBE growth
universality, and the crossover is from the MH universality, dominated by the $\nabla^4 h$ term, to
the MBE universality, dominated by the nonlinear $\nabla^2(\nabla h)^2$ term, in Eq. 4.4. Note that the
crossover time scale to see the MBE universality is approximately $\sim |\nu_4 / \lambda_{22}|^4$ and it should
show up only for substrate sizes larger than $\sim |\nu_4 / \lambda_{22}|$. Consistent with these expectations,
the observed crossover to MBE universality manifest itself [37] only for system sizes larger
than $100 \times 100$ — in smaller systems saturation occurs before the crossover and one sees
only the MH universality ($\beta \approx 0.25, \alpha \approx 0.9$). These findings \cite{37} in this simple limited mobility nonequilibrium growth model \cite{19} are in agreement with many experimental reports on dynamic scaling in epitaxy with the experimental $\beta \approx 0.2 - 0.3$ and the experimental $\alpha \approx 0.6 - 0.9$. I speculate that the dynamic scaling in most epitaxial kinetic roughening experiments is essentially in the crossover regime between the MH universality and the MBE universality class. It is certainly not possible to rule out the asymptotic existence of an EW universality in experimental systems at still larger scales; all one can say is that such an eventual crossover to the EW universality ($\beta = \alpha = 0$) has not been reported in the literature in the context of dynamic scaling in epitaxial growth experiments. Based on all of these observations, it is not unreasonable to conclude that the simple limited mobility nonequilibrium growth model of refs. \cite{19,37} captures the essence of the dynamic scaling behavior in epitaxial growth.

Before concluding this section I mention several features of the epitaxial atomistic growth model of ref. \cite{19,37} which are of potential importance:

1. Explicit calculation of the inclination dependent surface current on tilted substrates shows a vanishing current in both $d = 1 + 1$ and $2 + 1$ dimensions, implying the non-existence of any EW growth term in the model of ref. \cite{19,37}.

2. Very recent theoretical work \cite{39,40} using the master equation approach find that the model of ref. \cite{19,37} actually follows the MBE growth equation, Eq. 4.4 of this paper. (The model of Wolf and Villain \cite{18}, which is closely related to the model of ref. \cite{19}, is however found \cite{39,40} to contain the EW $\nabla^2 h$ term, which is consistent with the earlier finding \cite{31} of a tilt dependent surface current in the Wolf-Villain model.)

3. The model of ref. \cite{19,37} shows considerable evolving skewness in the growing surface (implying a breaking of the up-down symmetry under the nonequilibrium growth condition) with the best estimate for the steady state skewness in the surface morphology being $s \approx -0.5$ \cite{38,37,4].
4. For reasons not completely understood at the present time, the model exhibits an extremely long crossover regime \([19, 5, 4]\) in \(d = 1 + 1\) dimensions, with \(\beta \approx 0.37\) for upto \(10^8\) monolayers of growth on a \(L = 10^4\) substrate (the value of \(\alpha\) for smaller system sizes, upto \(L = 200\), is \(\alpha \approx 1.3\)) — thus the expected crossover to the MBE universality (\(\beta = 0.33, \alpha = 1.0\)) is extremely slow in one substrate dimension where the MH exponents (\(\beta = 0.375, \alpha = 1.5\)) seem to dominate for a long time except that the existence of a finite skewness definitively rules out a linear equation as the underlying continuum description.

5. Finally, the discrete model of ref. [19, 37] shows an extremely intriguing anomalous scaling [35] and multiaffine scaling [36] behavior where each moment of the height-height correlation function seems to have its own roughness exponent, indicating the growth problem to be similar to the intermittency phenomenon in fluid turbulence [36]. A recent detailed study [34] of the multiscaling phenomena [36] indicates that the continuum equation for the discrete nonequilibrium growth model of ref. [19] may actually be

\[
\frac{\partial h}{\partial t} = \left[ -\nu_4 \nabla^4 h + \lambda_{22} \nabla^2 (\nabla h)^2 + \eta \right] + \sum_{n=2,3,\ldots} \lambda_{2n} \nabla^2 (\nabla h)^{2n}, \quad (5.1)
\]

where the terms within the square brackets comprise the MBE growth equation, Eq. 4.4, and the infinite order series of \(\nabla^2 (\nabla h)^{2n}\) terms with \(2n = 4, 6, 8, \ldots\) defines a rather complex correction to scaling, arising from an infinite series of marginally relevant (irrelevant) terms in \(d = 1 + 1(2 + 1)\) dimensions. The multiscaling phenomenon seems to be transient, lasting only up to \(10^4-10^5\) layers of growth in \(d = 2 + 1\) dimensions [37], but is a very long lasting transient (at least up to \(10^9\) layers) in \(d = 1 + 1\) dimensions. A direct experimental measurement of the scaling properties of the higher moments of the height-height correlation functions in epitaxial growth will be very interesting in this context. Any experimential evidence for multiaffine growth, where different moments of the height-height correlation function scale with different exponents and where the step height distribution of the evolving morphology shows an
intermittent stretched exponential distribution \([36, 37]\), would not only be interesting from the kinetic surface roughening perspective, but will be of broad general interest as it will be an example of a rather simple stochastic nonequilibrium model exhibiting intermittency and turbulence.

VI. RELATED TOPICS

I will very briefly discuss two topics in this section without really doing much justice to their importance and significance. (Each of these topics deserves their own theoretical chapters.) The first topic is the role of growth temperature in dynamic scaling of epitaxial kinetic surface roughening. The second topic is the issue of dynamic scaling in “unstable” growth under ES step edge diffusion bias. In contrast to the standard lore in the literature, where temperature induced smooth layer by layer growth and growth under ES diffusion bias are thought of as phenomena quite distinct from kinetic surface roughening, I tend to take the view that the powerful dynamic scaling ideas describe all these growth scenarios with appropriate modifications and qualifications.

1. Temperature effects Note that the growth temperature \((T)\) plays no direct or explicit role in the dynamic scaling properties of kinetic surface roughening discussed so far in this article. This is in sharp contrast to equilibrium critical phenomena where \(T\) has to be tuned close to the critical temperature in order to observe the critical behavior and scaling. Kinetic surface roughening is thus generically scale invariant and the dynamic scaling behavior is present at long wavelengths without any tuning of growth parameters. The growth temperature does, however, play an extremely important role in controlling the various crossover regimes, finite size effects, and in determining the size of the transient layer by layer smooth growth regime. Growth temperature sets the distance/time scales which separate the transient and the dynamic scaling regimes. Temperature actually determines the important short distance cutoff in the growth problem by controlling the diffusion length \(\ell\) which scales as
\[ \ell \sim (D/F)^\gamma \] (6.1)

where the exponent \( \gamma \sim 1/2 - 1/6 \) depends explicitly on the temperature dependent minimum stable island size and can, in principle, be calculated \[8\] by stochastic Monte Carlo simulations or kinetic rate-theoretic arguments, and \( D, F \) are the diffusion rate and the deposition rate respectively. The diffusion rate \( D \) depends exponentially on the temperature via the Arrhenius activation law

\[ D \sim k_B T e^{-E_A/k_BT}, \] (6.2)

and therefore \( \ell \sim \frac{T^\gamma e^{-\gamma E_A/k_BT}}{F^\gamma} \) with the activation energy \( E_A \) depending explicitly on the size of the stable islands on the surface (i.e. how many bonds are being cut in the hopping process). The important point to note is that the characteristic diffusion length varies superexponentially \( \sim T^\gamma e^{-\gamma E_A/k_BT} \) with temperature, and therefore the crossover properties of dynamic scaling are expected to be strong functions of temperature in the appropriate temperature windows \[9,5,41,42\].

It has recently been shown \[9\] that the short distance cutoff in MBE growth is not the diffusion length itself, but the closely related coherence length \( \tilde{\ell} \) which varies as a power of the diffusion length \( \ell \):

\[ \tilde{\ell} \sim \ell^\delta \] (6.3)

with \( \delta = 4/(5 - d) \) for the MBE growth equation. Putting \( d = 2(3) \) one concludes therefore that the finite size scaling behavior of the critical exponents \( \alpha, \beta, \) etc. in the presence of the short distance cutoff defined by the coherence length \( \tilde{\ell} \) should show a characteristic \( L/\ell^2(d = 2 + 1) \) or \( L/\ell^{4/3}(d = 1 + 1) \) dependence. Such a finite size scaling behavior, in particular, an approximate \( L/\ell^{4/3} \) scaling of the effective growth exponent \( \beta \) on system size and diffusion length, has earlier been reported in \( d = 1 + 1 \) \[3,4\]. Since the diffusion length \( \ell \) itself depends strongly on temperature, this implies a potentially strong temperature dependence of the critical exponents arising just from
temperature dependent finite size effects. In particular, the dynamical exponent $\beta$ and the roughness exponent $\alpha$ should vary between their asymptotic values as defined by the appropriate universality for $L/\tilde{\ell} \to \infty$ to effectively zero as $L/\tilde{\ell} \to 0$. For Arrhenius activated full diffusion MBE model, however, the zero temperature ($L/\tilde{\ell} = \infty$) limit of $\beta$ is trivially $1/2$, corresponding to pure random deposition with no relaxation because at $T = 0$ the adatoms do not diffuse \cite{5,19}. Such a behavior of $\beta$, varying strongly with temperature and diffusion length, has been seen in computer simulations \cite{5,19,41,42}, and can easily be understood as manifestations of crossover/finite size scaling behavior in the presence of a characteristic short-distance cutoff $\tilde{\ell}$ over which the growing surface morphology is essentially smooth. In particular, for $\tilde{\ell} \geq L$ the layer by layer growth regime persists indefinitely \cite{3}, and $\beta, \alpha \equiv 0$ due to finite size effect. One can therefore think of the smooth layer by layer growth regime as a trivial dynamic scaling regime where finite size effects push down the growth and roughness exponents to zero values. Such an idea has been used in the literature to define and calculate the epitaxial growth temperature \cite{3,42}.

The basic point of physics is that kinetic roughening (for example, coarse-grained continuum descriptions) applies only at length scales above $\tilde{\ell}$, and below $\tilde{\ell}$ one has smooth layer by layer growth transient. Even at large scales the coefficients $\nu_2, \nu_4, \lambda_{22}$ etc. appearing in the growth Eqs. 4.2-4 depend on the growth temperature (and deposition rate), which could produce complex temperature dependent crossover behavior. Careful experimental work obtaining $\beta(T)$ as a function of temperature in epitaxial growth will be useful in the context of understanding finite size effects in dynamic scaling of epitaxy. Such systematic temperature dependent experimental information is lacking at the present time. I note that the so-called epitaxial growth temperature, $T_e$, is defined by the condition $\tilde{\ell}(T) = L$ in this picture, and the superexponential temperature dependence of $\tilde{\ell}$ implies a weak (sub-logarithmic) system size dependence of $T_e$ \cite{3,42}.
2. Unstable growth under ES barrier  In nonequilibrium growth under an ES step edge diffusion bias, where atoms preferentially attach to ascending over descending steps, a characteristic wedding cake morphology evolves on the surface with the formation of mounds/pyramids. These mounds coarsen and/or steepen with time — in the pre-saturation regime the typical mound radius (i.e. the lateral mound size), $R(t)$, increases with time according to a coarsening exponent $n$, and the mound slope, $m(t)$, increases with time according to a steepening exponent $\lambda$:

$$R(t) \sim t^n; \quad m(t) \sim t^\lambda.$$  \hspace{1cm} (6.4)

A crucial point (which is not always emphasized in the literature on the subject) is that the dynamic scaling law applies to this situation exactly in the same form as it does in the generically scale invariant kinetic surface roughening problem, $W \sim L^\alpha f(L/\xi(t))$ with $W(t, L \rightarrow \infty) \sim t^\beta$, except here the “surface roughness” $W(t)$ is essentially the same as the typical mound height, $H(t)$. Using the fact that the mound slope $m \sim H/R$ (i.e. mound height/mound size), one obtains the exponent identity

$$\beta = \lambda + n.$$  \hspace{1cm} (6.5)

in nonequilibrium growth under an ES barrier. (Alternative exponent definitions are, in principle, possible which may deviate somewhat from the above exponent identity, but in my view the definitions of $\beta$, $\lambda$, and $n$ used here are the natural ones both for the experimental and the numerical simulation purpose — an important point to note is that coarsening and steepening compete, as is directly implied by Eq. 6.5.) The dynamical exponent $z$ is essentially $1/n$ for most reasonable definitions of the mound size, implying that $R(t)$ for all practical purposes is the dynamical correlation length $\xi(t)$.

This leads to the conclusion that nonequilibrium growth on flat singular surfaces under an ES step edge diffusion bias follows the usual two exponent (eg. $\beta$ and $n$) dynamical
scaling behavior exactly in the same manner as in the kinetic roughening problem. There has been considerable earlier confusion in this subject based on erroneous claims in the theoretical literature of single exponent scaling in this problem. Note that the evolving mounds/pyramids etc. manifestly break generic scale invariance in this growth problem because obviously there are characteristic length scales (e.g., the mound size) dominating the growth morphology. But the dynamic scaling concept applies here at the same level of generality as it does in the generically scale invariant kinetic surface roughening phenomenon.

Incorporation of an ES barrier in nonequilibrium surface growth has turned out to be a rather formidable theoretical challenge. There is no suitable coarse-grained continuum growth equation which catches all aspects of the interesting mound formation and its subsequent coarsening. Although there are a number of proposed growth equations, and in some cases the exponents $\beta$, $n$, $\lambda$ have been calculated, there is no existing theoretical consensus on a continuum description for nonequilibrium surface growth under ES barriers. Surprisingly, numerical simulations of discrete nonequilibrium surface growth models under ES barriers have also turned out to be quite tricky, with the results depending strongly on the details of how the ES barrier is incorporated [43–51,27]. In fact, there is no consensus even on the basic nature of the instability [6] associated with surface growth under an ES bias — in particular, much debate and speculation can be found in the literature on whether or not there is slope selection (the exponent $\lambda \to 0$ if there is slope selection) during the coarsening of the mounds. Experimental studies seem to indicate that there may or may not be slope selection depending on the systems and growth temperatures one uses. I believe that a good part of the theoretical problem arises from our ignorance about how to incorporate the effect of ES barrier in the coarse-grained continuum description as well as in atomistic numerical simulations. In the stochastic Monte Carlo growth simulation, an ES bias can be included [46] either as a reflection barrier [46–48] or as an edge barrier [46,44].
In the reflection barrier case, an atom approaching a descending step is reflected back onto the upper terrace and is probabilistically prevented from reaching the top of the step edge. If it is already at the step edge, it may, however, go down and attach itself to the descending step without encountering any additional barrier. In the edge barrier case, there is a barrier for the atom to go down to the step edge, but there is no barrier to reach the top of the down-step (the ES bias only hinders it from going down once it is already at the top of the step). Both of these ways of incorporating ES barrier are simplifications of the realistic atomic potential near terrace edges [52] which have been calculated in a few cases. The correct situation is a complicated combination of edge and reflection barriers, neither by itself is adequate. Comparing with the realistic surface potential contours [52], however, it is quite obvious that the edge barrier model is a much better representation of the actual ES bias than the reflection barrier model. For reasons not very clear to me, most of the numerical growth simulations [47,48] utilize the reflection barrier approach (and make additional assumptions regarding the nature of surface relaxation to obtain slope selection). I myself believe that the edge barrier model is better suited to study surface growth under an ES bias than the reflection barrier model. Below I discuss our recent results [43] for nonequilibrium surface growth under an edge surface diffusion bias.

I conclude by providing the results of some very recent numerical calculations [43] of the exponents $\beta$, $\lambda$, and $n$ in the nonequilibrium growth under an ES barrier in the $1 + 1$ and $2 + 1$ dimensional SOS growth model. Our finding [43] is that the growth exponent $\beta$ is $1/2$ for this problem (both in $d = 2 + 1$ and $1 + 1$ dimensions), independent of the strength of the ES edge barrier. It has earlier been pointed out [38,44–46] that for a strong ES barrier, the growth exponent tends toward $1/2$, but our new finding is that $\beta = 1/2$ always under an edge ES barrier, except the crossover time to observe this asymptotic $\beta(= 0.5)$ is extremely long for weak ES barriers which is why the existing ES barrier simulations have not always unambiguously observed.
this asymptotic regime. Note that $\beta = 1/2$ here does not imply uncorrelated random Poisson growth because $n = z^{-1} \approx 0.2 - 0.1$. The other question of considerable interest to both theory and experiment is the issue of slope selection in nonequilibrium growth under an ES barrier, i.e. whether $\lambda = 0$ (i.e. $\beta = n$) asymptotically in this growth problem, and some magic slope is selected by the mounds which does not change with time and remains fixed. We find that within an SOS model, there is no slope selection $\lambda \neq 0$ in the edge barrier model, and any experimental observation of slope selection must derive either from the physics of crystallographic orientations or from some other processes which are not essential ingredients of the ES barrier physics in the SOS model. My own belief is that, although slope selection may happen at extremely long times when the typical mound slope $m(t)$ is very large, it is not a generic phenomenon at small slopes. We find $\lambda \approx 0.2 - 0.4$, $n \approx 0.2 - 0.1$, and $\beta \approx 0.5$ in all our edge barrier simulations without encountering any slope selection in either $1 + 1$ or $2 + 1$ dimensions.

VII. CONCLUDING REMARKS

In this article I have provided a theoretical review from my own perspective of our current understanding of dynamic scaling in nonequilibrium epitaxial growth on flat singular substrates in the high symmetry directions. The underlying theme has been the successful application of the dynamic scaling hypothesis, defined by two independent critical exponents, to a wide variety of epitaxial growth phenomena. I have tried to emphasize how local discrete rules for deposition and relaxation under nonequilibrium conditions lead at large scales to complex growth morphologies which obey dynamic scaling according to coarse-grained continuum equations. The subject is vast and necessarily my perspective is based on the work I am most familiar with. The list of references is by no means comprehensive. The cited review articles [1, 3, 23] as well as refs. [4, 8] provide more references to the literature.
VIII. ACKNOWLEDGEMENT

I am most grateful to the United States Office of Naval Research for their steadfast support of my research in this area. In particular, I wish to take this opportunity to thank Dr. Larry Cooper (ONR) for sponsoring my research on MBE growth.
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