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Kinetic Roughening in Molecular-Beam Epitaxy

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Abstract. Under certain conditions, kinetic roughening in vacuum deposition experiments is believed to be in a dynamic universality class different from that of the Kardar-Parisi-Zhang family due to a conservation law. We discuss results of dynamic renormalization group calculations for the dynamic scaling in the hydrodynamic regime and for the crossover from the equilibrium sine-Gordon model below the thermal roughening temperature.

The roughening of a vacuum deposited film is not only a topic of great technological importance but also of intense theoretical interest[1]. Even in the case of homoepitaxy where no mismatch between the lattice constants of the substrate and the film is present, a theoretical understanding of the growth kinetics is only begin to emerge[2,3]. For stable two-dimensional growth the driving force for surface roughness is the fluctuation in the incoming flux of particles at any given part of the surface. It is evident that, while the surface is moving at a finite velocity, its ability to relax into thermal equilibrium configurations can be kinetically constrained. Computer simulations of simple lattice models have shown that instead a nonequilibrium steady-state can be reached which exhibits interesting scaling properties both in space and time. In particular, starting from a flat surface at $t = 0$, the width of a surface of linear size L satisfies the scaling form $w(t, L) = L^{\zeta}\Phi(t/L^{z})$, where ζ and z are known as roughness and dynamic exponents, respectively.

Given the fact that dynamical scaling exists, one would like to identify universality classes and to understand what are the crucial ingredients which specify a particular class. It has been realized that one of the important elements in this respect is volumn conservation. Specifically, if we denote $Z(\mathbf{x}, t)$ as the thickness of the film above a substrate site $\mathbf{x}$ at time t in a suitable coarse-grained sense, and F the external beam intensity, volumn conservation means

$$\partial Z/\partial t = -\Omega\nabla\cdot\mathbf{j} + F \tag{1}$$

where $\mathbf{j}$ is a particle number current density in the surface and Ω the atomic volumn of the diffusing species. Equation (1) is inconsistent with the Kardar-Parisi-Zhang equation[2] which is the generic description of kinetic roughening in the absence of the conservation law. It has been argued that, when molecular-beam epitaxy (MBE) is carried out at not too low and not too high temperatures, (e.g., between room temperature and $500°C$,) (1) is a relevant constraint on the relaxation dynamics[3].

Under Eq. (1), a complete description of the relaxational process involves identifying the driving force for the surface diffusion current $\mathbf{j}$. This problem has been considered in the classical capillary wave theory by Herring and by Mullins[4]. There $\mathbf{j}$ is assumed to be proportional to the surface gradient of the chemical potential which is in turn expressed in terms of the local curvature of the surface. Under the "shot noise", the resulting fourth order equation yields $\zeta = (4-d)/2$ and $z = 4$. Here d is the dimension of the surface. In general, however, there is no need for the surface to

follow the dynamics derived from equilibrium thermodynamics when particles are added constantly to the surface. In fact, one can add new terms to the linear equation which maintain the conserving form of (1) but produce more efficient relaxation of surface fluctuations. One such equation was proposed by Villain[3] for MBE,

$$\partial Z/\partial t = -\gamma \nabla^4 Z + \frac{\sigma}{2}\nabla^2(\nabla Z)^2 + F_0 + \eta, \tag{2}$$

where we have split F into a constant part F_0 and a gaussian noise η. We[5], and independently Lai and Das Sarma[6], have performed one-loop dynamic renormalization group analysis of (2), and obtained exponents $\zeta = (4-d)/3$ and $z = (8+d)/3$ as conjectured by Villain[3].

In the dimension of physical interest, $d = 2$, the above nonlinear theory predicts $\zeta = 2/3$ while experimentally it is possible to achieve layer-by-layer growth at sufficiently high substrate temperatures, in which case the surface roughness is essentially absent. This raises the question concerning the applicability of hydrodynamic theories such as (2) on length and time scales of experimental interest. In the regime where the layer structure of the film can be identified, it appears sensible to consider the lattice discreteness effect on the surface dynamics. We have therefore generalized the Villain equation (2) to include a periodic term,

$$\partial Z/\partial t = -\gamma \nabla^4 Z + \frac{\sigma}{2}\nabla^2(\nabla Z)^2 + v\nabla^2 \sin(2\pi Z/a) + F_0 + \eta. \tag{3}$$

In addition, to take into account the stochastic nature of surface diffusion on the atomic scale, we have included in η a conserving component. From a scaling analysis we found that, while the nonconserving component arising from the beam fluctuation always dominates the conserving one on sufficiently large length scales and leads to the roughening of the surface at any temperature, the conserving component can be dominant on short length scales when surface diffusion is fast. In the latter case, flat areas (or terraces) of limited size can exist if the surface is below the equilibrium roughening temperature. The relevant length scale separating the two regimes as well as the crossover behavior can be discussed quantitatively in a renormalization group treatment of (3) [5].

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