Comment on "Transient Evolution of Surface Roughness on Patterned GaAs(001) During Homoepitaxial Growth"

Kan *et al.* [1] recently published intriguing experimental evidence that patterned GaAs surfaces are subject to a nonmonotonic amplitude decay during epitaxial growth. They compared the temporal evolution of their surface shapes with calculations based on four continuum growth models, including the Kardar-Parisi-Zhang (KPZ) equation, and found that none of them could reproduce the amplitude evolution, nor the shape of the experimental surfaces. We do not agree with their attempt to extend these conclusions to the much lower amplitude morphology ($\lesssim 3°$ surface slope) that we studied earlier, in which KPZ behavior was observed [2].

The continuum growth equations considered by Kan are asymptotic models, applicable for long times and low surface slopes ($\nabla h \ll 1$), and not for corrugated surfaces with steep slopes, like those considered in Kan's Letter. The KPZ model attempts to capture the spatio-temporal evolution of low-amplitude surfaces to lowest order in the surface gradient. Often cited objections to KPZ include (a) its lack of mass-conservation (of minute influence in the low-amplitude regime, as discussed in detail in Ref. [2]), and (b) the justification of the nonlinear term as being due to normal growth, an unphysical scenario in molecular-beam epitaxy (MBE) growth. However, the nonlinear term could be due to a different physical mechanism, for example, the lateral attachment of adatoms at step edges. Although the physical origin of the nonlinear term is not clear, Ref. [2] provides sound experimental and computational evidence that KPZ provides an accurate description of the low-amplitude surface morphological evolution for GaAs. As Kan points out, a more fruitful approach would be to develop "an atomic model based upon physical processes." Such a model should describe the surface evolution for large ∇h, and reduce to the KPZ model in the long-wavelength, low-amplitude regime.

We have recently developed such a model [3]. Adatoms, with density n, are deposited at a rate F; they diffuse randomly until they nucleate as dimers ($\sim Dn^2$), attach to a step at rate $\sim Dn$, or release from a step edge at rate κ. The interaction between surface adatoms and the surface with height h is described by

$$\partial_t n + \nabla \cdot \mathbf{j} = F - \partial_t h, \quad (1a)$$

$$\partial_t h = 2Dn^2 + (Dn - \kappa)S, \quad (1b)$$

where the adatom current in Eq. (1a) is written as: $\mathbf{j} = -D(\zeta n \nabla h + \nabla n)$, where the first term describes the net downhill flow of adatoms over steps, and the second term describes surface diffusion. The step density S is defined as the incoherent sum of the thermally generated steps S_0 and the steps associated with macroscopic topography as

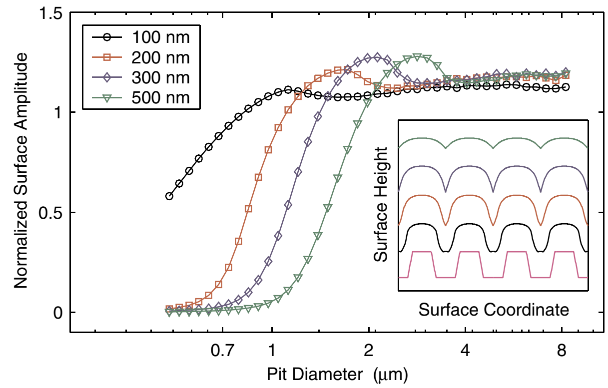

FIG. 1 (color online). Evolution of pit amplitude and surface shape (inset), for the film thicknesses indicated in the legend. The pitch and initial height in the inset is 2.8 μm and 50 nm, respectively. All offsets arbitrary.

$S = \sqrt{S_0^2 + (\nabla h)^2}$. A positive value for the downhill drift term ζ is consistent with a negative Ehrlich-Schwoebel barrier at the descending steps, although other mechanisms are possible.

Applying this model to starting surfaces similar to those used by Kan *et al.*, with the same growth rate and temperature, and parameters like those outlined in Ref. [3], we have reproduced Kan's amplitude overshoot [Fig. 1 and Kan's Fig. 2(a)], as well as the surface shape evolution to a high degree of accuracy [inset in Fig. 1 and Kan's Fig. 1(e)]. Our model shows KPZ behavior in the low-amplitude limit, as shown in the top curve in the inset. The surface profiles shown in the inset in the figure suggest an explanation for the nonmonotonic decrease in surface amplitude. The sidewalls expand laterally, which means that they grow faster vertically than the ridge tops and valleys. This is due to adatom attachment at the high density of steps on the sidewalls. As the width of the valley shrinks, the adatoms in the valley have a higher probability of migrating to the sidewalls than the adatoms that are deposited on top of the ridges which are now wider. This means the ridge tops grow faster than the valley bottoms, leading to a net increase in peak amplitude, as observed experimentally by Kan *et al.*

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