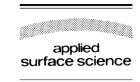


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Decay of silicon mounds: scaling laws and description with continuum step parameters

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Abstract

The decay of mounds about a dozen layers high on the Si(1 1 1)7 \times 7 surface [Surf. Sci. Rep. 34 (1999) 171] has been measured quantitatively by scanning tunneling microscopy and compared with analytic predictions for the power-law dependence on time predicted for a step-mediated decay mechanism [Mater. Res. Soc. Symp. Proc. 528 (1998) 237]. In accordance with these predictions, we find [Phys. Rev. Lett. 84 (2000) 3662] an exponent 1/4 associated with the (3D) decay of the mound height and exponent 1/3 associated with the (2D) decay of top-layer islands, appropriate to diffusion-limited behavior. The detailed effects of atomic-scale behavior at the step edges enter as the product of step stiffness and mobility; the measured value is consistent with earlier observations [http://www] of decay of single-layer structures. Using parameters from a continuum step model [Phys. Rev. Lett. 80 (1998) 552], we capture the essence of the kinetics. Qualitative features distinguish these mounds from multi-layer islands found on metals such as Cu(1 1 1). © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Silicon mounds; Continuum step model; Diffusion limited behavior

The continuum step model has proved a very fruitful approach to studying complex morphology on surfaces. In this perspective, a continuum approximation is made along the mean direction of the step, which allows the fluctuations of each step to be characterized by a single parameter, the stiffness. The steps are still treated as discrete entities, and their interactions are gauged by a second parameter, which

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gives the strength of the inverse-square (in step separation) repulsion that characterizes both the entropic and the elastic or dipolar repulsion between steps. A third coarse-scale parameter describes the atomic process that dominates the motion of the steps; it can either be a kinetic parameter or a combination of carrier density and the associated diffusion constant. The best test of this approach is not whether one can deduce these numbers from microscopic measurements or calculations of the key energies, whatever they may be, but rather whether the same set of mesoscale parameters can account for a broad range of seemingly disparate step phenomena. This viewpoint has been expounded often before [1,2].

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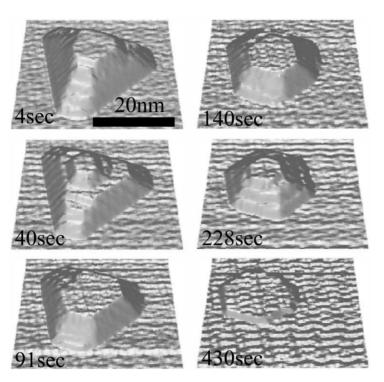


Fig. 1. STM "snapshots" of the decay of a typical nanomound studied on Si(1 1 1). The height is enhanced for clarity; the initial height is about 4 nm.

In this spirit, we have investigated the decay of nanoscale mounds of Si on Si(1 1 1) using scanning tunneling microscopy. The investigation is recounted in a recent letter [3], their results of which we summarize here. Sample still photos (not included in that letter) are given in Fig. 1, and a Quicktime[®] movie can be viewed on the web [4]. The islands are seen to decay layer by layer, with the top layer decaying most rapidly. Each STM image is obtained from (about 15) constant-height contour plots, from which the area of each layer (and the number of atoms in it) can be extracted. The hexagonal base is nearly triangular initially but becomes nearly equilateral at late times. At intermediate times, upper layers may form multilayer "hillocks" that have one side in close to the next lower layer, presumably to gain energy associated with the side facet orientation. This quantitative information is displayed for a particular case in Fig. 2 of Ref. [3]. The area of each layer decays essentially monotonically; an exception is that when a layer is the second highest, it has a brief increase just as the top

layer is extinguished. This behavior is quite different from the avalanche behavior found for metal mounds on metal (in particular, Cu(1 1 1) [5]) surfaces.

Quantitative investigations of mound decay on semiconductors heretofore have involved structures of a much larger scale. A particularly notable example was the study of the decay of micrometer-scale surface modulations on Si(1 0 0), which found the step crossing crucial to explain the details of the process [6]. In this investigation, we consider structures that are orders of magnitude smaller. Nonetheless, we find that the continuum step model provides a route to deal numerically with quantitative data and to gain a remarkable degree of understanding of the rate of nanomound decay.

As our theoretical models we use stacks of concentric circular "pucks"; a smooth envelope of simple analytic form describes the circle's height (relative to the apex) as a function of the radius. In the case of a conical envelope, this dependence is linear; this case is reminiscent of faceted sides. In the

other simple case of a parabolic envelope, the dependence is quadratic, indicative of rough sides. Most theoretical investigations focus on universal aspects of the decay of mounds, such as the exponent of the time dependence of the height, as a function of the mass-transport mode [7–9]. In [3] we tabulated the exponent associated with the time dependence of the decay of the radius of the top layer of the mound. Here we tabulate instead the exponent of the time dependence of the decay of the height. In the experiments, at three different temperatures (440, 465, and 485°C), this exponent is found to be 1/4 to within about 2%,

$$h_0 - h(t) = Bt^{1/4}$$

This exponent is the characteristic of an envelope with the shape of a cone rather than a paraboloid, but it does not clarify whether the dynamics are limited by kinetics or diffusion.

We next attempt to understand the prefactor B. We proceed by referring to earlier measurements of the decay of single-layer islands of Si on the same surface [10]. In that case the islands decayed at a rate of 3 atoms per second at 440°C, twice as fast as 465°C, and nearly twice again at 485°C. In the limit of kineticlimited behavior (called EC for evaporation-condensation or AD for attachment-detachment), this island decay rate is proportional to the kinetic coefficient times the stiffness divided by the thermal energy, so the measured island decay rate can be used to evaluate this combination. Furthermore, one finds that B^4 is proportional to this same combination, so that one can predict the value of B from the fourth root of the decay rate measured in the earlier experiment, presuming that the continuum step model is applicable. Remarkably, we find that the measured value of B in the current experiments is not quite twice as large as that predicted in the above way, i.e., semiquantitative agreement. In other words, the continuum step picture provides a viable way to study the decay of

Table 1 Exponent characterizing time dependence of the decay of the height of the mound, viz. the slope of $log(h_0 - h(t))$ vs. log t

Initial shape	Kinetics-limited	Diffusion-limited
Cone	1/4	1/4
Paraboloid	1/3	2/5

nanomounds that captures the essential physics of the problem (Table 1).

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