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Scaling properties of equilibrating semiconductor mounds of various initial shapes

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ABSTRACT

A surface below its roughening temperature consisting of two dimensional concentric circular monoatomic steps is discussed under step-flow model. Entropic interactions between the steps are considered and the diffusion equation is solved in two dimensional polar coordinates. It is assumed that the local mass transfer occurs due to surface diffusion only during the evolution of the initial surface. The evolution of initial surfaces bounded by both a sinusoidal and other envelope functions of the form x^{γ} are considered. The evolution of the height of surface as a function of time is analyzed for each surface in Diffusion Limited (DL) regime. We have determined three scaling characteristics of evolution of the height of the surface. For an initial sinusoidal surface profile we have the following findings: The height of surface approximately decreases as τ^{α} where α is independent of wavelength and initial height of the surface. The time dependence of the evolution of the height scales with the cube of the wavelength of the initial surface. Finally the normalized height of the initial surfaces of different amplitudes with the same wavelength scales linearly with the amplitude as a function of time. Similar findings are obtained for non-sinusoidal initial surfaces also.

1. Introduction

The growth of crystal surfaces and their evolution to their final equilibrium shape is important for technological reasons. Steps have important roles in crystal growth and in attaining the final equilibrium shape of crystal surface. For a surface consisting of steps separated by terraces, these processes occur only by the motion of steps on the surface. The motion of steps takes place through the attachment/detachment of particles to/from the step edges. The motion of steps at crystal surfaces were first studied by Burton et al. [1]. In their paper they considered a surface consisting of monoatomic steps separated by terraces and investigated the evolution of such a surface when the mechanism of particle transfer was surface diffusion. An initial surface shape which is studied extensively is a surface consisting of concentric circular monoatomic steps separated by terraces [2–12]. Israeli and Kandel [4,5] studied the equilibration of an initial surface which has a regular cone structure. They have considered the interaction between steps and studied the evolution of the initial surface in the Diffusion Limited (DL) and Attachment-Detachment Limited (ADL) regimes. Ichimiya et al. [7] studied the decay of silicon mounds experimentally. They found that the height of the mound decreases as $t^{1/4}$ or $t^{2/5}$ depending on the geometry of mound studied in DL case.

The atomic bonding and kink energy parameters, the orientation of the solid under consideration, the mass distribution on the surface (steps, clusters, etc.) and the temperature are the main parameters of the problem that determines whether the crystal evolves in DL, ADL or in a combination of both regimes. For example, Kodambaka et al. [8] have presented the result of in situ high-temperature (1550–1700 K) low-energy electron microscopy measurements of the coarsening/decay kinetics of concentrically stacked two-dimensional (2D) TiN adatom islands on TiN(1 1 1) terraces. They have determined that TiN(1 1 1) steps exhibit repulsive step-step interactions and that the TiN(1 1 1) mounds decay via surface mass tranport in the detachment-limited regime. They have also studied the coarsening/decay kinetics of 2D TiN adatom islands on TiN(0 0 1) terraces in high-temperature (1023–1223 K) range using scanning tunneling microscopy [9]. They found, among others, that island coarsening/decay depend on local environment and model their experimental results in a diffusion-limited island decay kinetics using steady-state diffusion equations. However, when the decay kinetics of two-dimensional TiN adatom and

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vacancy islands on atomically smooth TiN(1 1 1) terraces is investigated [10], they found size dependent island decay in the detachment-limited kinetics regime. In another study on copper surfaces, Schulze Icking-Konert et al. [11] investigated the decay of Cu adatom islands on Cu(1 1 1) as a function of temperature using scanning tunneling microscopy. By comparing the experimental results with the theory of Ostwald ripening and with numerical simulations they have found that the decay is limited by the diffusion of adatoms on the terrace.

In this study, the evolution of a surface below its roughening temperature consisting of two dimensional concentric circular steps is discussed. The existence of steps on the surface affects significantly the morphological evolution of the surface. The driving force for the evolution of surface morphology is the tendency of surface to decrease its free energy. In our study two distinct initial surfaces are considered: a surface consisting of concentric circles whose edges coincide with a sinusoidal envelope function and that of envelope functions which deviate from a regular cone either with a positive or negative curvature. Here we mainly concentrate on the variation of the height of the surface as a function of time during the evolution of the surface under consideration in Diffusion Limited (DL) regime only. Entropic interactions between the steps are considered and it is assumed that the local mass transfer occurs due to surface diffusion during the evolution of the initial surface. The diffusion equation is solved in two dimensional polar coordinates, and then an equation of motion for the radius of each circular step is written down and these coupled equations are solved numerically.

There are three main findings of the present study and they can be summarized as follows: First, it is found that the height of the surfaces considered in the present study approximately decreases as τ^{α} where α depends on the functional shape of the initial surface but is independent of wavelength for periodic surfaces. Second, for sinusodial surfaces the variation of the height of the surface scales with the cube of the wavelength of the initial surface. Similar behavior is found for non-sinusoidal surfaces where the details are presented in Section 3. Finally the normalized height of the initial sinusoidal surfaces of different amplitudes with the same wavelength scales linearly with the amplitude as a function of time.

The organization of the paper is as follows: In Section 2 a brief account of solution of diffusion equation and derivation of differential equations for the radius of each circular step is given. Section 3 is devoted to the main results of the study and their discussions. Our conclusions are provided in Section 4.

2. Theory

In this work, we consider a surface consisting of monoatomic height concentric circular steps. The number of steps on the surface is finite. The concentric circular steps with radius $r_i(t)$ are separated by flat terraces as shown in top panel of Fig. 1. The ith terrace is bounded from above and from below by steps i and $i+1$, respectively. The evolution of the surface takes place by the motion of steps by attachment/detachment of particles to/from step edges.

The diffusion equation for atom concentration ($C_i(\vec{r})$) on ith terrace in the absence of any flux to the surface can be written as

$$D_s \nabla^2 C_i(\vec{r}) = \frac{\partial C_i(\vec{r})}{\partial t} \tag{1}$$

where D_s is the surface diffusion constant and no particle desorption from the surface is allowed. At steady state the diffusion equation becomes [5]

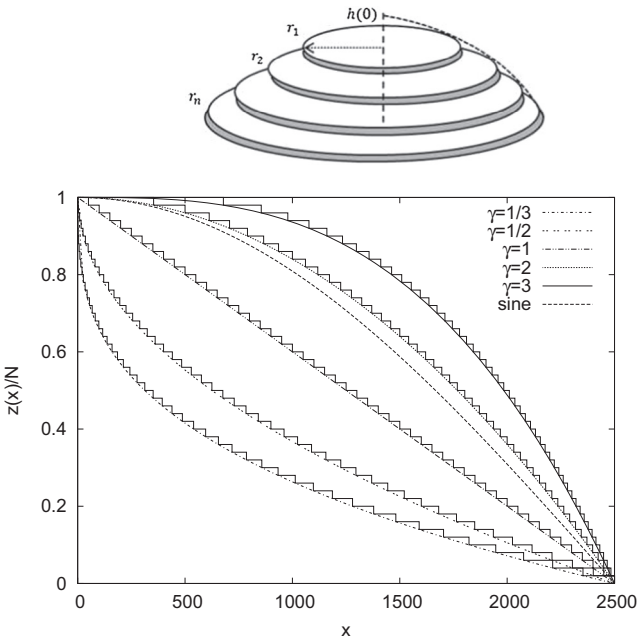

Fig. 1. Side view of various initial surfaces whose height is normalized. Except the sinusoidal surface of wavelength λ and amplitude A_0 (dashed lines), the other surfaces are of the form $z(x) = h(0) - ax^{\gamma}$ where $h(0)$ is the initial height of the surface. γ values considered in this study are as follows: 1/3, 1/2, 1, 2 and 3. The top panel shows the top of an arbitrary initial surface where the surface consists of monoatomic circular steps of radius r_i separated by terraces. All lengths are in units of a lattice constant a_0. In the present figure the following values are used: $N = A_0 = h(0) = 50$, $\lambda = 10000$ and $a = 3.68, 1, 2\times10^{-2}, 8\times10^{-6}, 32\times10^{-10}$ for γ values 1/3, 1/2, 1, 2 and 3 respectively.

$$\frac{\partial^2 C_i(\vec{r})}{\partial r^2} + \frac{1}{r}\frac{\partial C_i(\vec{r})}{\partial r} = 0 \tag{2}$$

The general solution of this equation is given as follows

$$C_i(\vec{r}) = A_i \ln r + B_i \tag{3}$$

where A_i and B_i are arbitrary constants to be determined by using appropriate boundary conditions described at the step edges. These conditions for the ith terrace can be written by assuming first-order kinetics as

$$D_s \left.\frac{\partial C_i}{\partial r}\right|_{r_i} = k\left[C_i|_{r_i} - C_i^{eq}\right] \tag{4}$$

$$-D_s \left.\frac{\partial C_i}{\partial r}\right|_{r_{i+1}} = k\left[C_i|_{r_{i+1}} - C_{i+1}^{eq}\right] \tag{5}$$

k is the attachment-detachment coefficient and C_i^{eq} is the equilibrium concentration of atoms on the terrace adjacent to the ith step. The up and down-step attachment-detachment coefficients are assumed to be the same. Using these boundary conditions, A_i is obtained as follows

$$A_i = \frac{C_i^{eq} - C_{i+1}^{eq}}{\ln\frac{r_i}{r_{i+1}} - \frac{D_s}{k}\left(\frac{1}{r_i} + \frac{1}{r_{i+1}}\right)} \tag{6}$$

Using mass conservation at the step edge, the velocity of the step can be written as

$$\frac{dr_i}{dt} = \Omega D_s \left(\frac{\partial C_i}{\partial r} - \frac{\partial C_{i-1}}{\partial r}\right)\Big|_{r_i} = \Omega D_s \frac{A_i - A_{i-1}}{r_i} \tag{7}$$

Ω is the area occupied by an atom on the surface. Due to the Gibbs-Thompson relation C_i^{eq} is given by