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Analyzing of the Evolution and the Scaling Properties of a Sinusoidal Mound

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ABSTRACT

The evolution of an initial surface (below its roughening temperature) bounded by a sinusoidal function and consisting of concentric circular steps in two dimensions has been investigated in the Diffusion Limited (DL) regime. Assuming that there were entropic interactions between steps and the local mass transfer took place due to the surface diffusion, the solution of the diffusion equation has been obtained by using polar coordinates in two dimensions. The results obtained in this investigation with analyzing the surface height's evolution as a function of time are as follows: The surface's height approximately decreases as τ^{α} $(\alpha \approx 0.35)$ and α is independent of the amplitude and the wavelength of the initial surface. The variations in the heights of the surfaces which have different amplitudes (A_{01}, A_{02}) and wavelengths (λ_1, λ_2) scale as $(A_{01}/A_{02})(\lambda_1/\lambda_2)^3$.

Keywords: Mass transfer, Surface structure, Surface processes, Diffusion limited regime.

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Introduction

Knowing the morphological structures of semiconductor crystal surfaces and how they reach their equilibrium surface structures are issues that need to be emphasized in terms of designing and fabricating new semiconductor devices. The dynamics in the surface's evolution to equilibrium structure provide us detailed information about the surface's structure and the driving forces that enable the surface to reach its equilibrium structure. Monatomic steps which have terraces between them are observed on the surfaces under their roughening temperature. The events in the growth and reaching the equilibrium shape of a crystal take place through monatomic steps and the existence of steps on the surface affects significantly the morphological evolution of the surface. The evolution of surface morphology occurs due to the tendency to decrease the free energy of the surface.

There are lots of theoretical and experimental works done from past to present about decaying of crystalline surfaces. Rettori and Villain [1] have studied on a crystal surface below its roughening temperature and examined the decaying of a profile produced artificially. Uwaha [2] investigated the relaxation of crystal shapes caused by step movement. The flattening of a corrugated crystal surface which has monoatomic steps where mass transport occurs by surface diffusion has been studied by Ozdemir and Zangwill [3]. In their study where they explained the morphological changes of the gratings with annealing, Umbach et al. [4] have studied on atomic step arrays on Si(001) using scanning tunneling microscope. Israeli and Kandel [5] have examined a cone surface's equilibration which has a regular shape for Diffusion Limited (DL) and Attachment-Detachment Limited (ADL) regimes. Ichimiya et al. [6] have studied the silicon mounds' decay experimentally in the DL regime and determined that the mound's height decreases as a function of time as $t^{1/4}$ or $t^{2/5}$. In another study the decay characteristics of three-dimensional (3D) islands have been examined theoretically by Li et al. [7]. Kodambaka et al [8, 9] presented the coarsening/decay kinetics of 2D TiN adatom islands in their experimental works. Kellogg and Bartelt [10] have investigated the island decay on Rh(001) surface using low-energy electron microscopy. Esen et al. [11] put forth a study about the equilibration of a conic shaped surface using the Kinetic Monte Carlo method. In Diffusion Limited (DL) regime, the different shaped surfaces owned circular monoatomic steps have been examined by Tüzemen et al. [12]. They have assumed that there were only repulsive interactions between the steps. They found that the scaling characteristics of the surfaces' height variations. In addition, they determined that the surfaces' heights characteristically decreased with τ^{α} $(\alpha \approx 0.36$ for the sinusoidal surface they dealt with) in time. Moreover, Tüzemen et al. [13] have investigated the morphology of a conic shaped initial surface in two dimensions in DL regime. They have included the repulsive interaction as well as the attractive interaction between steps in their calculations. The surface's height evolution and morphology have been studied in the presence of only repulsive interactions and both attractive and repulsive interactions between steps.

In this work, the evolution of an initial surface (below its roughening temperature) which consists of concentric circular steps in two dimensions and whose edge structure coincide with a sinusoidal function has been investigated. In our investigation, we examined the changes in interested surfaces' heights as a function of time during the surface's evolution for only Diffusion Limited (DL) regime. It was supposed that the local mass transfer takes place because of the surface diffusion while the initial surface's evolution happens. In addition, it was considered that there are entropic interactions between steps on the surface. With these admissions, the diffusion equation

has been solved in two dimensions by using polar coordinates and an equation of motion for each circular step's radius was obtained. Later the solution of these coupled equations was achieved numerically. The organization of the work is as follows: the definitions and the problem's theoretical solution are given in section 2, in section 3 obtained numerical results and their discussions are presented and in the section 4 conclusions are given.

Theory

In this study, an initial surface which consisting of concentric circular steps owned monoatomic height is examined. There are finite number of steps on the surface. The flat terraces separate these steps, as shown in Figure 1. The borders of i^{th} terrace are i and $i+1$ from above and below respectively. The surface's evolution occurs by the steps' motion by attachment (detachment) of particles to (from) step edges. In the case of no flux to the surface, the diffusion equation for i^{th} terrace atom concentration can be given as follows,

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

Here D_s represents the surface diffusion constant. There isn't any desorption from the surface. The steady state diffusion equation is written as [5]

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

The solution of Eqn. (2) is $C_i(\vec{r}) = A_i \ln r + B_i$. The arbitrary constants A_i and B_i are calculated by using suitable boundary conditions which are defined at the step edges and given as below,

$$D_s \frac{\partial C_i}{\partial r}\Big|_{r_i} = k\left[C_i|_{r_i} - C_i^{eq}\right] \quad (3)$$
$$-D_s \frac{\partial C_i}{\partial r}\Big|_{r_{i+1}} = k\left[C_i|_{r_{i+1}} - C_{i+1}^{eq}\right]$$

while k shows the attachment/detachment coefficient (it is assumed that attachment/detachment coefficients belonging to the up and down steps have the same value) and C_i^{eq} expresses the value of atoms' equilibrium concentration on the adjacent terrace to the i^{th} step.

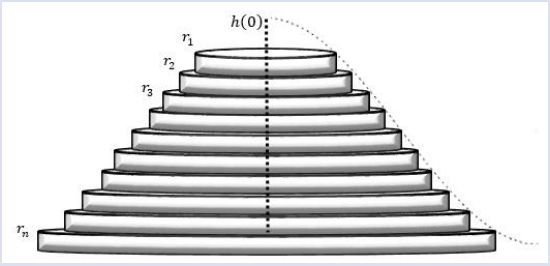

Figure 1. The initial surface consists of monoatomic circular steps with radii $r_1, r_2, r_3, \ldots\ldots r_n$ of separated by terraces and $h(0)$ shows the extrapolated initial surface height. The shape of the sinusoidal function in which the edge structure is coincident is also given with dashed lines.

The expressions of the arbitrary constant A_i and the step's velocity can be given as follows by using boundary conditions in Eqn. (3) and conservation of mass at the step edge respectively,

$$A_i = \frac{c_i^{eq} - C_{i+1}^{eq}}{ln\frac{r_i}{r_{i+1}} - \frac{D_S}{k}\left(\frac{1}{r_i} + \frac{1}{r_{i+1}}\right)} \quad (4)$$

$$\frac{dr_i}{dt} = \Omega D_s \left(\frac{\partial C_i}{\partial r} - \frac{\partial C_{i-1}}{\partial r}\right)\Big|_{r_i} = \Omega D_s \frac{A_i - A_{i-1}}{r_i} \quad (5)$$

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

$$C_i^{eq} = \bar{C}^{eq} exp\left(\frac{\mu_i}{T}\right) \approx \bar{C}^{eq}\left(1 + \frac{\mu_i}{T}\right) \quad (6)$$

Boltzman's constant is used as 1 in the calculation because of the used units. The step chemical potential (μ_i) which is dependent on entropic [14] and elastic [15,16] interactions between the nearest neighbor steps with the island curvature can be approximately given as under the assumption that the distances between steps are smaller than the radii [5,17,18].

$$\mu_i = \frac{\Omega\Gamma}{r_i} + \Omega G\left(\frac{2r_{i+1}}{(r_{i+1}+r_i)}\frac{1}{(r_{i+1}-r_i)^3} - \frac{2r_{i-1}}{(r_i+r_{i-1})}\frac{1}{(r_i-r_{i-1})^3}\right) \quad (7)$$

Here, while G shows the strength of the interaction between steps and Γ expresses the step line tension. The dimensionless expressions (ρ_i and τ) of the radii and time can be written as follows by using Ref. [5],

$$\rho_i = \frac{T}{\Omega\Gamma} r_i \quad (8)$$

$$\tau = D_s \bar{C}^{eq} \Omega \left(\frac{T}{\Omega\Gamma}\right)^2 \left(1 + \frac{D_S T}{k\Omega\Gamma}\right)^{-1} t \quad (9)$$

By using these expressions with the Eqns. (3)-(5), the equations of the steps' motion can be obtained as below.

$$\dot{\rho}_\iota = \frac{d\rho_i}{d\tau} = \frac{a_i - a_{i-1}}{\rho_i} \quad (10)$$

The arbitrary constant a_i is given by

$$a_i = \frac{\varepsilon_i - \varepsilon_{i+1}}{(1-q)ln\frac{\rho_i}{\rho_{i+1}} - q\left(\frac{1}{\rho_i}+\frac{1}{\rho_{i+1}}\right)} \quad (11)$$

and ε_i is written as

$$\varepsilon_i = \frac{1}{\rho_i} + g\left(\frac{2\rho_{i+1}}{(\rho_{i+1}+\rho_i)}\frac{1}{(\rho_{i+1}-\rho_i)^3} - \frac{2\rho_{i-1}}{(\rho_i+\rho_{i-1})}\frac{1}{(\rho_i-\rho_{i-1})^3}\right) \quad (12)$$

where g measures G relative to Γ and equals to $(T^2G/\Omega^2\,\Gamma^3)$. If the constant a_i is analyzed, it can be easily seen that it depends on q and g. The parameter q determines the surface evolution regime. In the case of $q = 0$, the evolution of the surface comes true in the Diffusion Limited (DL) regime. On the other hand, the surface evolves in the Attachment/Detachment Limited (ADL) regime for $q = 1$.

Results and Discussion

In this work, We consider an initial surface which consists of monoatomic circular steps of separated by flat terraces and whose edge structure coincide with a sinusoidal function in the form of $A_0 \sin(2\pi x/\lambda)$ and investigate its approach to equilibrium in time. A_0 and λ are the amplitude and the wavelength of the sinusoidal surface respectively. The side view of this surface is shown in Figure 2. During the investigation, we have studied the evolutions of the initial surfaces only in the Diffusion Limited regime ($q = 0$ in Eqn. (11)). The cases in which the initial surfaces' evolutions take place in the Attachment/Detachment Limited regime ($q = 1$) have not been examined.

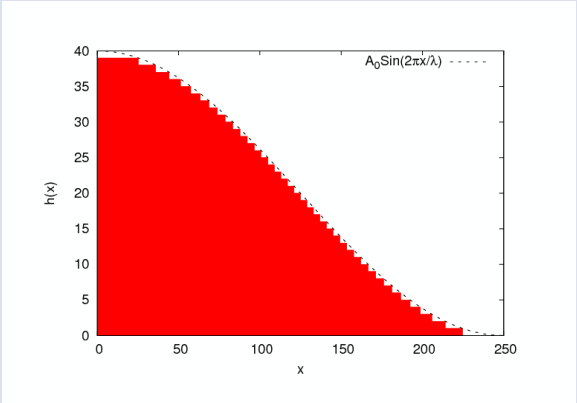

Figure 2. An example of investigated surface which has a sine structure. The units of all used lengths are a lattice constant a_0.

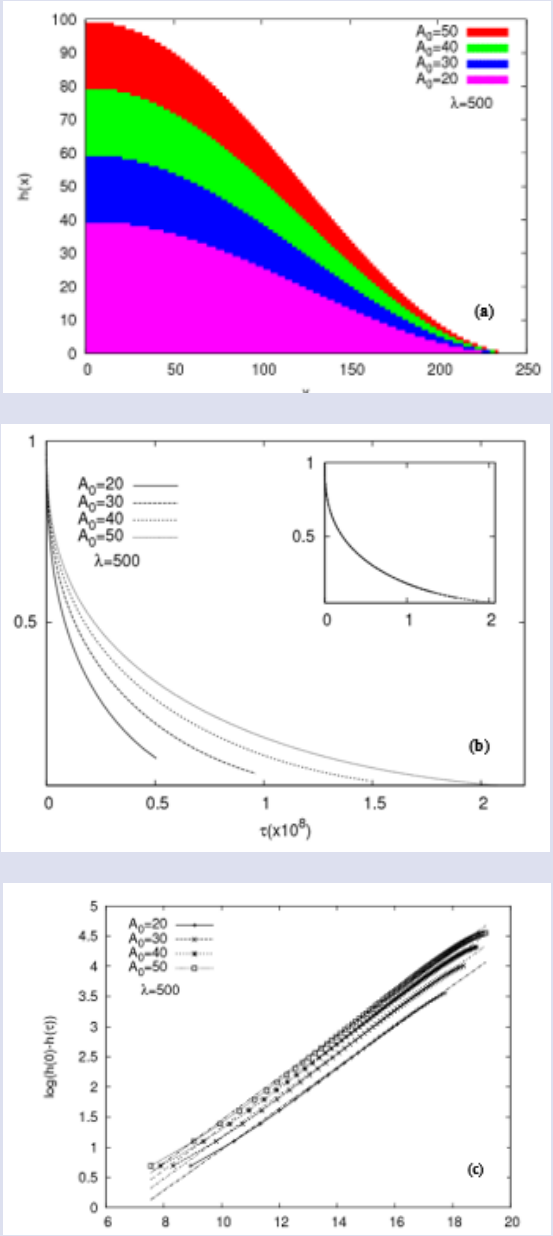

Figure 3. (a) The initial surfaces which have the same wavelength $(\lambda = 500)$ and different amplitudes $(A_0 = 20, 30, 40, 50)$ (b) The variations in the surface's scaled heights as a function of time for the initial surfaces defined in (a). The inset gives the scaling relation in the surface's height with respect to scaled time. All curves are scaled with respect to the curve with $A_0 = 50$. Scaling parameter is given by $\beta' = (A_{01}/A_{02})$. The scaling factors are given as follows $(5/2)$ $(5/3)$, $(5/4)$ and 1 for the amplitudes of the initial surfaces $A_0 = 20, 30, 40$ and 50 respectively, (c) The $log\big(h(0) - h(\tau)\big) - log(\tau)$ plots of the initial surfaces given in (a). The slope values (α) of all curves are equal and nearly 0.35.

Firstly, we considered the initial surfaces that have the same wavelength $(\lambda = 500)$ and different amplitudes (as 20, 30, 40 and 50). The number of steps on these initial surfaces

were $40, 60, 80$ and 100 (shown in Figure 3a). The variations of these surfaces' heights as a function of time have been examined for $g = 10^{-6}$ (in Eqn. 12) firstly. When the evolution of studied surface starts, the radius of the top most step starts to reduce and it disappears from the surface after a while. The surface height also decreases with the disappearance of the topmost step. This phenomenon also applies to other steps. During these events, the particles continuously transfer from the disappeared step to other steps and they grow them. This process continues to take place until last few steps remain. The normalized height variation of the surface happens as given in Figure 3b in this case.

It can be easily seen that all surface heights decrease depending on time. The initial surface, which has the greater wavelength (more steps), needs more time to complete its evolution. The scaling here is related to the surfaces' normalized heights evolution in time forms with the amplitudes' ratios (the number of steps' ratios) of the initial surface.

$$h_{A_{01}}(\tau) = h_{A_{02}}(\beta\tau') \tag{13}$$

Here β equals the ratio A_{01}/A_{02}. The inset in Figure 3b shows the scaling behavior for two initial surfaces which have the same wavelength and different amplitudes. Other finding from this investigation is that the surface's height decreases as follows [19, 6]

$$h(0) - h(\tau) = k\tau^{\alpha} \tag{14}$$

$h(0)$ expresses the initial height of the surface and k is a constant. The $log\big(h(0) - h(\tau)\big) - log(\tau)$ plots of the initial surfaces given in Figure 3a are shown in Figure 3c. The slopes of all curves are obtained as approximately (independent of wavelength) $\alpha \approx 0.35$. The advantage of determining the form of the surface height decreases is that it gives us about the events (driving forces that cause events) took place during evolution. The driving forces which affect the evolution of the interested initial surfaces are the entropic interaction between the steps and the line tension due to the step curvature. The same results have been obtained for $g = 10^{-5}, 10^{-4}$ and 10^{-3} values under the same initial surface conditions.

In the second part, we examined the initial surfaces that have the same amplitude (number of steps) $(A_0 = 40)$ and the different wave lengths $(\lambda = 300, 400, 500, 600)$ (Figure 4a). The value of g was again taken as 10^{-6} firstly, when the heights' variations of the surfaces are investigated. Figure 4b shows the variations of the heights of the surfaces as a function of time. The surface which has the biggest wavelength completes its evolution in the longest time. The scaling of the curves belonging to the height variations is shown in the inset of Figure 4b. In this situation, the scaling happens with the cube of the ratio of the initial surfaces' wavelengths.

$$h_{\lambda_1}(\tau) = h_{\lambda_2}(\beta'\tau') \tag{15}$$

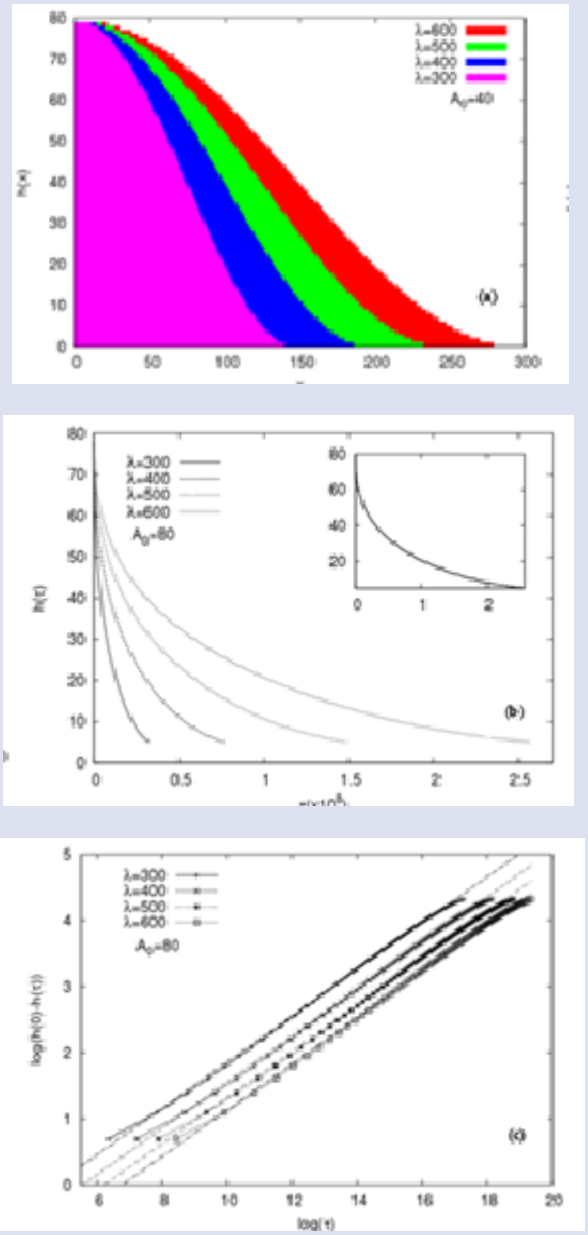

Figure 4. (a) The initial surfaces which have the same amplitude $(A_0 = 40)$ and different wavelengths $(\lambda = 300, 400, 500, 600)$ (b) The changes in the surface's scaled heights as a function of time for the initial surfaces defined in (a). The scaling relation between the surfaces' heights is given inset. All curves are scaled with respect to the curve with $\lambda = 600$. Scaling parameter is given by $\beta' = (\lambda_1/\lambda_2)^3$. The scaling factors are given as follows $(6/3)^3$, $(6/4)^3$, $(6/5)^3$ and 1 for the wavelengths of the initial surfaces $\lambda = 300, 400, 500$ and 600 respectively (c) The $log\big(h(0) - h(\tau)\big) - log(\tau)$ plots belonging the initial surfaces indicated in (a). The slope values (α) of all curves are approximately 0.35..

β' is equal to $(\lambda_1/\lambda_2)^3$. Figure 4c shows the $log\big(h(0)-h(\tau)\big)-log(\tau)$ curves for the cases examined in Figure 3b. The slope of all curves is $\alpha \approx 0.35$. In this part of the investigation, we acquired the same scaling behaviors and the α values for $g = 10^{-5}, 10^{-4}$ and 10^{-3} values under the same initial surface conditions. In our old study [12], we have examined a sinusoidal initial surface similar to the one studied here. Because of this, the scaling characteristics obtained in equations (13) and (15) are the same with found out ones in Ref. [12] as expected. While the slope of the $log\big(h(0)-h(\tau)\big)-log(\tau)$ curves belonging to the studied sinusoidal surfaces was found as $\alpha \approx 0.36$ in Ref. [12], it was found as $\alpha \approx 0.35$ for the sinusoidal surfaces studied here. The α values are close to each other due to the surface similarity.

In the last part of the study, we analyzed the initial surfaces which have different amplitudes and different wavelengths. While the amplitudes of the chosen initial surfaces are $20, 30, 40$ and 50, the wavelengths of these surfaces are $300, 400, 500$ and 600 respectively (shown in Figure 5a). Similarly, first of all we examined that how these surfaces' scaled heights vary as a function of time for $g = 10^{-6}$. The curves drawn for this investigation are given in Figure 5b. As a result, it has been found that the evolutions of the surfaces' normalized heights scales according to the following expression,

$$h_{A_{01},\lambda_1}(\tau) = h_{A_{02},\lambda_2}(\eta\tau') \qquad (16)$$

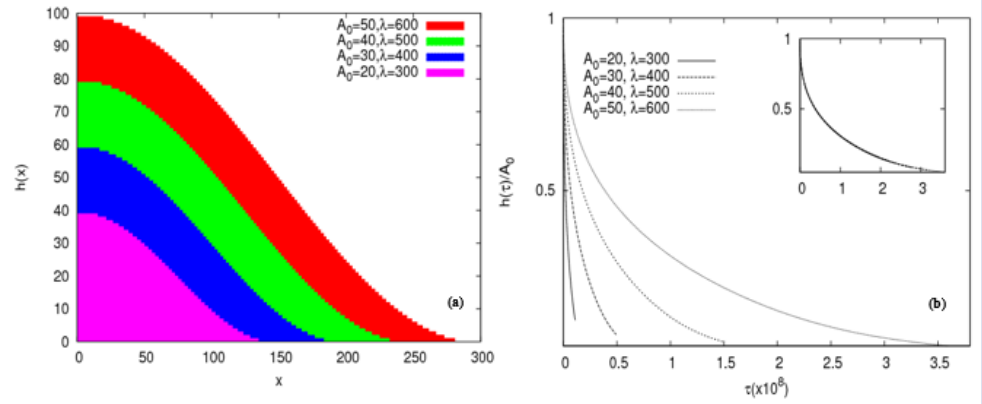

Figure 5. (a) The initial surfaces which have the different amplitudes $(A_0 = 20, 30, 40, 50)$ and wavelengths $(\lambda = 300, 400, 500, 600)$ (b) The changes in the surface's scaled heights as a function of time for the initial surfaces. The scaling behaviors of the surfaces' heights is given inset. All curves are scaled with respect to the curve with $A_0 = 50$ and $\lambda = 600$. Scaling parameter is given by $\eta = (A_{01}/A_{02})(\lambda_1/\lambda_2)^3$. The scaling factors are given as follows $(5/2)(6/3)^3$, $(5/3)(6/4)^3$, $(5/4)(6/5)^3$ and 1 for the amplitudes of the initial surfaces $A_0 = 20, 30, 40$ and 50 respectively.

Here, η is given by $\beta.\beta'$. So $\eta = \left(\frac{A_{01}}{A_{02}}\right)\left(\frac{\lambda_1}{\lambda_2}\right)^3$. The scaled curves are given in inset of Figure 5b. In addition, we plotted the $log\big(h(0)-h(\tau)\big)-log(\tau)$ plots of initial surfaces which are given in Figure 5a and determined that all obtained curves' slopes were $\alpha \approx 0.35$. Again, in the last part of the study, we determined that the scaling property and α value has not been changed in the cases of taking the values of g as $10^{-5}, 10^{-4}$ and 10^{-3}.

Although it is not shown here, the different initial surfaces (surfaces in the form of $z(x) = h(0) - ax^{\gamma}$ for the values of $\gamma = 1/3, 1/2, 1, 2, 3$) which have been discussed in our study [12] have been examined under the last investigation's conditions. When these initial surfaces had different numbers of steps (N) and the different intersection points (x_0) with the x axis (similar to the initial surfaces investigated in Figure 5), it has been determined that the scaling property of the changes of these surfaces' scaled heights as a function of time was similar to the expression given in eqn. (16). It can be written as follows,

$$h_{N_1,x_{01}}(\tau) = h_{N_2,x_{02}}(\eta'\tau') \qquad (17)$$

The value of η' has been found as $\left(\frac{N_1}{N_2}\right)\left(\frac{x_{01}}{x_{02}}\right)^3$ independent of the g value.

Conclusions

We examined the evolution of a sinusoidal initial surface (below its roughening temperature) in Diffusion Limited regime. The examined surface consists of concentric monoatomic circular steps in two dimensions separated by terraces. The diffusion equation has been solved in two dimensions by using polar coordinates and an equation of motion for each circular step's radius was obtained by assuming the line tension of steps and the entropic repulsion between neighboring steps. In this investigation, we obtained the results by analyzing the surface height's evolution as a function of time are as follows: The surface's height approximately decreases as τ^{α} $(\alpha \approx 0.35)$ and α is independent of the amplitude and the wavelength of the initial surface. The variations in the heights of the surfaces which have different amplitudes (A_{01}, A_{02}) and wavelengths (λ_1, λ_2) scale as $\left(\frac{A_{01}}{A_{02}}\right)\left(\frac{\lambda_1}{\lambda_2}\right)^3$. Moreover, we determined that obtained results were independent of the "g" value.

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Conflicts of interest

There are no conflicts of interest in this work.

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