

The Investigation of Bunching and No Bunching Regions of Sinusoidal Mounds

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ABSTRACT

We studied the evolution of an initial surface which was sinusoidal mound shaped for Diffusion Limited (DL) regime. We supposed that there were two dimensional concentric circular steps on initial surface and attractive/repulsive interactions between these monoatomic steps. While following the surface's evolution, the equation of motion related to each step radius's change and diffusion equation have been solved. We obtained bunching and no bunching regions of studied initial surfaces in a parameter space with their scaling characteristics. Our results in this examination can be summarized as; bunching (no bunching) region expands (shrinks) with increasing of wavelength or amplitude of the initial surface. The curves separating bunching/no bunching regions scale with each other. In the case of the amplitude (wavelength) is changed, the scaling factor is $(A_0/A'_0)^{1/6} ((\lambda/\lambda')^{1/2})$. When both the wavelength and amplitude of the surface are changed at the same time, the scaling factor is equal to $(A_0/A'_0)^{1/6} \times (\lambda/\lambda')^{1/2}$.

Keywords: Diffusion, Surface structure, Semiconducting Materials, Step Bunching.

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Introduction

Studies on crystal morphology, which provides information about the structural properties and growth mechanisms of various materials, have long been an interesting field in material science. Crystal morphology is also important for understanding the complex dynamics of mass transfer, surface structure and surface processes. Vicinal surfaces are characterized by a conscious deviation from the crystallographic orientation and they play an important role in understanding surface dynamics with growth kinetics [1-7]. This deviation causes the formation of step bunches that affects the surface roughness and morphology. Vicinal surfaces consist of steps and terraces under their roughening temperature. We have to know the interaction type between these steps to understand surface dynamics. There are repulsive and attractive interactions between steps on the surface [8-12]. The repulsive interaction which arises from the elastic [13-15] or entropic [16] interactions varies inversely with the square of the average step separation. It has been demonstrated through experimental studies that the attractive interaction is inversely proportional to the step separation [17-21]. This type of interaction appears from dipole-dipole interactions [22,23] or indirect electronic interactions [24,25]. Step bunching that occurs in semiconductor materials is significant because of its effects on device performance and fabrication [4,26-30]. Discovering the dynamics of step bunching and mound formation finds out the interplays between surface diffusion and adatom kinetics. The crystals can growth under different regimes like Diffusion-Limited (DL) and Attachment-Detachment-Limited (ADL) regimes. In DL regime, the growth rate is determined by the mass

transport rate. On the other hand, atoms' attachment/detachment at/from the surface direct the growth kinetics in the ADL regime. Particularly, DL regime governs the evolutions of step bunches and the semiconductor mounds. A lot of works have been done on the step bunching phenomenon from past to present. Some of the studies carried out in recent years are as follows; Siewierska and Tonchev [31] studied on the scaling of the minimum distance between consecutive two steps in the bunch. Sato [32] examined that how the surface diffusion field affects the growth law of the bunch size in the step bunching induced by immobile impurities. In the model they created Popova et al. [33] investigated step bunches on the surface of growing and sublimating crystals and showed that the overall picture of the bunching process changes entirely when steps cannot overlap, thus forming macrosteps. In another study Popova [34] studied the effect of step-step exclusion on growing vicinal surfaces destabilized by a step-up (SU) or step-down (SD) driving force in Diffusion-Limited (DL) and Kinetics Limited (KL) growth regimes. In the presence of repulsive and attractive interactions between steps, Tüzemen et al. [35] searched a surface which consists of two dimensional concentric circular monoatomic steps in DL regime. They obtained a phase diagram separating the step bunching and no step bunching regions for the surface they examined. In addition, Tüzemen [36] investigated the bunching - no bunching regions for different initial surfaces consist of concentric circular monoatomic steps in a parameter space. He found out the scaling characteristics of these bunching/no bunching

regions under the effects of attractive and repulsive interactions between steps.

In this investigation, we studied a sinusoidal mound shaped initial surface in two dimensions for Diffusion Limited (DL) regime. We assumed that this surface had concentric circular steps with attractive and repulsive interactions between them. We determined bunching and no bunching regions of examined initial surfaces in a parameter space with their scaling features. To achieve our goals, we solved the diffusion equation and obtained an equation of motion regarding the change of radius of each circular step. After that we achieved the solution of these coupled equations numerically

Theory

We investigate that how an initial surface whose edge structure coincide with a sinusoidal function in the form of $A_0 \sin(2\pi x/\lambda)$ reaches to equilibrium situation in course of time in this study. The wavelength and amplitude variables that define sinusoidal surface structure are identified by λ and A_0 respectively. The working surface has monoatomic and concentric circular steps in two dimensions. There are flat terraces between consecutive two steps. Figure 1 shows the general structure and side view of the initial surface. The radii of the each circular steps are defined as r_1, r_2, r_3, \dots etc. in Figure 1. The movements of steps on the surface under roughening temperature provide the surface evolving. The mechanism that controls these movements is by the attachment and/or detachment of particles to/from step edges. In the absence of bulk diffusion or evaporation/condensation processes, local mass transfer takes place with surface diffusion. The borders belonging to i^{th} terrace are specified by i (from above) and $i + 1$ (from below). In the case where we assume that there is no flux to the surface, we can write the general diffusion and steady state diffusion equations for i^{th} terrace atom concentration in polar coordinates as follows respectively [37],

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

and

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

D_s is the surface diffusion constant. The solution of Eqn. (2) is given by $C_i(\vec{r}) = A_i \ln r + B_i$. We calculate the constant A_i in expression by doing mathematical solution details of which are given in Ref. [35].

$$A_i = \frac{C_i^{eq} - C_{i+1}^{eq}}{\ln \frac{r_i}{r_{i+1}} - \frac{D_s}{k} \left(\frac{1}{r_i} + \frac{1}{r_{i+1}} \right)} \tag{3}$$

C_i^{eq} defines the equilibrium concentration of atoms on the adjacent terrace to the i^{th} step. The value of C_i^{eq} (according to the Gibbs-Thompson relation) is given as,

$$C_i^{eq} = \bar{C}^{eq} \exp\left(\frac{\mu_i}{T}\right) \approx \bar{C}^{eq} \left(1 + \frac{\mu_i}{T}\right) \tag{4}$$

The value of Boltzman's constant is taken as 1 due to the used units in the calculations. μ_i indicates the step chemical potential written depending on the line tension, repulsive and attractive interactions between the nearest neighbor steps.

For ease of mathematical calculation we can write the equations of motion related with the change of radii of circular steps in dimensionless form. To do this we make the following definitions respectively [21,35,37]

$$\dot{\sigma}_i = \frac{d\sigma_i}{d\tau} = \frac{A'_i - A'_{i-1}}{\sigma_i} \tag{5}$$

Here σ and τ are the dimensionless radius and time. A'_i corresponds the dimensionless form of arbitrary constant A_i given in Eqn. (3). The expressions of σ, τ and A'_i can be written as,

$$\sigma_i = \frac{T}{\Omega \Gamma} r_i \tag{6}$$

$$\tau = D_s \bar{C}^{eq} \Omega \left(\frac{T}{\Omega \Gamma} \right)^2 \left(1 + \frac{D_s T}{k \Omega \Gamma} \right)^{-1} t \tag{7}$$

$$A'_i = \frac{\mu'_i - \mu'_{i+1}}{(1-q) \ln \frac{\sigma_i}{\sigma_{i+1}} - q \left(\frac{1}{\sigma_i} + \frac{1}{\sigma_{i+1}} \right)} \tag{8}$$

where $T, \Omega,$ and Γ express the absolute temperature value, the area owned of a diffusing particle and the steps' line tension respectively. The equilibrium value of particle concentration at the step edge is shown by \bar{C}^{eq} . k characterizes the step attachment/detachment coefficient. The q parameter in Eqn. (8) identifies in which regime the surface will evolve. When $q = 0$, the surface evolves in the DL regime. If $q = 1$, surface evolution regime is ADL. The value of chemical potential μ'_i obtained with dimensionless radii can be written as

$$\mu'_i = \frac{1}{\sigma_i} + \gamma \left[\left(\frac{2\sigma_{i+1}}{(\sigma_{i+1} + \sigma_i)(\sigma_{i+1} - \sigma_i)^3} - \frac{1}{2\sigma_{i-1}(\sigma_i + \sigma_{i-1})(\sigma_i - \sigma_{i-1})^3} \right) - \beta \left(\frac{\sigma_{i+1}}{(\sigma_{i+1} + \sigma_i)(\sigma_{i+1} - \sigma_i)^2} - \frac{\sigma_{i-1}}{(\sigma_i + \sigma_{i-1})(\sigma_i - \sigma_{i-1})^2} \right) \right] \tag{9}$$

The first term is the line tension, the second and the third terms are repulsive and attractive interactions between the nearest neighbor steps respectively. Dimensionless coefficients are $\gamma = (T^2 \gamma' / \Omega^2 \Gamma^3)$ and $\beta = (\Omega \Gamma / T) (\beta' / \gamma')$. γ' and β' indicates the repulsive and attractive interaction strengths respectively.

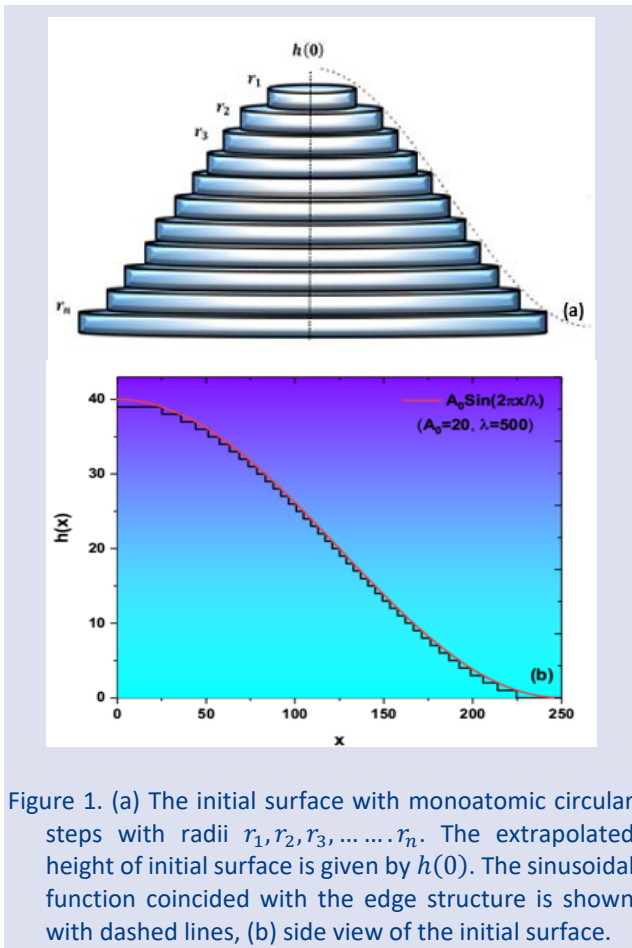


Figure 1. (a) The initial surface with monoatomic circular steps with radii $r_1, r_2, r_3, \dots, r_n$. The extrapolated height of initial surface is given by $h(0)$. The sinusoidal function coincided with the edge structure is shown with dashed lines, (b) side view of the initial surface.

Results and Discussion

For Diffusion Limited (DL) regime, we discussed initial surfaces which have sinusoidal shaped and its edge structures fit $A_0 \sin(2\pi x/\lambda)$ function in two dimensions. Initial surfaces have circular and concentric monoatomic steps. Surface evolution takes place by disappearing some top steps on the surface because of transferring particles on it to other terraces and steps. We investigated bunching/no bunching regions of different initial surface structures as a function of the repulsive and attractive interaction parameters γ and β by following the step bunchings formed throughout the surface evolution. We changed the values of the repulsive interaction parameter γ from 5×10^{-7} to 1×10^{-3} in all examinations.

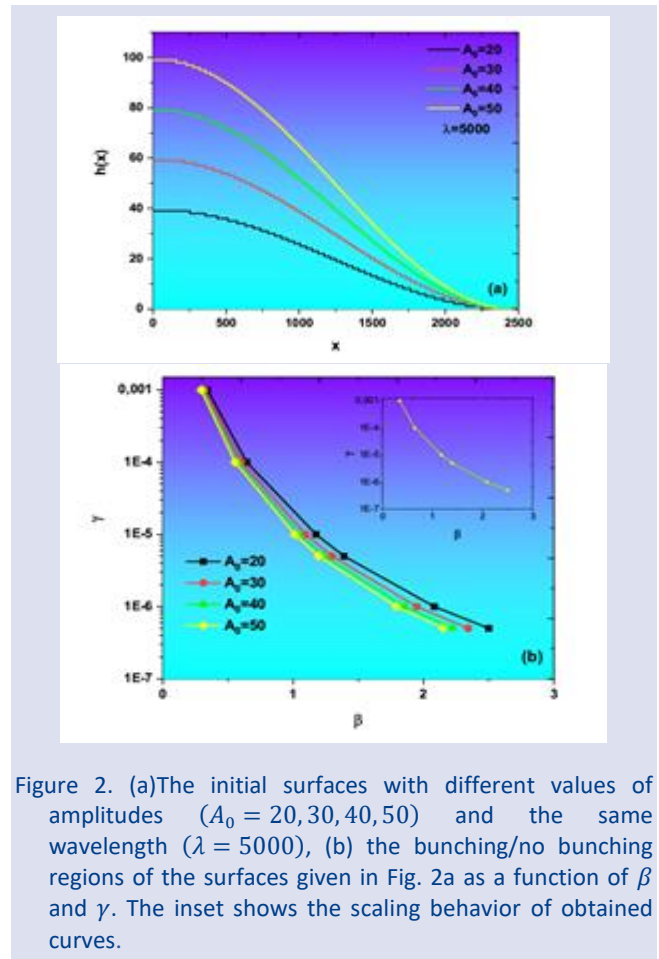


Figure 2. (a) The initial surfaces with different values of amplitudes ($A_0 = 20, 30, 40, 50$) and the same wavelength ($\lambda = 5000$), (b) the bunching/no bunching regions of the surfaces given in Fig. 2a as a function of β and γ . The inset shows the scaling behavior of obtained curves.

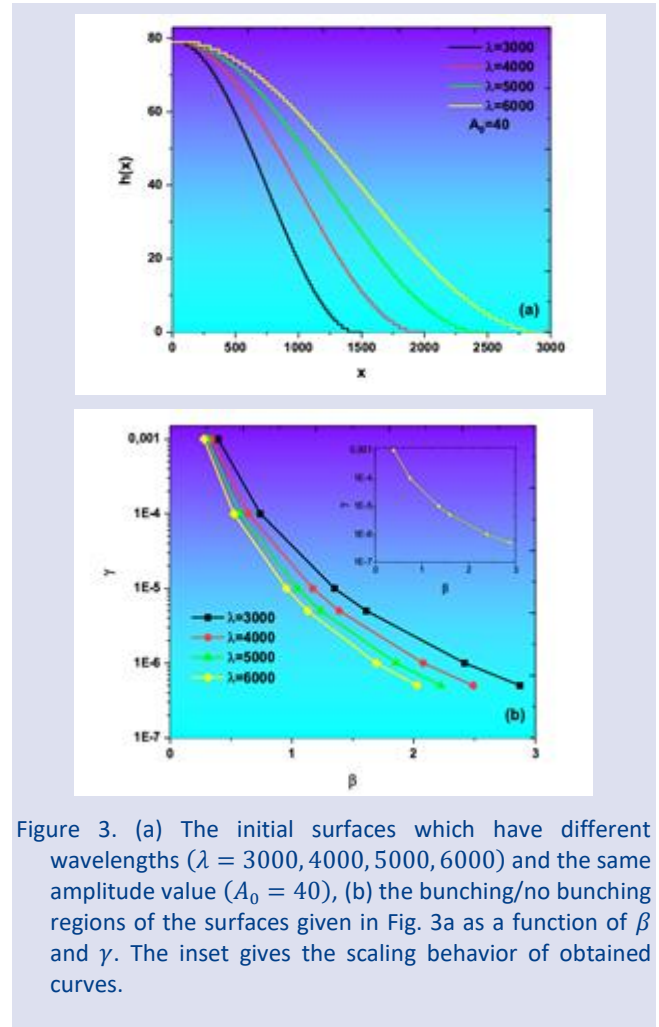


Figure 3. (a) The initial surfaces which have different wavelengths ($\lambda = 3000, 4000, 5000, 6000$) and the same amplitude value ($A_0 = 40$), (b) the bunching/no bunching regions of the surfaces given in Fig. 3a as a function of β and γ . The inset gives the scaling behavior of obtained curves.

We studied the initial surfaces with the same wavelength for the first part of our work (Figure 2a). While we took the wavelength's value as 5000, we altered the amplitudes of the surfaces by increasing by 10 from 20 to 50. In other words, we kept fixed the point where the rightmost parts of the initial surfaces intersect the x-axis and changed the steps' numbers owned by these surfaces. We numerically obtained the bunching/no bunching regions of the step interaction parameters γ and β by revealing the β value corresponding to each γ value mentioned above [35,36]. The results are given in Figure 2b. The regions above and below obtained curves indicate the bunching and no bunching regions, respectively. The relations between the line tension of a step and repulsive/attractive interactions between nearest neighbor circular steps ensure the determining these two regions. If Figure 2b is analyzed carefully, it can be seen that the bunching region of the surface expands with increasing the surface's amplitude (number of the steps on initial surface). Besides we found that the bunching/no bunching regions were scaled as $(A_0/A'_0)^{1/6}$ for initial surfaces which had different amplitudes as A_0 and A'_0 respectively. The inset in Figure 2b shows the scaled case of the curves. All curves have been scaled according to the curve with $A_0 = 20$. The scaling factors are $(5/2)^{1/6}$, $(4/2)^{1/6}$, $(3/2)^{1/6}$ and 1 for the amplitude's value of the initial surfaces $A_0 = 50, 40, 30$ and 20.

In the second part of the study, we examined the effect of altering the wavelength belonging to the initial surface on the surface's evolution in time and the areas of the bunching/no bunching regions. While doing this, we assumed the value of amplitude as constant while changing the wavelength values. Figure 3a indicates the initial surfaces with the same amplitude ($A_0 = 40$) and different wavelengths ($\lambda = 3000, 4000, 5000, 6000$).

In these conditions, the behaviors of obtained bunching/no bunching regions relating to given surfaces in Fig. 3a are presented in Figure 3b. We found that when we increase the surface's wavelength, the bunching region expands. In addition to this result, we identified that the curves (which separates the bunching/no bunching regions) scaled as $(\lambda/\lambda')^{1/2}$ for initial surfaces which have different wavelength values as λ and λ' respectively. The inset gives the scaled behavior of the curves. The curves have been scaled according to the curve with $\lambda = 3000$. The scaling factors are $(6/3)^{1/2}$, $(5/3)^{1/2}$, $(4/3)^{1/2}$, 1 for $\lambda = 6000, 5000, 4000, 3000$ respectively.

As last part, we changed both of the amplitudes and the wavelengths of the all initial surfaces. While we took the values of amplitudes as 20, 30, 40 and 50, we used the values from 3000 to 6000 in increments of 1000 for the wavelength respectively. The initial surfaces studied here are given in Figure 4a. When we analyzed the curves obtained as a function of β and γ in Figure 4b, we found that when both the amplitude and wavelength were increased, the bunching region expanded and these curves were scaled among themselves. The scaling coefficient here was appeared as the product of the scaling coefficients we found before $((A_0/A'_0)^{1/6} (\lambda/\lambda')^{1/2})$. All curves have been scaled according to the curve with $A_0 = 20$ and $\lambda = 3000$. The

scaling factors are $(5/2)^{1/6} (6/3)^{1/2}$, $(4/2)^{1/6} (5/3)^{1/2}$, $(3/2)^{1/6} (4/3)^{1/2}$ and 1

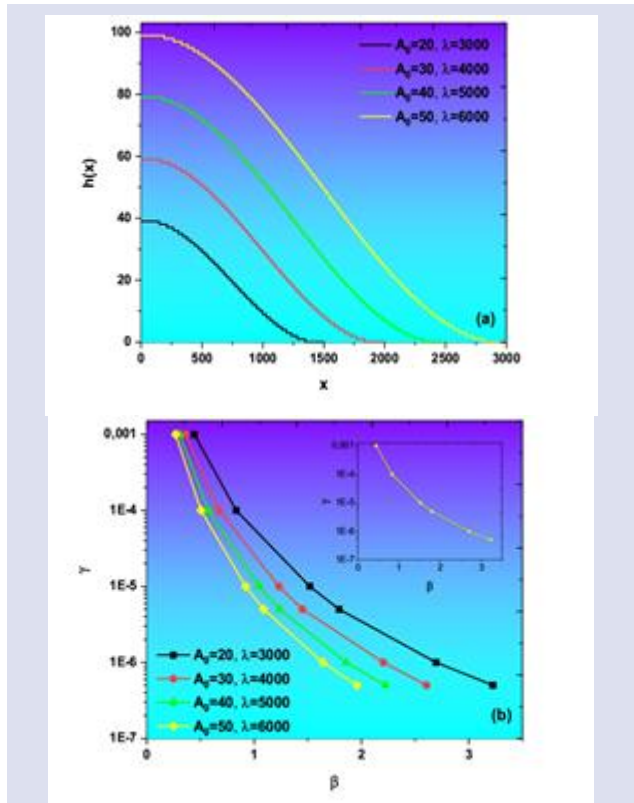


Figure 4. (a) The initial surfaces which have different amplitudes ($A_0 = 20, 30, 40, 50$) and the wavelengths ($\lambda = 3000, 4000, 5000, 6000$), (b) the bunching/no bunching regions of the given surfaces as a function of β and γ . The scaling behavior of obtained curves is given in inset.

Conclusions

In this study, we investigated the evolution of a two dimensional initial surface which is sinusoidal mound shaped for Diffusion Limited (DL) regime. We supposed that there were concentric circular steps on initial surface and attractive/repulsive interactions between steps. We obtained the equation of motion regarding the change of radius of each circular step together with the solution of the diffusion equation to follow surface's evolution. We examined bunching and no bunching regions of studied initial surfaces in a parameter space with their scaling properties. We can summarize our results as follows: while the wavelength λ (amplitude A_0) of the initial surface under consideration is constant, increasing its amplitude (wavelength) causes the bunching area of the surface to grow. In both cases, the resulting curves scale with each other. In case where the amplitude (wavelength) is changed and the wavelength (amplitude) is constant, the scaling factor is $(A_0/A'_0)^{1/6} ((\lambda/\lambda')^{1/2})$. In the condition that both the wavelength and amplitude of the surface are changed, the scaling factor is equal to the product of the expressions obtained above $((A_0/A'_0)^{1/6} (\lambda/\lambda')^{1/2})$.

Conflict of interest

The author declares no conflicts of interest.

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