Cumhuriyet Sci. J., 46(1) (2025) 167-171
DOI: https://doi.org/10.17776/csj.1593496

Cumhuriyet Science Journal

| csj.cumhuriyet.edu.tr | Founded: 2002 ISSN: 2587-2680 e-ISSN: 2587-246X Publisher: Sivas Cumhuriyet University

Investigation of Step Growth on Nano Surfaces Depending on Temperature and Flux Rates Using the KMC Method

Mehmet Esen [1,a,*]

[1] *Adana Vocational School Computer Programming Department, Çukurova University, Adana, Türkiye.*
**Corresponding author*

Research Article

History
Received: 02/12/2024
Accepted: 19/03/2025

ABSTRACT

In this study, the growth of nano-sized surface step structures was examined using the Kinetic Monte Carlo (KMC) simulation technique. The step growth and correlation function on the nano surfaces were analyzed at surface energy values of Eb = 100 meV, Ed = 80 meV, Eds = 150 meV, and Ek = 80 meV, where Eb is the bonding enegy, Eds is the step edge diffusion , Ed is the surface diffusion and Ek Schwoebel energy barrier values , with a surface flux of 1 atom every 10 ns directed towards the pre-formed stepped surfaces on the nano surfaces. The simulation temperature was set to T = 250 K. In this case, step growth was limited, but cluster structures played an important role in stepped surface growth. In a different scenario, at T = 300 K, the amplitude increased at a constant rate, and there were no step fluctuations. Surface growth increased, and the surface fluctuation amplitude also grew. At T = 350 K, when the temperature was raised further, step fluctuations has become dominant, the step fluctuation continued to increase at a constant rate, the step amplitude grew, and the number of islands decreased compared to the other two cases. In addition the correlation of steps is investigated for each temperature.
According to these results, the dynamics of step growth can be controlled by selecting an appropriate temperature and balancing the surface energy parameters.

Keywords: KMC method, Nano surfaces, Step growth, Surface diffusion energy, Temperature

[a] *mehesen@cukurova.edu.tr* *https://orcid.org/0009-0000-2057-4536*

Introduction

Semiconductor surface production technologies play a crucial role in advancing science and technology. Semiconductor surfaces have an important role in the production of many semiconductor devices. Experimental production of semiconductor surfaces is generally provided by sending atoms or molecules to a sub-surface with different methods. Chemical vapor deposition(CVD), molecular beam epitaxy(MBE) methods are experimental methods that provide experimental surface formation. Before conducting surface formation experiments, the development of the surfaces is guided by predictions from theoretical studies. These theoretical approaches examine factors such as the base material's effect, atom types and their movement to the surface, surface temperature, atomic diffusion properties, temperature variations during the experiment, and the evolution of the formed structures into different configurations. Simulation methods are essential for establishing the theoretical framework. Using these methods, predictions about surfaces and structures can be simulated, guided by the results obtained from the simulations, thereby saving time and resources. In cases where real-world testing is not possible, simulations allow predictions by modeling specific features as parameters. Among surface simulation techniques, Monte Carlo (MC) methods hold significant importance. These include molecular dynamics MC, direct MC, and the Kinetic Monte Carlo (KMC) technique . The KMC method is based on the important studies of Bortz et al. [1], and Fichthorn and Weinberg [2] and Haneman et al. [3]. There are more recent studies on step simulations using the KMC method [4,5].

Method

In this study, a custom Fortran program utilizing the KMC method was developed, and data were collected using this program. In this method, possible states of the surface sites were analyzed, and their transition probabilities were calculated. The transition probabilities of atoms from one site to another, depend on the energy barriers between them. In the KMC method, atoms moving on the surface, overcome specific energy barriers and settle somewhere on the surface. With a certain probability, these atoms can be displaced by thermal fluctuations (surface diffusion), bond with previously fixed atoms to become part of the structure, or leave the surface and become part of the vapor above the surface. The probability of a particle moving from one site to another on the surface given is as,

$$P \propto e^{-E_b/k_B T} \tag{1}$$

where E_b is the energy barrier the particle must surmount is in going from one site to a neighboring one. If we call this transition probability *i* events, there can be *n* total transition events for the particles on the surface. The rate at which a particle can make transition to state *i* with a rate r_i is given as,

$$r_i = w_i e^{-E_i/k_B T} \tag{2}$$

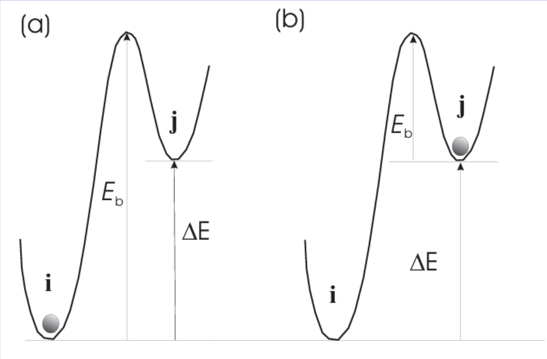

Figure 1. The barrier energies required to be crossed for states i and j are shown, the probability of transition is low in case (a) but the probability is high compared to the other in case (b). The energy barrier Eb is higher in(a).

In equation(2) w_i represents the number of attempts to pass through the potential well per unit time for the defined event i to occur, and generally $w_i = 10^{12}\ s^{-1}$. E_i is the size of the energy barrier that the particle tries to cross, k_B is Boltzmann's constant and T is the absolute temperature. As shown in Figure 1, the transition probability from state i to state j is difficult, whereas the transition from j to i is more probable. If the transition probabilities of all particles in all directions are determined by the surface configuration energy, and the probability of one of these events is proportional to the transition probability, then only one particle moves at a time. This is one of the strengths of the KMC method. Another advantage of this method is that a link relation can be established between real time and simulation time [1]. The necessary conditions for establishing this link were outlined by Fichthorn et al. [2]. These criteria are as follows: transitions must be a Poisson event, transition events must be independent of each other, the time between successive events can be calculated in a convenient way, transition probabilities must obey a 'dynamic hierarchy' such that the 'comprehensive equilibrium' condition is satisfied.

The KMC method can be used for systems in equilibrium or far from equilibrium. The current independent Poisson distribution for the transition from state *i* to state *j* in the interval from instant *t* to *t+ τ is given by*

$$P(n_i) = \frac{(r_i t)^{n_i}}{n_i!} e^{-r_i t} \tag{3}$$

One feature of Poisson events is that a collection of independent events behaves as a single Poisson event. An important property of a Poisson event is that the time elapsed between successive events can be found, and this is the probability of occurring at an instant *t* can be given as [7],

$$P(t) = Re^{-Rt} \tag{4}$$

Average time between these events

$$\bar{t} = \int_0^\infty tP(t)dt = \int_0^\tau t\,Re^{-Rt}dt = 1 - e^{R\tau} \tag{5}$$

The right hand side of eqn (5) is between zero and 1,therefore it can be equated to a random number *u* between 0 and 1, as a result the time elapsed between two consecutive events becomes

$$\tau = -\frac{\ln u}{R} \tag{6}$$

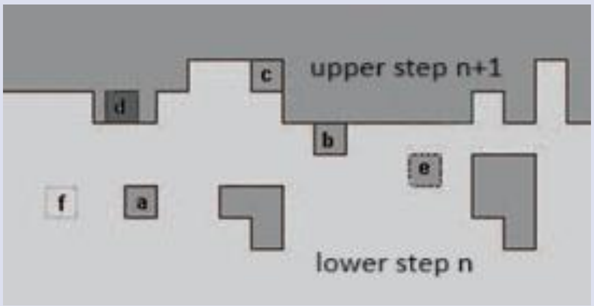

Figure 2. Schematic representation of atoms on a stepped surface, dark regions are one atomic length higher than light colored regions. Only two steps are shown on the surface; a cubic structure located at the step edge, a single atom on the surface, b at the step edge, c attached to the corner, d embedded in the step, e inside the surface, f sample atoms embedded in the crystal depth .

As seen in Figure 2, schematic views of the atoms that can be found on the sample surface are given. The number of nearest (nn), next nearest (nnn) and nex next nearest neigbor (nnnn) atoms for each specific location shown in Figure 2 is given Table 1.

Table 1. Nearest neighboring (nn) atom numbers of crystal atoms [8]

Position	index	nn	nnn	Next nnn
Above the surface	a	1	4	4
Step Edge	b	2	6	4
Around the corner	c	3	6	4
Inside the step	d	4	6	4
Inside the surface	e	5	8	4
Deep in crystal	f	6	12	8

Each bond of the atoms appearing in Table 1 can have different combinations of threshold energies, accordingly the transition barrier energies for several configurations are given in Table 2.

Table 2. Sample transition probabilities of some crystal atoms

Event	Energy Barrier	Probability of occuring
Free diffusion on the surface (a)	E_d	$\exp(-E_d/k_BT)$
Step edge detachment (b downward direction)	$E_b + E_d$	$\exp(-(E_b + E_d)/k_BT)$
Detaching from the edge of the step to the top (b upward direction)	$E_b + E_k$	$\exp(-(E_b+E_k)/k_BT)$
Going down from the terrace (d down direction)	E_k	$\exp(-E_k/k_BT)$
Movement along the edge of the step (b movement in two directions)	E_{ds}	$\exp(-E_{ds}/k_BT)$

When Figure 1 and Table 2 are examined together, it is seen that each atom on the surface has the possibility of moving in 4 different directions, and each atom can make different types of bonds with 4 atoms that may be around it depending on its position on the surface, It should be known that it must break different bond combinations in each direction of movement and the algorithm we developed calculates and groups these probabilities for thousands of different combination cases. In addition, the location of atomic islands and steps were found using specially developed unique difference and fill algorithms [8]. These are necessary for a proper analysis of the resulting surface.

The KMC algorithm used in the present study is given in the following steps:

1. Time is reset $t = 0$
2. All transition rate r_i s for all particles in the system are calculated
3. The cumulative sum of the transition rates are calculated. $R_i = \sum_{j=1}^{i} r_i R = R_N$
4. A random number u is chosen between 0 and 1.
5. The i *th* event to occur is chosen to satisfy the equation $R_{i-1} \leq uR < R_i$.
6. The selected *i*.th event is performed (atom location changes)
7. The changed probabilities are recalculated and added to the unchanged ones.
8. A new random number u is selected and $\tau = -\frac{\ln u}{R}$ calculated
9. Time is updated $t = t + \tau$
10. Goto step 1.

The step position random walk behavior, related to step movements on the surface, is described by the position correlation function as [9]:

$$G(y) =< ((x(y) - X(y_0))^2 \geq \frac{b^2}{a\|} |y| \tag{7}$$

In this equation *G(y)*, is a function of distance *y* along the step edge. The term *b*^{2} in the equation is the step diffusivity term, |y| is the everage position of the step, a|| is the distance between nearest neighbor atoms.

Results And Discussion

The structures formed on the surface were simulated using different surface energy parameters. The growth and fluctuation of the steps were investigated, and it was observed that these properties depend on the particle flux to the surface and the surface energy parameters. In this section, the growth of a single step on a large surface is studied at different temperatures. By choosing a large surface, the effects of periodic boundary conditions and the limited size of the surface are minimized. For all cases considered in this section, the temperature is varied while the other energy parameters are kept constant. These are as follows: the atomic bond energy Eb = 100 meV, free surface diffusion barrier Ed = 80 meV, the step edge diffusion barrier Eds = 150 meV, and the Schwoebel energy barrier Ek = 80 meV. The Schwoebel energy barrier is the the energy a particle must overcome when joining a step edge from an upper step. The atomic flux to the surface is 1 particle per 10 ns. In the first case, T = 250 K was chosen, and the resulting surface morphology is shown in Figure 3. For these parameters, surface diffusion of particles is more difficult, so island formation begins immediately upon particle flux to the surface. Since the binding energy is higher than the diffusion energy, particles bound to steps or islands are more difficult to detach. Furthermore, the particle density near the step edge is low. Because particles in this region are absorbed by the step, sufficient density for island formation near the step cannot be achieved for a long time. However, as the previously formed islands grow and the step edge advances, the islands and the step edge approach each other and eventually merge.

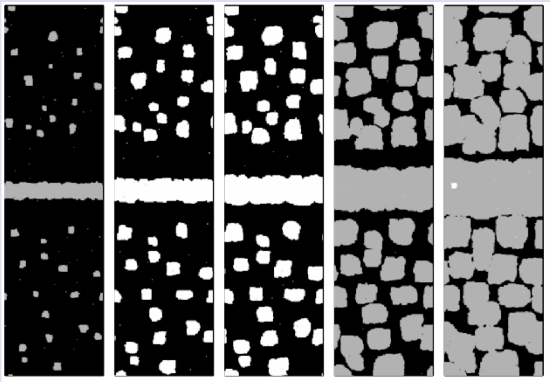

Figure 3. The time evolution of the surface is shown from left to right. The surface size is 160x600, with energy parameters of Eb = 100 meV, Ed = 80 meV, Eds = 150 meV, and Ek = 80 meV at T = 250 K. The flux is 1 atom per 10 ns. As seen in the figure, the growth of islands is more dominant than the growth of steps. A single step is surrounded by two terraces of the same height on each side of the step.

Figure 4 shows the correlation function of the step edge shown in Figure 3. The correlations obtained at later times of the surface are indicated by t_3 in Figure 4. Initially, the step oscillates with small wavelengths. Over time, small wavelength oscillations are eliminated and longer wavelength structures remain on the surface.

When these reach a stable equilibrium, the step grows in this way as expected. The change in correlation varies almost linearly for small step lengths as given in equation(7)[8].

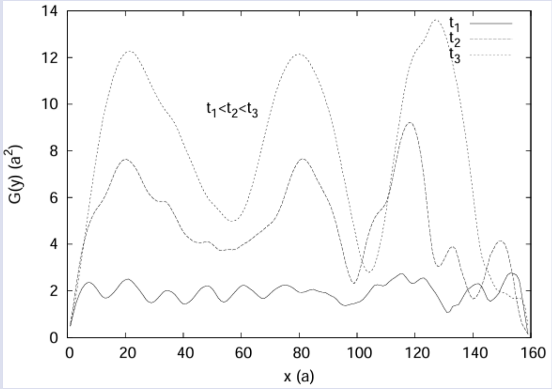

Figure 4. Correlation function of a step given in figure 3.

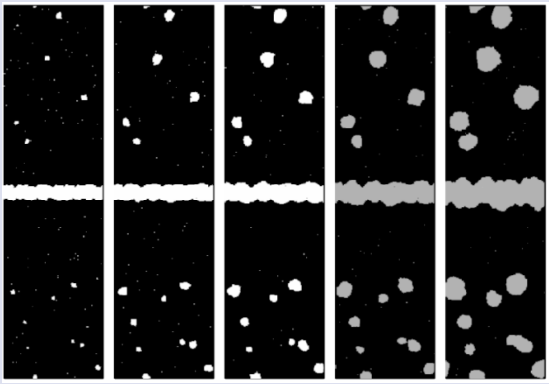

Figure 5. The time evolution of steps and islands on a 160x600 surface at E_b = 100, E_d = 80, E_{ds} = 150 and E_k = 80 meV at T = 300K. The flux is 1 atom at 10 ns. As can be seen in the figure, the growth of the islands is not dominant and the islands grow in small numbers.

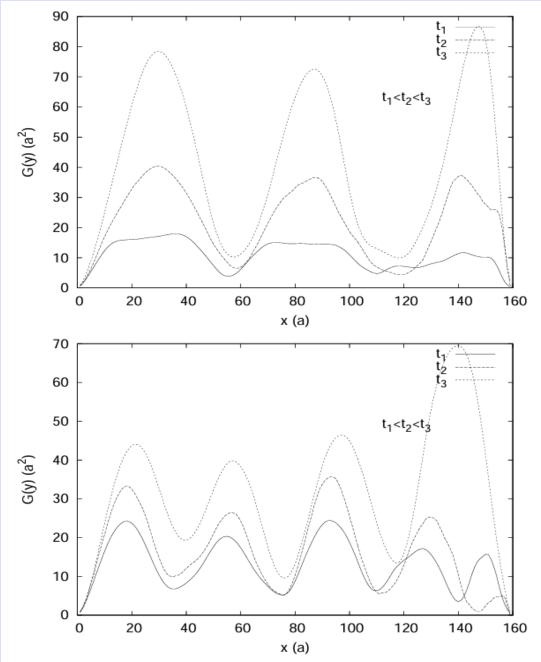

Figure 6. Correlation function for the two sides of the growing step shown in Figure 5. The step fluctuation strength and behavior depends on the cluster distribution near the step edge.

In another case the surface temperature was increased at T=300K. As seen in Figure 5, island formation is low. Since the temperature is higher, the diffusion of particles on the surface is higher. It is easier for atoms to merge and separate at the edges of the step or at the edges of the island. Therefore, island formation is low.

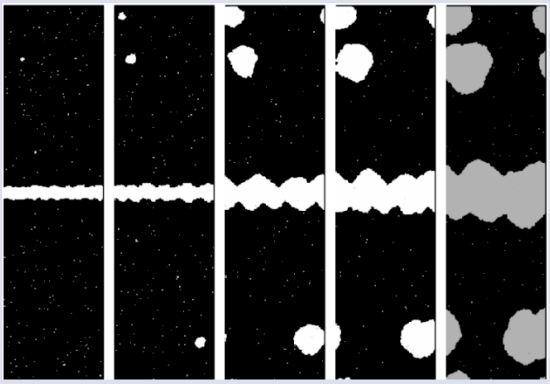

Figure 7. The time evolution of steps and islands on a 160x600 surface at E_b = 100, E_d = 80, E_{ds} = 150 and E_k = 80 meV at T = 350K. The flux is 1 atom at 10 ns. As seen in the figure, the growth of the islands is not dominant and the islands grow in very small numbers.

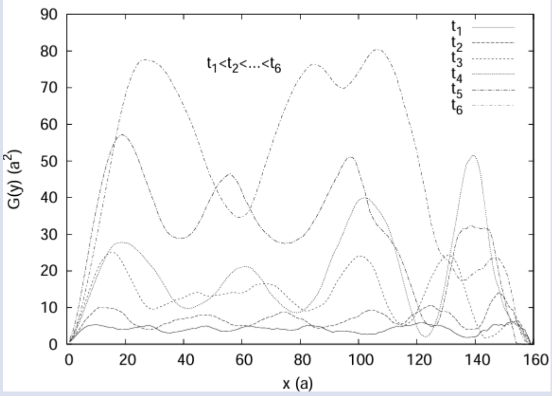

Figure 8. Correlation function for the two sides of the growing step shown in Figure 7.

As in the case of Figures 5 and 6, the step fluctuation behavior depends on the cluster distribution near the step edge. In the present case we have less number of clusters with a considerable size.

In Figure 7, a higher temperature of T = 350 K is simulated. At this temperature, step growth dominates, and no islands form in the terrace region where the step is fed. Instead, a few very large islands form far from the step edges. When the step correlation is analyzed in Figure 8, the amplitude increases significantly and the oscillation mode numbers decrease in the later stages of growth.

Conclusions

Considering all the results, the effect of material parameter selections on step growth processes—a key phenomenon in surface growth—is evident. The selection of growth temperatures suitable for the atomic binding energies of the material plays a crucial role in determining the step growth phases.

Based on these results, if the temperature is increased and the surface flux is maintained at an adequate level, step growth can dominate surface growth. However, if the temperature is increased excessively, step decomposition may become excessive, causing the entire step structure to disappear and the surface to decompose into small clusters of 2 or 3 atoms. This study provides valuable guidance for determining the temperature at which experimental studies should be conducted.

Conflict of interest

The author declare that he has no conflict of interest.

Acknowledgement

This study is supported by Çukurova University BAP unit with the project number BAP-2024-16928.

References

[1] Bortz A.B., Kalos M.H., Lebowitz J.L.,1975, *J. Comp. Physics*, 17.

[2] Fichthorn K. A., & Weinberg W. H., Theoretical foundations of dynamical Monte Carlo simulations. *The Journal of chemical physics*, 95(2) (1991) 1090-1096.

[3] Haneman D., & Chernov A. A., Thermal conversion of Si (111) 2× 1 cleaved surface structure to Si (111) 7× 7 structure. *Surface science*, 215(1-2) (1989) 135-146.

[4] Nagpal S., Sitapure N., Gagnon Z., & Kwon, J. S. I., Advancing crystal growth prediction: An adaptive kMC model spanning multiple regimes. *Chemical Engineering Science*, 299 (2024) 120472.

[5] Li, Y., Chen, X., & Ai W., Kinetic Monte Carlo simulation study of the early stages of epitaxial SiC (0001) growth. *Journal of Crystal Growth*, 617 (2023) 127291.

[6] Bulmer M. G. *Principles of statistics*. (2012). Courier Corporation.

[7] ÇINLAR E., An Introduction to Stochastic Processes, Prentice-Hall, 1975.

[8] Esen M., Atomik Basamaklı Kristal Yüzeylerinin Kinetik Monte Carlo Yöntemi ile İncelenmesi, Çukurova Üniversitesi, Fen Bilimleri Enstitüsü, Fizik Bölümü Anabilim Dalı, *Doktora Tezi*, tez no: 5907, (2006)

[9] Bartelt N. C. (et al.), Brownian motion of steps on Si(111) *Phys. Rev. B*, 48 (1993) 15453-15456.