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SURFACE MORPHOLOGY OF LATTICE MISMATCHED THIN FILMS

Mr. Piti Panichayunon

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Thesis Title	Surface Morphology of Lattice Mismatched Thin Films
By	Mr. Piti Panichayunon
Field of Study	Physics
Thesis Advisor	Patcha Chatraphorn, Ph.D.
Thesis Co-Advisor	Sojiphong Chatraphorn, Ph.D.

Accepted by the Faculty of Science, Chulalongkorn University in Partial Fulfillment of the Requirements for the Master's Degree

..... Dean of the Faculty of Science
(Professor Piamsak Menasveta, Ph.D.)

THESIS COMMITTEE

..... Chairman
(Assistant Professor Kajornyod Yoodee, Ph.D.)

..... Thesis Advisor
(Patcha Chatraphorn, Ph.D.)

..... Thesis Co-Advisor
(Sojiphong Chatraphorn, Ph.D.)

..... Member
(Assistant Professor Sukkaneste Tungasmita, Ph.D.)

..... Member
(Nuttakorn Thubthong, Ph.D.)

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ในงานนี้ได้ทำการศึกษาแบบจำลองเอ็มบีอีแบบเอสโอเอส (SOS-MBE) ซึ่งใช้สำหรับศึกษาการเตรียมฟิล์มซึ่งแผ่นรองรับและสารที่นำมาเตรียมฟิล์มเป็นสารชนิดเดียวกัน ซึ่งภายในแบบจำลองนี้อะตอมจะถูกปล่อยลงมายังแผ่นรองรับแบบสุ่มตำแหน่งโดยอะตอมที่อยู่ที่ผิวสามารถเคลื่อนที่ได้ตลอดเวลาจนกว่าจะถูกทับโดยอะตอมอื่น ทำการศึกษาโดยการเปลี่ยนค่าอุณหภูมิของแผ่นรองรับ และสังเกตลักษณะของพื้นผิวและค่าอินเตอร์เฟสวิดท์ พบว่าเมื่ออุณหภูมิของแผ่นรองรับมีค่าต่ำ ค่าอินเตอร์เฟสวิดท์จะเพิ่มขึ้นอย่างรวดเร็ว และเมื่ออุณหภูมิของแผ่นรองรับมีค่าสูงขึ้น ลักษณะพื้นผิวของฟิล์มจะมีความขรุขระลดลงและจะกลายเป็นการเตรียมฟิล์มเป็นชั้นๆเมื่ออุณหภูมิของแผ่นรองรับมีค่าสูงมากๆ หลังจากนั้นได้ทำการปรับปรุงแบบจำลองเอ็มบีอีเพื่อใช้ในการศึกษาการเตรียมฟิล์มซึ่งแผ่นรองรับและสารที่นำมาเตรียมฟิล์มเป็นสารต่างชนิดกัน โดยเพิ่มผลของความเครียดเนื่องจากค่าคงที่โครงผลึกของแผ่นรองรับและฟิล์มบางไม่เท่ากัน และเรียกว่าแบบจำลอง Lattice Mismatch พบว่าผลของความเครียดทำให้เกิด mound บนพื้นผิวของฟิล์มเมื่อความแรงของความเครียดถึงค่าวิกฤต สำหรับการศึกษานี้ค่าวิกฤตของความเครียดอยู่ระหว่าง 0.8 eV. และ 1.2 eV. และค่าความหนาวิกฤตที่ทำให้เกิด mound อยู่ระหว่างชั้นที่1 และ 2 และยังพบอีกว่า รัศมีเฉลี่ยของ mound ขึ้นอยู่กับความหนาของฟิล์มและอุณหภูมิของแผ่นรองรับโดยรัศมีเฉลี่ยของ mound จะเพิ่มขึ้นเมื่อความหนามีค่าเพิ่มขึ้นและจะเพิ่มแบบเอกซ์โพเนนเชียล เมื่ออุณหภูมิเพิ่มสูงขึ้น โดยการเพิ่มความแรงของความเครียดไม่ผลต่อการขยายตัวของรัศมีเฉลี่ยของ mound

ภาควิชา ฟิสิกส์	ลายมือชื่อนิสิต.....
สาขาวิชา ฟิสิกส์	ลายมือชื่ออาจารย์ที่ปรึกษา.....
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PITI PANICHAYUNON : SURFACE MORPHOLOGY OF LATTICE MISMATCHED THIN FILMS. THESIS ADVISOR : PATCHA CHATRAPHORN, PH.D.,THESIS CO-ADVISOR : SOJIPHONG CHATRAPHORN, PH.D., 53 pp. ISBN 974-17-6663-7.

In this work, we study a Solid-On-Solid (SOS) MBE growth model, for homoepitaxial growth, where atoms are dropped or deposited on randomly chosen lattice sites. Surface atoms may continue to hop at any time until they are buried by other atoms. We varied the substrate temperature and obtained the surface morphology and interface width (W). Our study shows that surface atoms do not hop much when the substrate temperature is low, resulting in a fast growing width. For higher temperature, the surface becomes kinetically rough that eventually turns into a layer-by-layer growth at very high temperature. We then expand this model to heteroepitaxial growth by including an effect of a strain caused by a lattice mismatch between the substrate and film materials and ,namely *Lattice Mismatch* model. We find that the effect of strain leads to a mound formation when strain strength reach the critical value. For this work, the critical strength of strain should be between 0.8 and 1.2 eV while the critical thickness that lead to a mound formation should be between 1 and 2 ML. Moreover, our study shows that average mound radius depends on the thickness and the substrate temperature. The average mound radius increases when thickness increases and exponentially increases when temperature increases. While the increase of strain strength does not effect the evolution of mound radius.

Department Physics — Student's signature .....

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Chapter 1

Introduction

1.1 Introduction

Thin films grown by molecular beam epitaxy (MBE) technique have drawn a lot of attention in the past decades due to its high quality and potential for many applications such as solar cells, eletronic devices, quantum devices, etc. Typically, the MBE experiments are usually performed under ultra-high vacuum with the pressure in the order of 10^{-10} torr or less. This working pressure leads to a long mean free path of atoms or molecules of source materials. This is the origin of term "beam" in MBE. The term "epitaxy" refers to the fact that the surface growth process allows only one layer at a time, i.e. a new layer does not begin to form until the one below it is complete. Generally, MBE growth is divided into two types. First, homoepitaxial growth of which the substrate and the thin film are the same material. Second, heteroepitaxial growth of which the substrate and the thin film material are different. In the latter case, the lattice constants of the substrate and the thin film are not the same. This difference in the lattice constants, i.e. lattice mismatch causes strain in the thin film. Experiments show island formation or mound formation on the film[1, 2, 3]. The island shapes and sizes depend on various growth conditions such as deposition rate, substrate temperature, etc. But, there has not been any clear theoretical explanation on how the islands are formed. The nature of the island formation is an interesting topic in recent years. This is because when the mechanism is understood, it would be easy to control

the island pattern on thin film surface. The objective of this work is to investigate effects of strain due to lattice mismatch on surface morphology of the film grown by molecular beam epitaxy technique.

In this thesis, we use computer simulation to study the kinetic nonequilibrium surface roughening of homoepitaxy and heteroepitaxy growths. Computer simulation is a convenient tool to use. One of the reasons is that it is easy to control parameters such as substrate temperature or bonding energy in simulations. It is also a bridge between theories and experiments. Nowadays, there are many discrete growth models [4] used to describe MBE growth process. Among this many discrete growth models we are interested in the model called *MBE model* [6]. This model is used to study homoepitaxial growth. We can modify this model to incorporate the effect of strain in heteroepitaxial growth system.

1.2 Overview of The Thesis

In the next chapter, chapter 2, we introduce the theoretical background, MBE growth mechanism, interface width and height-height correlation function, which needed for our computational MBE growth studies. Moreover, we introduce the discrete growth model used extensively to study MBE growth. The *MBE* model [6], a model for homoepitaxial growth, is an important model because it is very realistic compare to many other models. It also has a lot of flexibility in its diffusion rule and we are able to modify the MBE model for a study of heteroepitaxial growth that is the main focus of our studies. However, some other models, *Das Sarma-Tamborenea* (DT) model[8] and *Wolf-Villain* (WV) model[9], are also discussed for the sake of completeness. The detail descriptions of all the models and method of modification that we study are presented in chapter 2.

We present our simulation results along with analyses and discussions in chapter 3. The chapter is divided into two sections. The first section is the

homoepitaxial growth simulation results that we study via MBE model. In this section, effects of substrate temperature on the MBE model are discussed. In the second section, simulation results of *Lattice Mismatch model* [5], a modified model used in our study of heteroepitaxial growth are presented. We also discuss effects of substrate temperature and strength of strain in this section. However, we note that although most of our work here is presented with completed analyses, there are several issues, which are still not completely understood. The conclusions of our work are offered in Chapter 4.

Chapter 2

Theoretical Aspect and Models

To understand kinetic properties of the growth model we must have some background tools in the study. In this chapter, we will introduce theoretical background of mechanisms taking place on the growing surface in MBE growth. Discrete growth models used in our study are also explained. Furthermore, we briefly describe the interface width, which is the quantity used to study roughness of the surface, and the correlation function used to detect the mound formation on surface.

2.1 MBE Growth Mechanism

To understand the kinetics process on the surface, we will review the most relavant processes, i.e., *deposition, desorption*, and *surface diffusion*, that take place on the surface (see Fig. 2.1). The interplay of these processes results in the characteristic of thin film.

2.1.1 Deposition

In this process, atoms or molecules of source material are thermally evaporated and forming a beam with corresponding thermal velocity. This beam is directed to the substrate to form a film. Each atom is deposited on a random site of the surface, forming bonds with the surface atoms (atom A in Fig. 2.1). In this work,

the deposition rate is taken to be one monolayer (ML) per second for simplicity in the computer simulation algorithm.

2.1.2 Desorption

Desorption is a contrary process to deposition. In this process, some atoms deposited on the surface may be ejected from the surface (atom B in Fig. 2.1). The desorption probability depends on how strongly the atom is bonded to the surface and the growth temperature. The strength of the bonds depends on the type of the atom and the local geometry of the surface where the atom sticks to. For the same type of atom, desorption probability increases when growth temperature increases. This is because higher temperature means atoms have more energy. More energetic atoms have higher probability to be able to break free from the surface. However, desorption rate in typical MBE experiment is rather small. For this work, we assume that there is no desorption in the growth model.

2.1.3 Surface Diffusion

Surface diffusion is the process that deposited atoms move around on the surface (atom C in Fig. 2.1) searching for the most energetically favorable position. The diffusion length, i.e. the distance that an atom can move from its deposition site, depends on the substrate temperature and binding energy. The diffusion rule for each discrete growth models are presented in the next chapter.

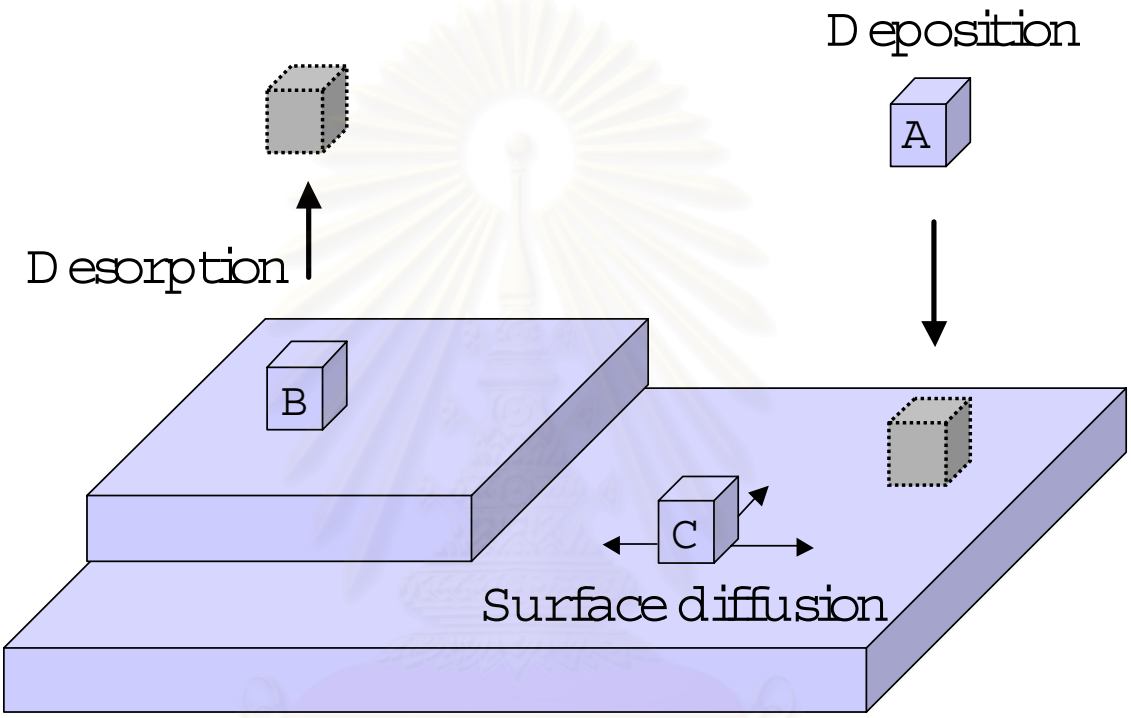

Figure 2.1: The MBE growth mechanism that taking place on the surface. (A) Atoms arrive on the surface, where they are deposited. (B) An atom on the surface may desorb, leaving the surface of the thin film. (C) Atoms diffuse in random directions on the surface.

2.2 Models and Methods

In this section, discrete growth models used to study the MBE growth are introduced. We will start with the simplest model that can be used to study the growth problem, known as *Random Deposition* (RD) model[4]. More complicated models such as *Das Sarma-Tamborenea* (DT) model [8], *Wolf-Villain* (WV) model [9], and *MBE* model [6] will be followed. The DT and WV models are more realistic than the RD model because they are models that include the dynamical diffusion/relaxation process. However, the MBE model, which we are interested and focus on in our work, is the most complicated and most realistic among all models discussed here since it includes the effect of substrate temperature. Moreover, bonding energy is also an adjustable parameter in this model. The original MBE model[6] simply applies for a homoepitaxial growth but we can modify it to study the heteroepitaxial growth which is the main focus of this work. One may call this modified model as *Lattice Mismatch* model.

All the models mentioned above are nonequilibrium discrete growth model. They are under the *solid-on-solid(SOS)* restrictions, i.e. no bulk vacancy, no overhanging and no desorption. An adatom is deposited on a randomly chosen site on an initially flat substrate and then allowed to diffuse, according to a specific set of diffusion rules for each model. The movement of an adatom is a lateral move, i.e. it hop from the top of one site to another. In this work, we assume the deposition rate to be 1 monolayer(ML) per second for simplicity in simulations, and all simulations are done with periodic boundary condition to avoid the finite size effect. All simulations are carried out on one dimensional substrate(d = 1+1) system.

2.2.1 Random Deposition Model

The Random Deposition (RD)[4] model is the simplest growth model in the literature. An adatom is deposited on a randomly selected site above the initially flat

substrate and then sticks instantaneously on the deposited site with no diffusion. This model refers to very low temperature MBE condition in which there is no diffusion since the activation energy is too low to overcome the bonding energy that the atom forms with the neighbor beneath it. This effectively gives the RD model an absolute zero diffusion length. In other words, the diffusion precess is not included in the RD model. In the simulation algorithm, we choose a random site x on a flat substrate size L and increase its height $h(x,t)$ by one. So the surface height of the RD model grows independently and the surface of the growing film is *uncorrelated*. Since the surface height are uncorrelated, the growth front can be described by the *Poisson distribution* [4] and we can find the exact solution [4] for the growth exponent to be $\beta = 0.5$.

2.2.2 DT and WV Models

The Das Sarma-Tamborenea (DT) model [8] is a simple model for the study of the kinetic surface roughening growth which followed the MBE growth condition and under the SOS restrictions. In the DT model, after an adatom is deposited randomly on a chosen site on a one dimensional flat substrate (d = 1+1), it instantaneously diffuses and tries to increase its coordination number. While an adatom diffuses, it searches around the deposited site for a site that offers more bonds than at its original position. The search is done within its diffusion length ℓ. In other words, an adatom tries to increase its coordination number or its bondings. If the neighboring sites around the initial deposited site under diffusion length ℓ do not offer higher coordination number than the initial deposited site, the adatom will incorporate itself at its original deposited site. And the adatom at a kink site, a site where it has one lateral nearest neighbor bond, does not move (see Fig. 2.1). Furthermore, if there is more than one suitable final site, the adatom will randomly select its final site from those choices. After an adatom find its selected final site, it moves to that site and incorporate itself there permanently. Then the next adatom will be deposited on a substrate randomly and repeat the

diffusion process.

Wolf-Villain (WV) model [9] is very similar to the DT model. It is also under the SOS restrictions and used to study the kinetic surface roughening growth which followed the MBE growth condition. The difference is that, in the diffusion of WV adatom, it tries to *maximize* the coordination number or its bonding. In other words, while the adatom is diffusing, it searches around the deposited site within its diffusion length for a site that offers the maximum bonds (see Fig. 2.1). The WV adatom at a kink site is also able to move if the sites around the initial deposited site under its diffusion length can offer higher coordination number than the initial deposited site.

In conclusion, there are two important differences between DT and WV diffusion rules. First, an adatom at a kink site cannot move in DT model while a WV adatom can always move to a site with higher coordination number. That can be inferred to the difference of the substrate temperature between the DT and the WV applications. The substrate temperature of DT model is less than that of the WV model so the DT adatoms does not have enough energy to break two bonds at akink site. Second, the DT adatoms try to increase, not maximize, their coordination number while the WV adatoms try to maximize their coordination number. The DT and WV models are certaining better than the RD model for study of MBE model growth. This is because in the DT and WV models, two crucial mechanisms : deposition and surface diffusion are included. The RD model neglects the diffusion mechanism and has only the deposition process. However, there are still things that The DT and WV models oversimplify in some sense, so we move to a more realistic model in the next topic.

2.2.3 MBE Model

The MBE model [6] is another model for studying the kinetic surface roughening process in molecular beam epitaxy growth. It is more complicated and closer to

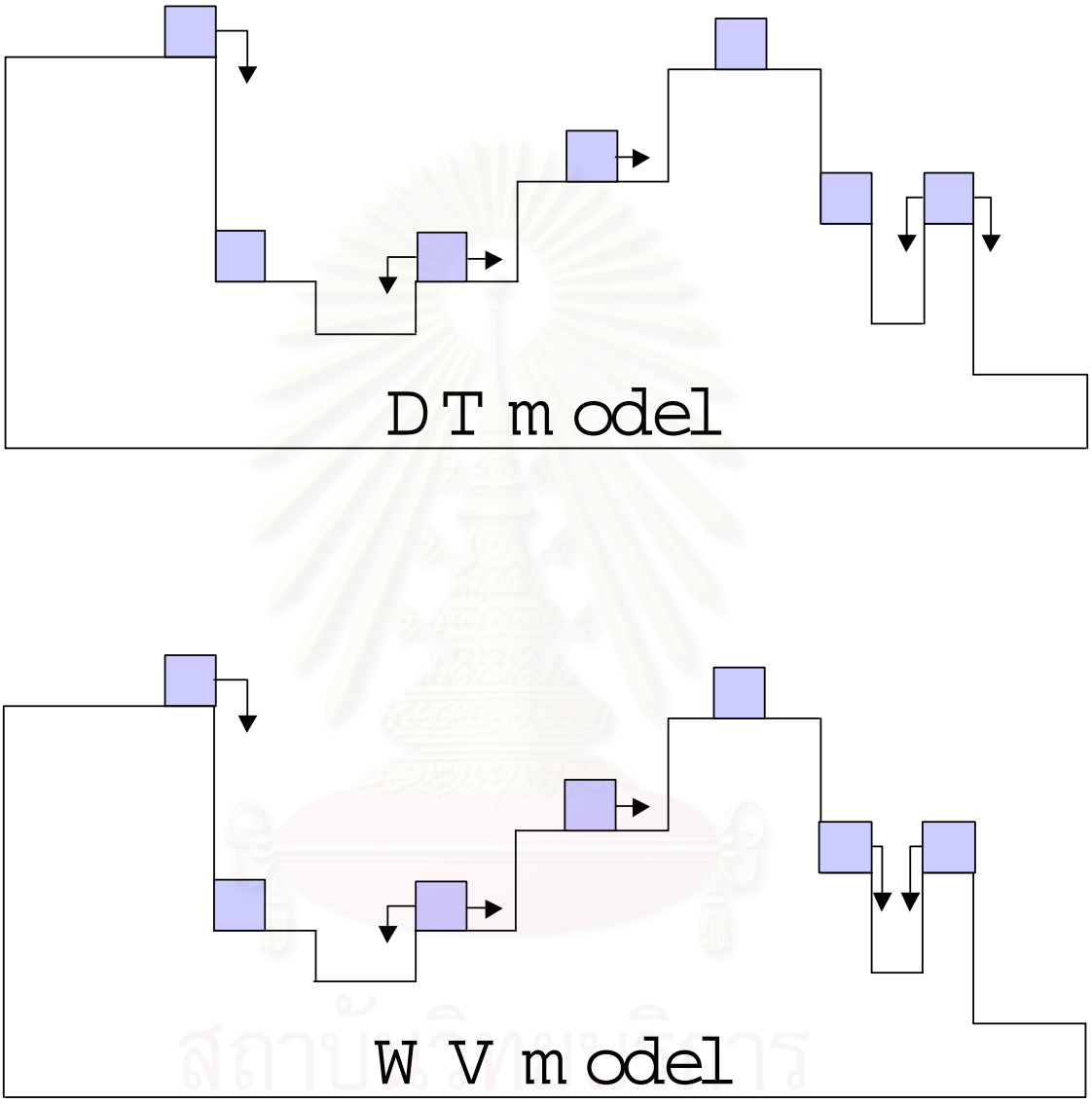

Figure 2.2: The schematic configurations defining the diffusion growth rules for the DT and the WV models.

the real MBE experiment than previously discussed models. While the DT and the WV models do not include the effect of the substrate temperature, the MBE model takes the substrate temperature into account. In this model, adatoms are deposited on randomly chosen substrate sites and they still move under the SOS constraint. Any surface atom, an atom on the surface, (not just the most recently deposited atom) can hop randomly to a neighboring site at any time until they are completely buried. This is a somewhat more realistic situation for the diffusion process. The hopping activation energy, the energy that the atom need to break its bond before hopping, depends on the bonding environment and the substrate temperature. The hopping rate at a substrate temperature T is calculated from the Arrhenius expression [5, 10]:

$$R_n = R_0 \exp^{-E/k_b T}, \tag{2.1}$$

where $R_0 = dk_bT/h$ is characteristic vibrational frequency, d is the substrate dimension, k_b is the Boltzmann constant, and h is the Planck' constant. For this work we study a one dimensional substrate, thus $d = 1$. The activation energy $E = E_0 + nE_b$, where E_0 is the crystal potential energy, E_b is the bonding energy, and n is the number of nearest neighbors at that site. In table 2.1, we calculate the hopping rate as a function of a number of bonds and the substrate temperature. The hopping rate obviously increases when the substrate temperature increases. Since the increase of the substrate temperature lead to the increase of the energy of an atom, that results in higher hopping ability or the increase of the hopping rate. In contrast, the hopping rate decreases dramatically when the number of bonds increase. When the number of bonds increase, the activation energy that the atom needs to break its bonds also increase. So the more number of bonds, the more difficult of the atom to move. That leads to the decrease of hopping ability or hopping rate of the atom.

In the computational algorithm, we initially choose the substrate site x randomly and increase the height $h(x, t)$ at that site by one, which is the simulation of an adatom being deposited onto site x. Then we calculate the hopping rate of

all surface atoms (not just the most recently deposited one), and select the atom with highest hopping rate to hop. The atom can hop to one of its nearest neighbor, i.e. site $x + 1$ or $x - 1$. If there are more than one atom with the same highest hopping rate, only one atom will be randomly selected and allowed to hop. The inverse of hopping rate is the time that the moving atom uses for its diffusion. In the next step, we compare the deposition time of new atom with the diffusion time of the hopping atom. If the new atom is not due to arrive the surface, the diffusion process continues by a hop of the atom with the highest rate at that time. After the combined hopping time of all atoms reaches the deposition time, a new adatom is deposited on the substrate. The hopping rate is calculated every time when the configuration of surface changes due to the diffusion. This results in an extensive time-consuming computation and requires high performance computing resources. The flow chart of the computing algorithm is shown in Fig. 2.3

In this thesis, we began with the study of the effect of the substrate temperature on homoepitaxial growth of the MBE model. After that, we modified the model to study the heteroepitaxial growth. The details and descriptions of the modified model, the Lattice Mismatch model, are in the next topic.

2.2.4 Lattice Mismatch Model

All of previous models are used to study homoepitaxial growth systems. In this section, we will describe the heteroepitaxial growth system. This model is modified from the MBE model and called a *Lattice Mismatch model* [5]. In heteroepitaxial growth system, substrate and thin film material are diffrent, that means the lattice constant of the substrate and the film can be different. Under epitaxy growth, atoms in thin film layer try to change their lattice constant to match the lattice constant of the substrate material. Since the volume of each atoms must

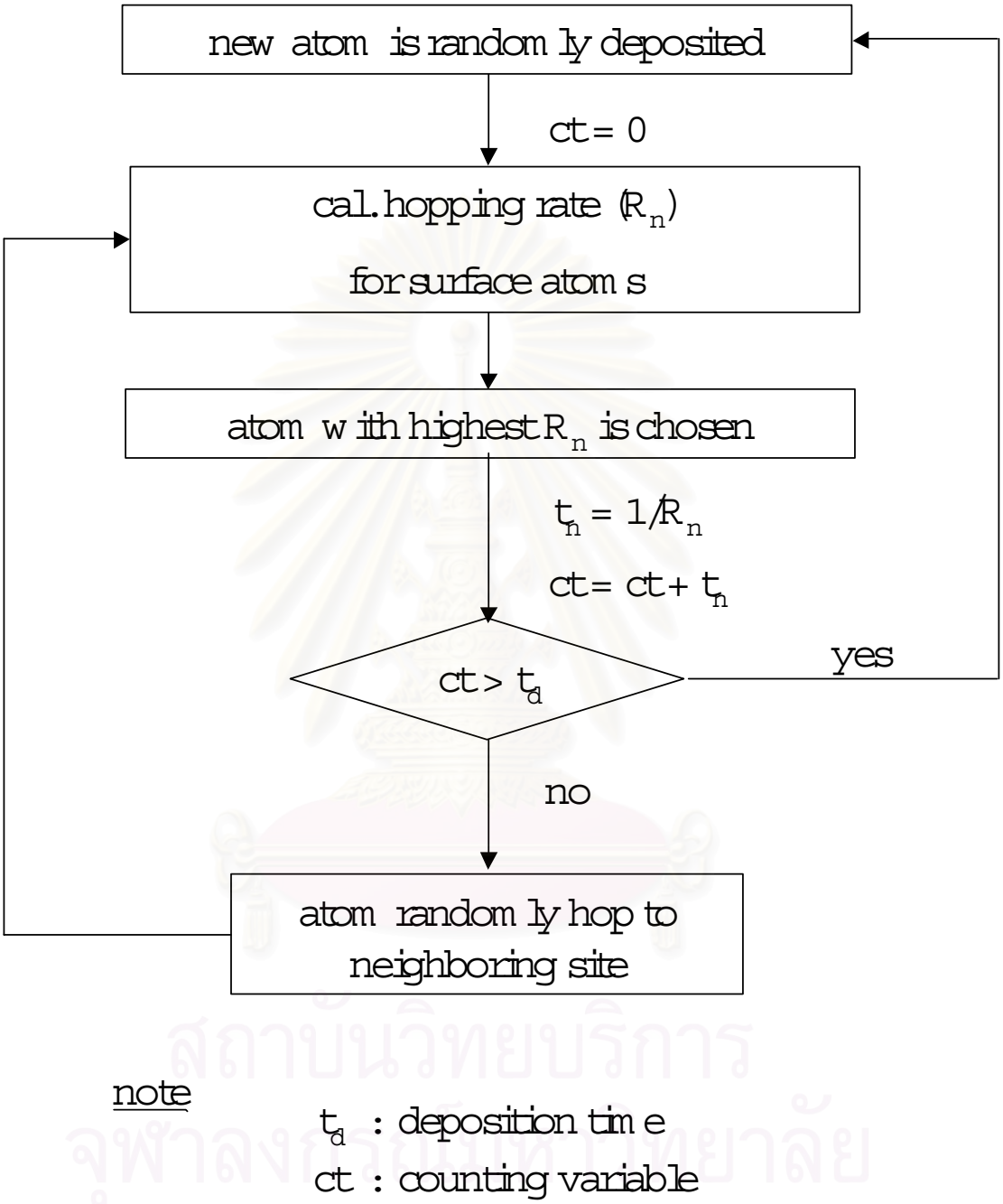

Figure 2.3: Flowchart of algorithm for MBE model

T(K)	$R_{n=1}$	$R_{n=2}$	$R_{n=3}$
300	8.9×10^{-10}	8.1×10^{-15}	7.3×10^{-20}
400	3.4×10^{-4}	5.7×10^{-8}	9.4×10^{-12}
500	0.81	7.7×10^{-4}	7.2×10^{-7}
600	149	0.45	1.4×10^{-3}
700	6320	43.6	0.30

Table 2.1: The Arrhenius hopping rates R_n in Eq. 2.1 at several substrate temperatures T and $n = 1, 2, 3$ for the MBE model.

be conserved, the shape of an atom changes when it changes its lattice constant. For example, if the atom compresses horizontally, it must extend vertically. When the atom changes its shape, the strain occurs in this heteroepitaxial growth. If the difference in the lattice constant of the two material is large, then atoms in the thin film layer need a big change in their shape and this lead to a strong strain in the crystal. We include the effect of strain in a new model to study the heteroepitaxial growth. The lattice mismatch model follows the same principle as the MBE model. The strain energy is incorporated into the hopping activation energy E of the Arrhenius hopping rate. Thus $E = E_{bond} - E_{strain}$ where E_{bond} is chosen to be

$$E_{bond} = \begin{cases} E_0 = (0.7NN + 0.2NNN) \quad eV. & ; \text{if } NN \leq 2 \\ E_1 = 4.0 \quad eV. & ; \text{if } NN = 3 \\ E_2 = 1.45 \quad eV. & ; \text{if step of height} \geq 2 \end{cases} \tag{2.2}$$

where NN is a number of nearest neighbors and NNN is a number of the next

nearest neighbors. E_{strain} is the strength of strain energy that is always positive. E_0 applies to single atoms, atom which has one nearest neighbor bond with atom beneath it, or atoms at step edges, except when step heights are of two layers or greater. E_2, a reduced barrier height, is applied to surface atoms on top of these steps so that the inclined(11) facets in our simulations are favored over the vertical ones. E_2 is chosen a little lower than that given by bond counting, E_0, since it was found in experiments that the inclined(111) facets are preferable over the vertical ones. Therefore, surface atoms on top of these steps should be promoted to diffuse to other sites. E_1 is the barrier for the rest of the surface atoms which have maximum coordination number of three. It is chosen a little higher than that given by bond counting to eliminate intrasubstrate breaking which is not seen experimentally [3]. The bonding energy in this model is also modified from the MBE model by extending the consideration to the next nearest neighbor bond. For edge atoms, the influence of strain is stronger than other atoms. So we normalize the strain energy and set it to be zero for all atoms except atoms at the edge. An edge atom is the atom at the edge of a terrace, i.e. an atom with one nearest neighbor of equal height and the other nearest nieghbor with lower height.

The computer simulation algorithm can be summarized as follows:

1. Choose a site x randomly and deposite one atom at that site by increasing the height $h(x,t)$ at that site by one.

2. Count the number of nearest neighbor and next nearest neighbor bonds of the surface atoms.

3. Select the corresponding E_{bond} according to Eq.(2.2) and calculate hopping rates of all surface atoms

4. Select the atom with the highest hopping rate. If there are more than one atom with the same highest rate, only one of those atoms will be randomly selected and allowed to hop.

5. The selected atom hops randomly to a nearest neighboring site. The diffusing time of the atom is calculated and kept in a counter variable.

6. The deposition time is compared with the diffusing time counter. If the time in the counter is still less than the deposition time, the algorithm in step 2-5 are repeated. In contrast, if the time in the counter is equal to the deposition time, the next atom is deposited and all algorithms starting from step 1 are repeated.

Results of our numerical simulations will be discussed in the next chapter.

2.3 Interface Width

When trying to understand the kinetic surface roughening behavior, one of the important quantities is the *interface width*, W, which is the root mean square height fluctuation around the average height of the surface. It is a function of the substrate size L and time t, and is defined as [4]

$$W(L,t) \equiv \langle (h(x,t) - \langle h(t) \rangle)^2 \rangle^{1/2}, \tag{2.3}$$

where $h(x,t)$ is the height of the growing surface at the site x and at time t above the flat substrate. The angular brackets represent an average over the entire substrate. $\langle h(t) \rangle$ is the averaged height of the growing surface at time t which is calculated from

$$\langle h(t) \rangle \equiv \frac{1}{L} \sum_{x=1}^{N} h(x,t). \tag{2.4}$$

The interface width can be used to quantitatively describe the roughness of the growing surface. We can plot the interface width versus the growing time in a log-log scale, namely *W-t plot*. Behavior of a typical *W-t plot* is shown in Fig 2.4. This plot shows the time evolution of the surface roughness. Typically, the *W-t plot* has two regions separated by the time t_c which is called the crossover time. In the region where $t \ll t_c$ we can see that the interface width increases as a power of time as

$$W(L,t) \sim t^{\beta}. \tag{2.5}$$

The exponent β or the *growth exponent* characterizes the time-dependent dynamics of the roughening process at $t \ll t_c$ region.

The second region, $t \gg t_c$, is the saturation region. The power-law behavior in the width does not continue indefinitely, but it is followed by a saturation region during which the interface width reaches an approximately constant value, W_{sat}. In Fig. 2.5, five different curves corresponding to the time evolution of the interface width from five different system sizes L are shown. As L increases, it can be seen that the saturation width, W_{sat}, increases as well. Further investigation shows that the dependence of W_{sat} on L also follows a power law as

$$W_{sat}(L) \sim L^{\alpha}. \tag{2.6}$$

This can be seen clearly in Fig. 2.6. The exponent α, called the *roughness exponent*, is another critical exponent that characterizes the roughness of the saturated interface. Moreover, we also found that the crossover time of the systems also increases as the substrate size increases. It was found that the crossover time depends on the substrate size L as the power law of L as

$$t_c \sim L^{z} \tag{2.7}$$

where z is called the *dynamical exponent*.

2.4 Height-Height Correlation Function

Mound or island formation are sometimes found in MBE growth films. There are many factors that can cause mound formation. One of the very well known factors is the Ehrlich-Schwoebel (ES) barrier exists in some homoepitaxy growth [19, 21, 22]. However, strain in heteroepitaxy growth also induce mounds on the surfaces. In the study of surface with island or mound formation in early time, the interface width is not an appropriate tool to study the surface. A useful

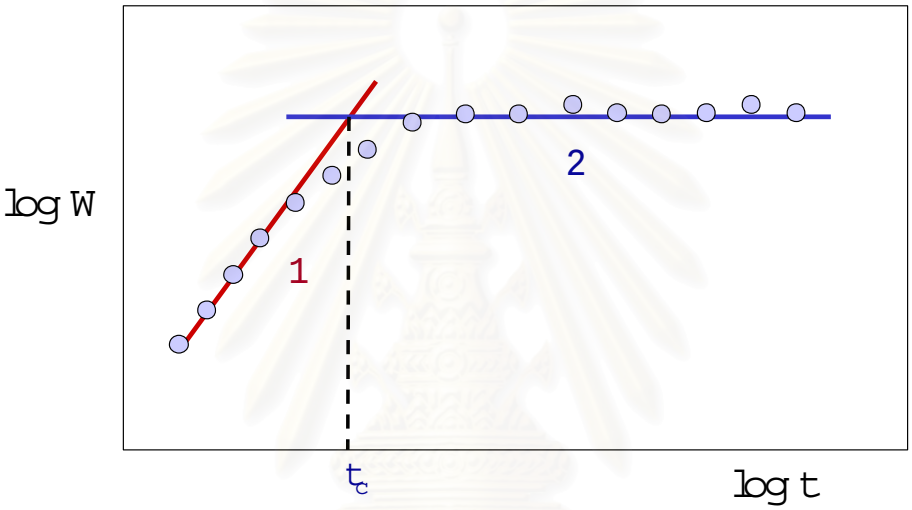

Figure 2.4: Time evolution of the interface width which has two regions separated by a crossover time t_c.

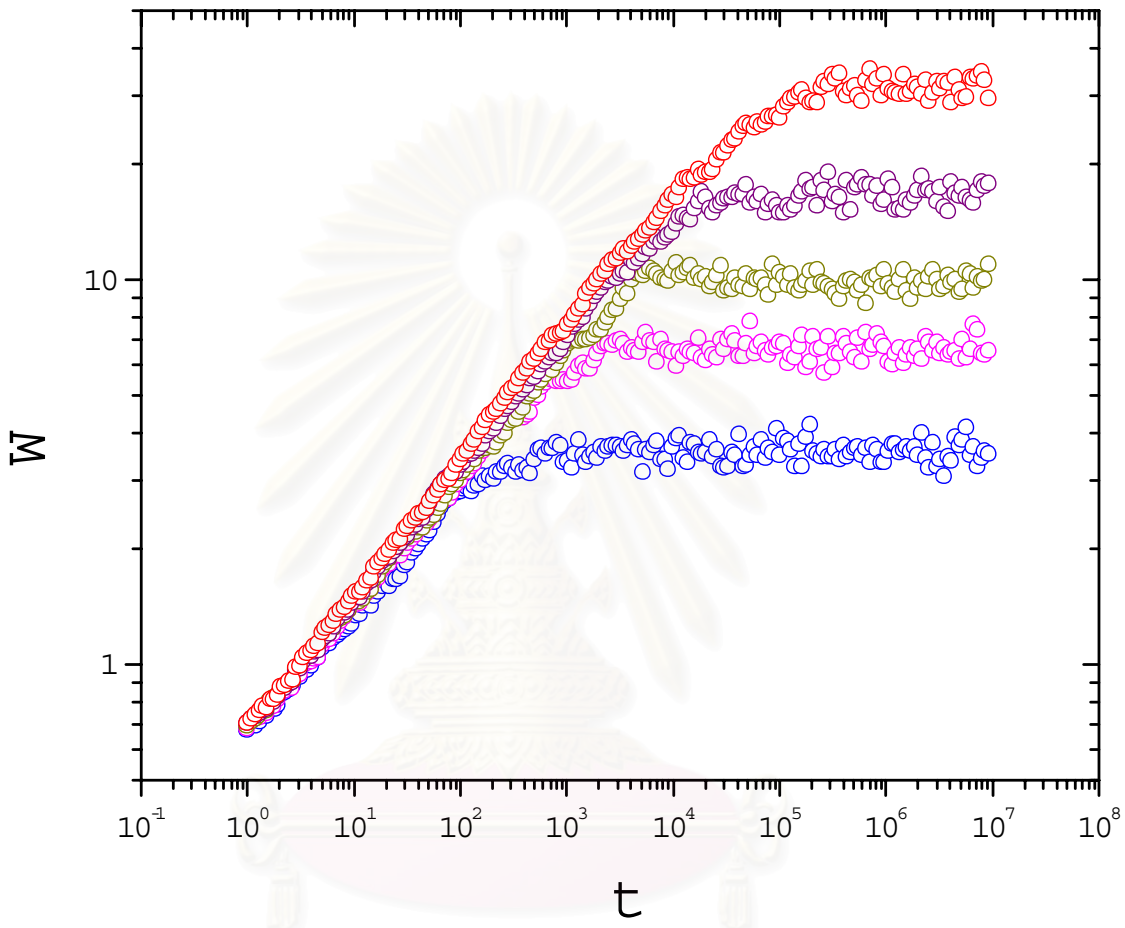

Figure 2.5: The plot of the interface width versus time t of the systems with different substrate size $L = 20, 30, 40, 60$ and 100 from bottom to top. We found the saturation regime and the crossover time increases when the substrate size L is increased.

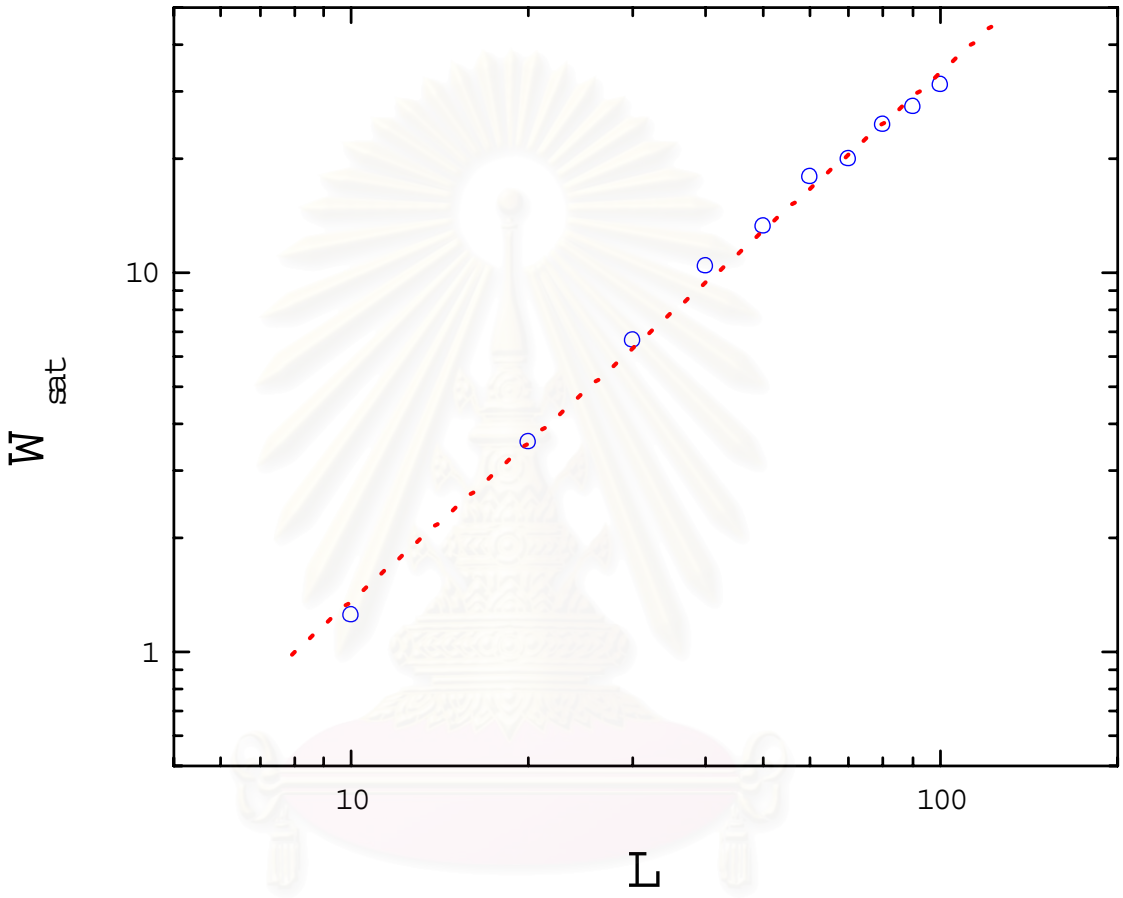

Figure 2.6: The plot of the W_{sat} versus substrate size L. As L increases, the saturation width, W_{sat}, increase as well, and the dependence also follows a power law.

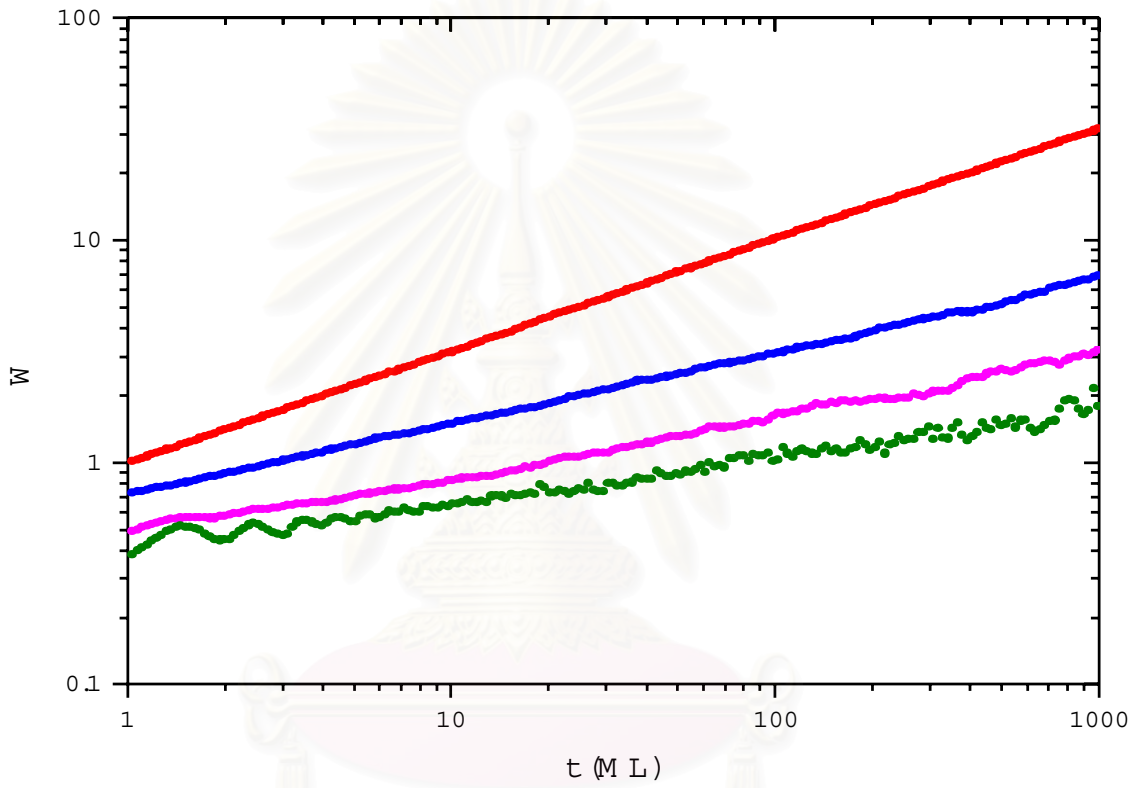

Figure 2.7: The interface width as afunction of time in log-log scale. The oscillation of the green line is a signature of the layer-by-layer growth.

quantity conventionally used to determine mounds or islands on the surface is the *height-height correlation function* $H(r)$, defined as [19, 20]

$$H(\mathbf{r}) \equiv \langle h(\mathbf{x})h(\mathbf{x}+\mathbf{r})\rangle_x, \tag{2.8}$$

where $< ... >$ represents the overall substrate averaging, h refer to the deviation of the surface height from the average height, and $r = |\mathbf{r}|$ is the distance between two sites on the substrate. The calculated $H(r)$ oscillates as a function of r, see Fig. 2.8, when the surface has regular mounded patterns. Other important characteristics of mounded patterns are the average mound radius and averege mound slope. Conventionally, the distance of the first zero-crossing of correlation function $H(r)$ is taken to be the average mound radius, and $[H(r=0)]^{1/2}$ is the average mound height.

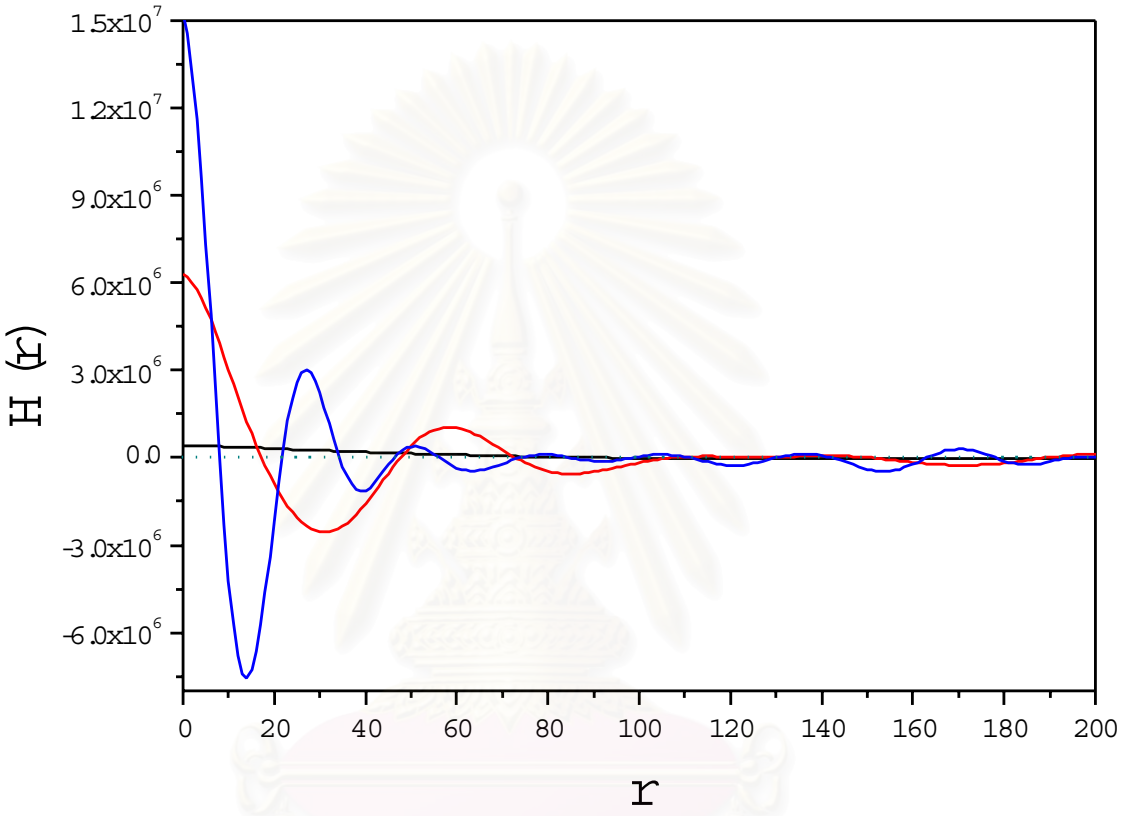

Figure 2.8: The height-height correlation function $H(r)$ which shown the oscillations as a function of r implies mound formation on the surface (the blue line and the red lines). But if there is no mound formation on the surface, there is no oscillation (black line).

Chapter 3

Simulation Results and Discussions

In this chapter, we will show all of our simulation results and analysis. First, we present our results from the homoepitaxial MBE growth system, i.e. the system which has no strain. Next, the simulation results of the heteroepitaxial growth system, i.e. the system with strain due to the lattice mismatch, will be presented. Our study is based on the one dimensional substrate that is flat at the initial time. Even though the one dimensional substrate growth has never been seen in the experimental laboratories, it is still important to study due to the existance of one dimensional interface roughening in real phenomena such as the snowflakes falling on the car windshield, waves clashing on the shoreline. Furthermore, we gain more insight in the dynamical properties of the MBE growth models by using less time in the simulations for the one dimensional growth models. For both models, atoms are deposited on randomly chosen sites on the flat substrate. Then, the diffusion process previously described in the last chapter will take place. In this work, the deposition rate of all simulations is taken to be one monolayer(ML) per second.

We will be looking at the morphology-the characteristic of the surface in both models. Next we calculate the interface width W for the MBE model and the height-height correlation function $H(r)$ for the Lattice Mismatch model. For the homoepitaxial growth, we are interested in the effect of the substrate temperature. In the case of the lattice mismatch model results, we are interested in the effect of

the substrate temperature and the strength of strain on the surface morphology. Although the main focus of this thesis is to study the MBE heteroepitaxial growth, the study of homoepitaxial growth using MBE model is still necessary since it is the basic model we started from.

3.1 Results of The MBE Model

The MBE model is designed to study the MBE homoepitaxial growth system under SOS constraints. It is somewhat more realistic than the other models in term of the diffusion rules as previously described in chapter 2. Any atoms on the surface (not just the most recently deposited atom) can hop randomly to a neighboring site at any time until they are completely buried while in other models, only the most recently deposited atom is able to move and after that it will be incorporated there permanently (with no longer move). For this work, we carry out the simulation using MBE model and investigate the effect of substrate temperature(T) from 400 K to 900 K. Parameters for activation energy were chosen to be $E_0 = 1.0$ eV, $E_b = 0.3$ eV [6] and the deposition rate is taken to be one monolayer per second. The substrate size of our systems is chosen to be 1000 lattice sites and films thickness are 1000 ML. In Fig. 3.1, we show the surface morphologies for the substrate temperature T = 400 K to 900 K. When the substrate temperatures are relatively low, in the range of 400 K to 600 K, the surface morphologies are very rough. The plot of interface width(W) as a function of time(t) is shown in Fig. 3.2. For 400 K and 600 K, the W-t plots for both substrate temperatures (red line and blue line in Fig. 3.2) overlap and the slope of this plot is 0.5 corresponding to the characteristic of the Random Deposition (RD) model [4], i.e. a model without diffusion, as discussed in the previous chapter. This implies that the MBE model at 400 K and 600 K show no diffusion of deposited atoms. Atoms which are deposited on randomly chosen sites cannot hop since they do not have enough energy to overcome the bonds originally formed. That leads to the domination of

the random deposition process. This is the cause of very rough surfaces for 400 K and 600 K. For higher substrate temperatures, the surface morphologies become smoother, see Fig. 3.1. As shown in the plot of the interface width as a function of time, in Fig. 3.2, for T = 650, 700, 750 K, the slopes of the W-t plot decrease from 0.5. This means that the growing rate of roughness is decreasing. When the substrate temperature increases, the energy of the atoms also increase, until they have enough energy to overcome the bonding energy, thus they are able to hop. The increase of the substrate temperature leads to the increase of the diffusion length[12, 13]. So the gaps on the surface are filled up when substrate temperature increases. Futhermore, the increase of the substrate temperature leads to the decrease of hopping time which, by comparing with lower T, is equivalent to the extension of the period that the new atom will arrive the surface in the simulation. That results in the increase of the diffusion time by comparison. The surface atoms have more time to diffuse to the suitable site leading to a smooth surface. When the layer is more complete, surface morphologies become smoother resulting in the decrease of growing rate of roughness. For higher substrate temperature at 800 K and 900 K, the surface morphologies are very smooth compared to those lower temperature ones, see Fig. 3.1. This is because the increase of substrate temperature to very high values results in the increase of the probability for surface atoms to continue to hop until they find the maximum bonding sites. In Fig. 3.2, we can see the oscillation of interface width which is the characteristic of a very smooth surface of a layer-by-layer growth. Why does the oscillation of interface width refer to the layer-by-layer growth ? It can be explained as the following. The interface width is the root mean square height fluctuation aroud the average height, in other word, it is the standard diviation of the height that represents a distribution of height around the average height. In the beginning when the atoms are deposited on the substrate under the layer-by-layer mode, the average height is zero that results in the increase of interface width. After that the average height increases and at the same time more atoms are filling the layer more and

more until they fill a half of the layer, the distribution of the height come near the average height at 1 that result in the decrease of interface width. When atoms fill up the layer the interface width must be zero again. This will repeat when the new layer is deposited. If the growth is absolutely layer-by-layer, then the width will continue its oscillation with the average value of W remaining at constant. Nevertheless, for our result, it is not an absolute layer-by-layer growth so that the average interface width still gradually increases as a function of time while the oscillation slowly damps out as seen in Fig 3.2.

3.2 Results of The Lattice Mismatch Model

The lattice mismatch model is modified from the MBE model, and is used to study the heteroepitaxial growth. The activation energy in the Arrhenius hopping rate is changed by including the strain effect resulted from lattice mismatch between the lattice constant of the substrate and the thin film material. Moreover, while the MBE model concerns just the nearest neighbor bonding energy, the lattice mismatch model extends the calculation to the next nearest neighbor bonding energy. The other part of the model follows the same principle as the MBE model. For this work, we observe the characteristic of the surface when the substrate temperature and the strength of strain are varied. The *height-height correlation function*, $H(r)$, is used to determine the mound formation and the average mound radius. In our simulation, we varied the strength of the strain from 0.8 eV to 2.0 eV which is a half of the maximum bonding energy E_1 in Eq. 2.2 and varied the substrate temperatures from 550 K to 750 K. In general, the effect of strain is active for every atom but more so for edge atoms. We can simply normalize and set strain energy to be zero for all atoms except atoms at the edges because the most important thing is the comparison of the hopping rate of each atom, not the absolute value of the hopping rate itself. An edge atom is defined as an atom which one side of it is a step with the height higher than the neighboring site and

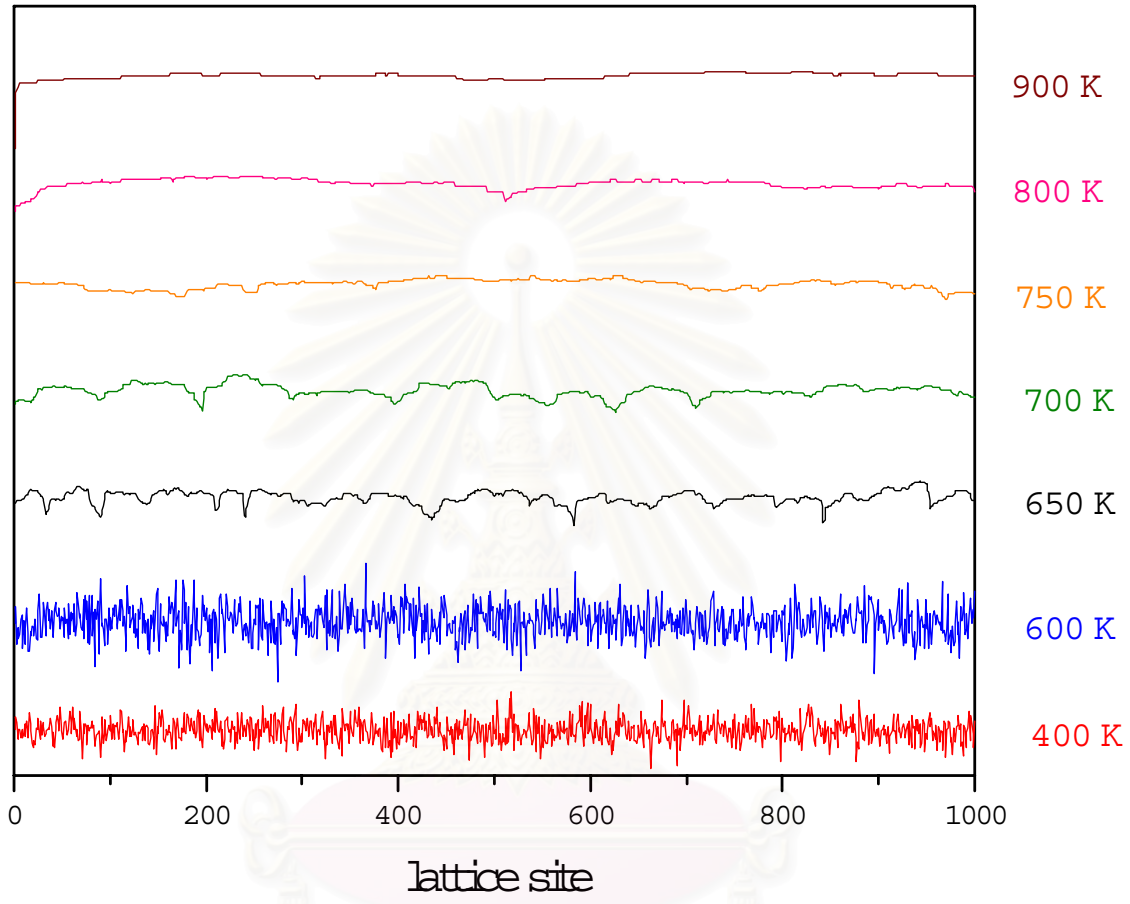

Figure 3.1: The surface morphologies of the MBE model for T= 400 K, 600 K, 650 K, 700 K, 750 K, 800 K, and 900 K after depositing 10^3 ML on a substrate of size $L = 10^3$ lattice sites. For low substrate temperature T = 400 K and 600 K, the surface is very rough. For higher temperature, the surface morpholgies become smoother.

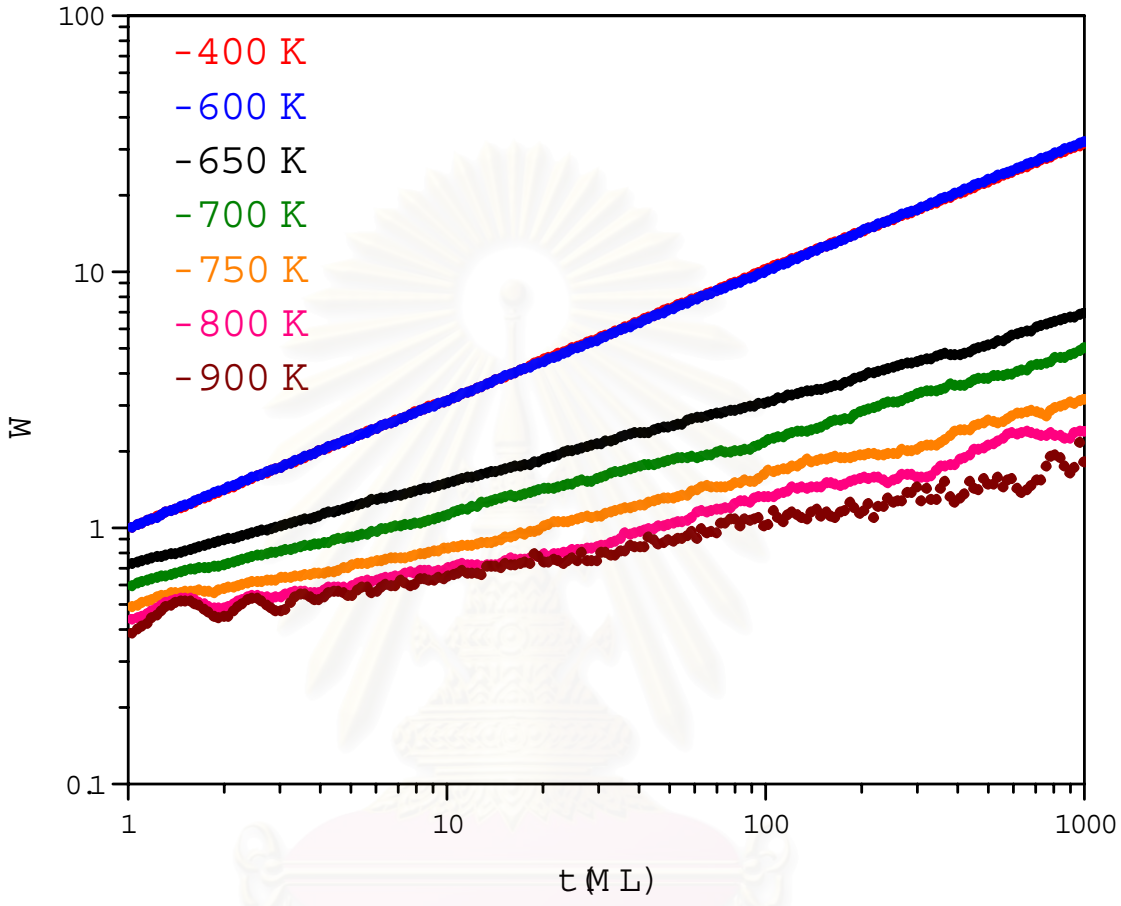

Figure 3.2: The w-t plot of the MBE model for T= 400 K, 600 K, 650 K, 700 K, 750 K, 800 K, and 900 K after depositing 10^3 ML on a substrate of size $L = 10^3$ lattice sites. The w-t plot for low temperature, 400 K and 600 K, are overlap and give the growth exponent $\beta = 0.5$ same as RD model. For higher T, the growing rate of interface width decrease. And for high T at 900 K, we can see the oscillation of interface width which is the characteristic of very smooth layer-by-layer growth.

the another side is the terrace. We carry out the simulation with the initial flat substrate and substrate size and thickness deposited are chosen to be 1000 and 10 ML, respectively.

3.2.1 The Lattice Mismatch Model with No Strain

The bonding energy in the lattice mismatch model is different from the MBE model as shown in Eq.(2.2). Therefore, we carry out our simulations of the Lattice Mismatch model without effect of strain and compare with the original MBE model. In Fig. 3.3, we show the surface morphologies of the lattice mismatch model at 10 ML when the substrate temperature is increased from 550 K to 750 K. We found that the surfaces become smoother when substrate temperature increases, similar to the MBE model. The increase of substrate temperature results in the increase of energy of atoms, corresponding to the increase of the probability for the atoms to continue hopping until they find maximum bonding sites. The growing rate of the interface width decreases when the substrate temperature increases, see Fig. 3.4, and the oscillation of the interface width which is the charateristic of a very smooth layer-by-layer growth appears at high temperature of 750 K. We did not find the oscillation of the height-height correlation function in all substrate temperatures in this case, see Fig. 3.5. This implies that no mound appears on the surface. From all the results, The Lattice Mismatch model with no strain tends to be the same as the MBE model.

3.2.2 The Lattice Mismatch Model with Strain Effect

In this work, we varied the strength of the strain from 0.8 eV to 2.0 eV. The increase of the strain energy relates to the increase of the lattice mismatch between the substrate and the thin film material. First, we investigate the effect of strain on the model when substrate temperature is fixed. At T = 550 K (Fig. 3.6), when we apply the strain effect on the model, the surface morphologies change its shape.

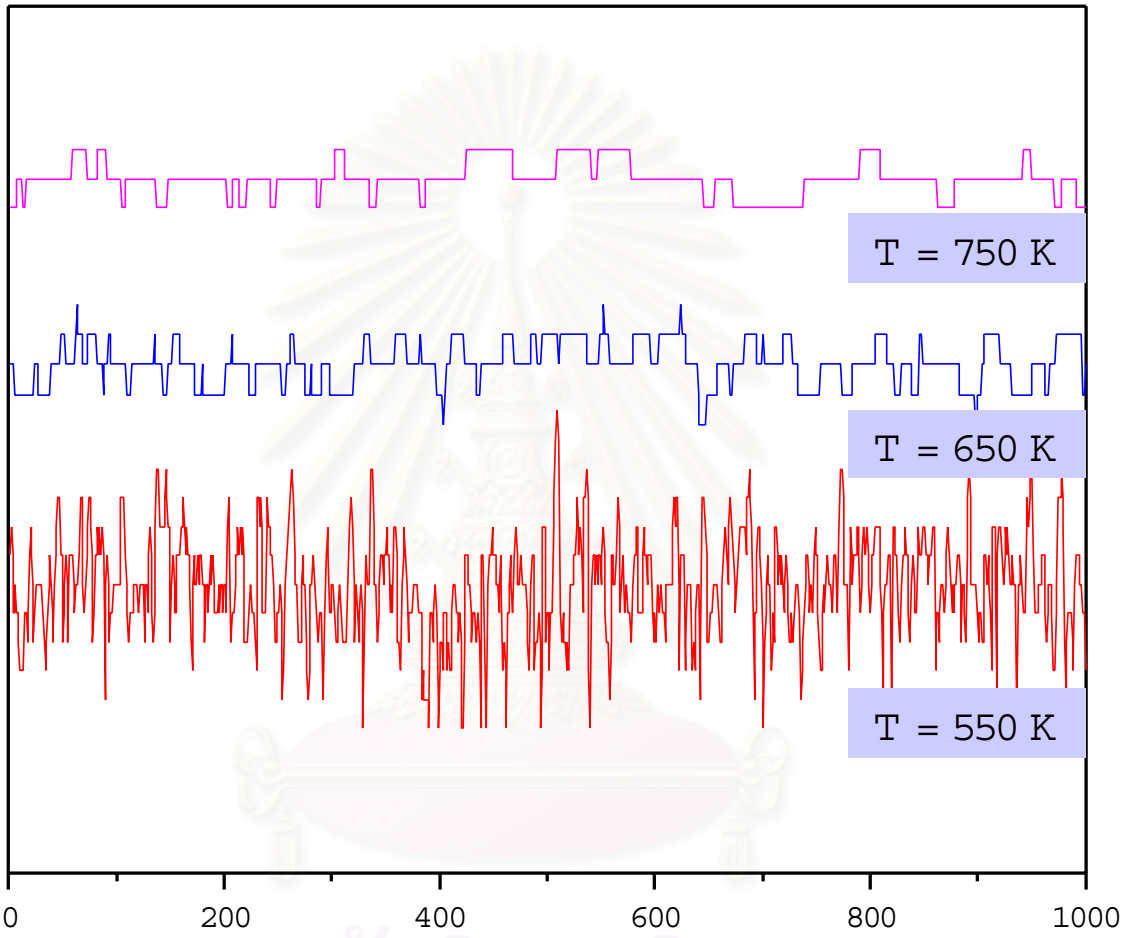

Figure 3.3: The surface morphologies of lattice mismatch model without strain for substrate temperature 550 K, 650 K and 750 K from bottom to top at 10 ML.

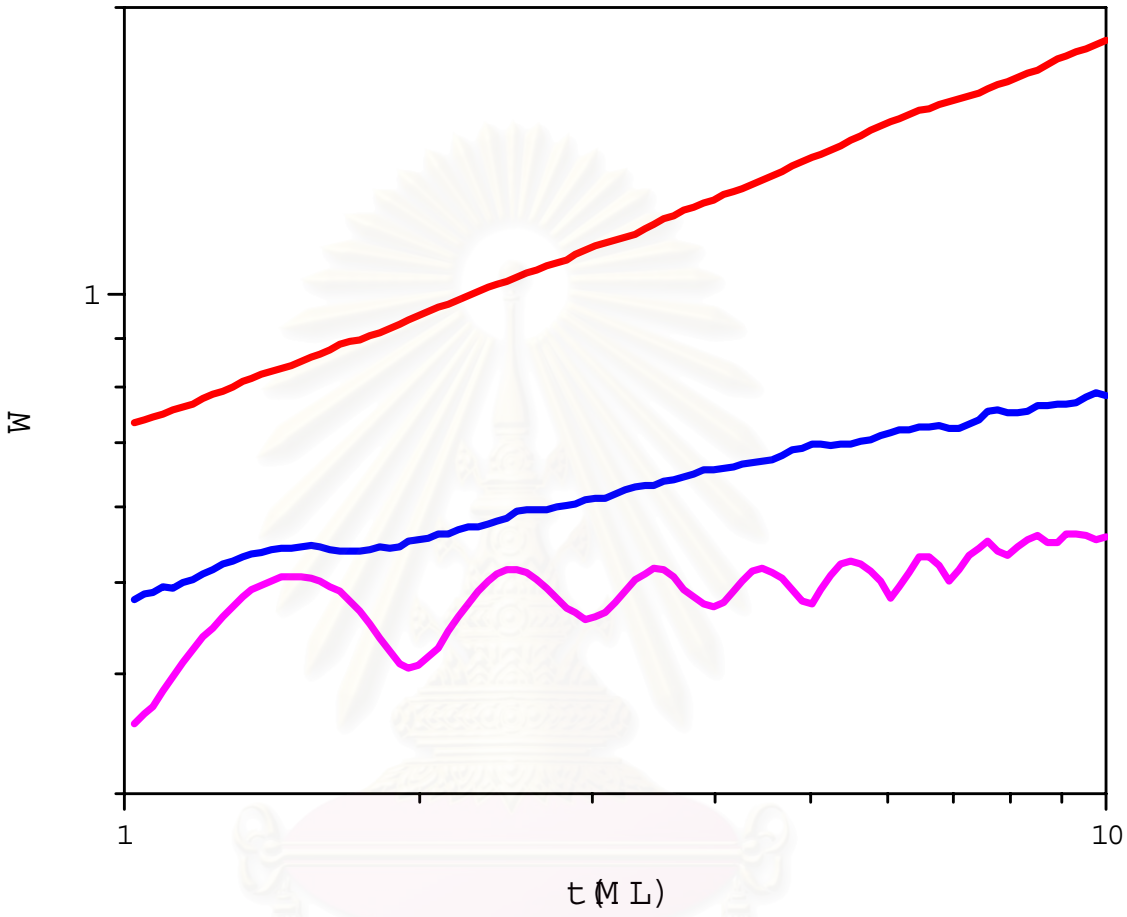

Figure 3.4: The w-t plot of lattice mismatch model without strain for substrate temperature T = 550 K, 650 K and 750 K from top to bottom at 10 ML. The growing rate of interface width decrease when substrate temperature increase and the oscillation, which is the characteristic of very smooth layer-by-layer growth, appear at high temperature.

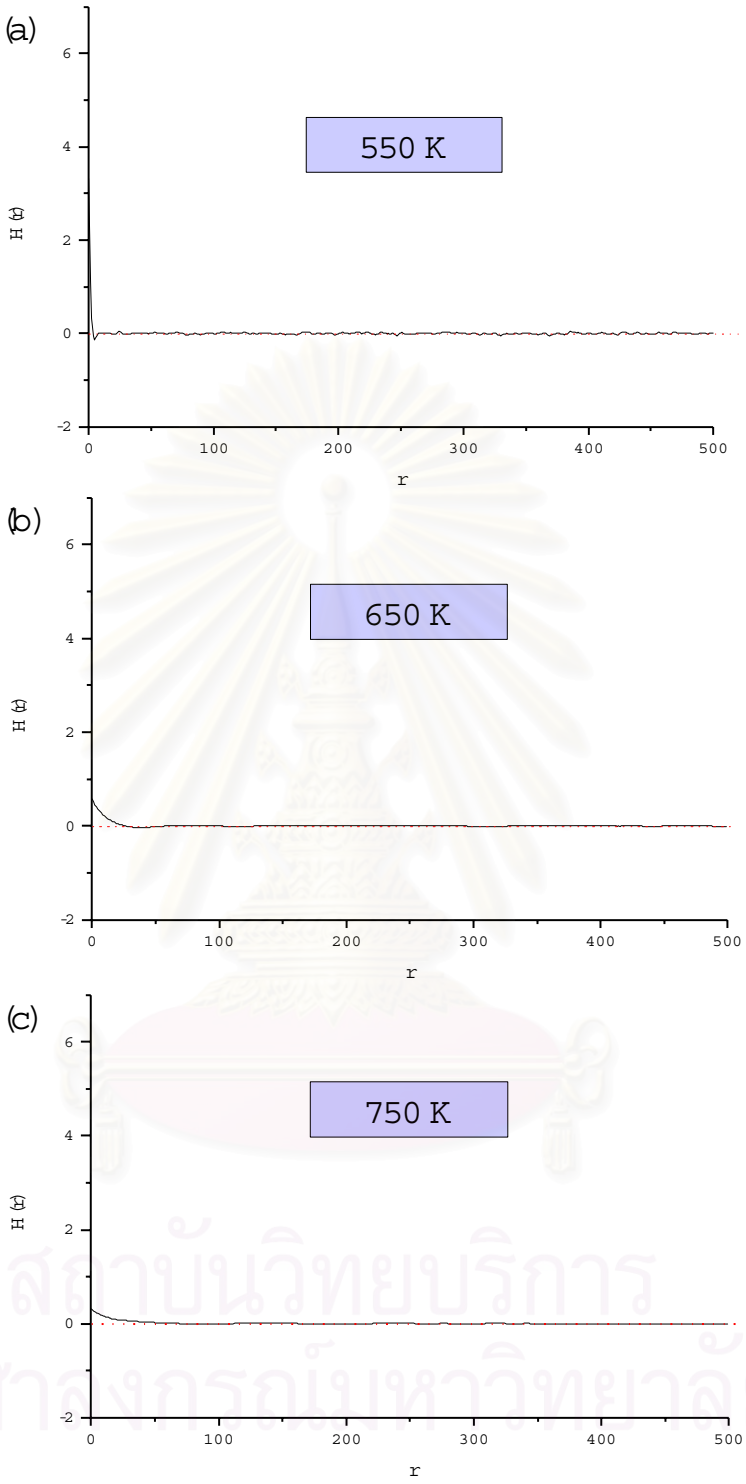

Figure 3.5: The height-height correlation function $H(r)$ of lattice mismatch model without strain for substrate temperature T = 550 K, 650 K, 750 K at 10 ML from top to bottom.

When we zoom in the surface morphologies, see Fig. 3.6 b, surface morphologies show pyramid-type structure. For 650K and 750 K, the effect of the strain is obviously observed on the surface morphologies. The smooth surfaces become kinetically rough. The formation of mound occurs, see Figs. 3.7 and 3.8, which can be determined by the oscillatory height-height correlation function. It can be explained that more surface atoms diffuse to the upper terrace with increasing probability due to the effect of strain. From the height-height correlation function $H(r)$, shown in Fig. 3.9, the oscillation of $H(r)$ is obviously seen beginning when the strain energy = 1.2 eV for all substrate temperatures. It implies that the effect of the strain leads to the mound formation on the surface when the strength of strain reach a critical value [14]. If the strain is too weak, however, it will not induce mound formation in the system. The strength of the strain 0.8 eV is not enough to cause mound formation in our case. The 0.8 eV strain leads to just a rough surface as shown in Figs. 3.7 and 3.8. From our results, the critical value for the strain should be between 0.8 eV and 1.2 eV. In other words, the heteroepitaxial growth leads to a mound formation on the surface when the lattice mismatch between substrate and thin film is large enough. We also found that the oscillation of $H(r)$ started and was obvious at thickness of 2 ML for all substrate temperatures and all values of strain that lead to mound formation, see Fig. 3.10.

An interesting question arises from our finding: why do we not see the oscillation in H(r) at 1 ML ? Our answer is that because at the beginning, there are very few atoms on the surface and the atoms are far apart. IT is very unlikely for the diffusing atoms to come together and form an assemble. However, the assemble of the diffusing atoms is what leads to mound formation because the effect of strain is felt at the atoms a the edge of the assemble. So mound formation does not occur at 1 ML. It may be implied that the critical thickness leading to the mound formation on the surface should be between 1 ML and 2 ML in our simulations, agreeing with previous works [1, 5, 15, 16, 17]. Furthermore, we found

that the average mound radius increases when the film thickness increases for all substrate temperatures and all values of strain, see Fig. 3.11. When the thickness increases, number of atoms increases and the distance of free space between atoms decreases. That results in the high chance that diffusing atoms and small mounds can form an assemble. That causes the average mound radius to increase. In Fig. 3.11, at the same thickness, the average mound radius increases with the increasing substrate temperature. In Fig. 3.12, we plot the average mound radius as a function of the substrate temperature for the strain energy of 2.0 eV. We found that the average mound radius increased exponentially when the substrate temperature increased as observed in the experiment[23, 24]. For other systems with different values of the strain energy, this exponential growth behavior is still observed. It was found that the diffusion length of surface atoms increase exponentially when the substrate temperature increases[12, 13]. This mean the atoms can diffuse farther when the substrate temperature is higher. So that atoms can diffuse faraway and assemble themself with other atoms or mounds to form a larger mounds or sometime called islands. That results in the increase of average mound radius. Furthermore, at higher temperature, the diffusion time is shorter, i.e. the atom uses a shorter time to move from its initial site to a new site. So atoms can diffuse many steps before a new atom is deposited, which is equivalent to the increase of the probability of atoms to continue hopping until they assemble with other atoms or mounds.

Next, we are interested in the result of the strength of the strain on the average mound radius. We plot the average mound radius as a function of strain energy for T = 550 K and 650 K at 3, 4 ,10 ML, as shown in Fig. 3.13. We found that the evolution of the average mound radius shows the same tendency. At the same thickness, we can detect the mound formation at the strain energy of 1.2 eV. and the average mound radius does not significantly change when the strain energy increases. According to the previous result, the strain effect leads to the jump of the diffusing atom up to the upper terrace. So, we propose that the

effect of the strain should have an effect on the vertical growth of the mound size. Therefore we cannot find a specific relationship between the increase of the strain energy and the average mound radius. Moreover, we cannot see any relationship between the increase of the strain energy and the average mound height since the thickness used in the simulation is not enough. That reults in the average mound height not being obviously different for all systems with different strain energies, substrate temperatures, and thicknesses.

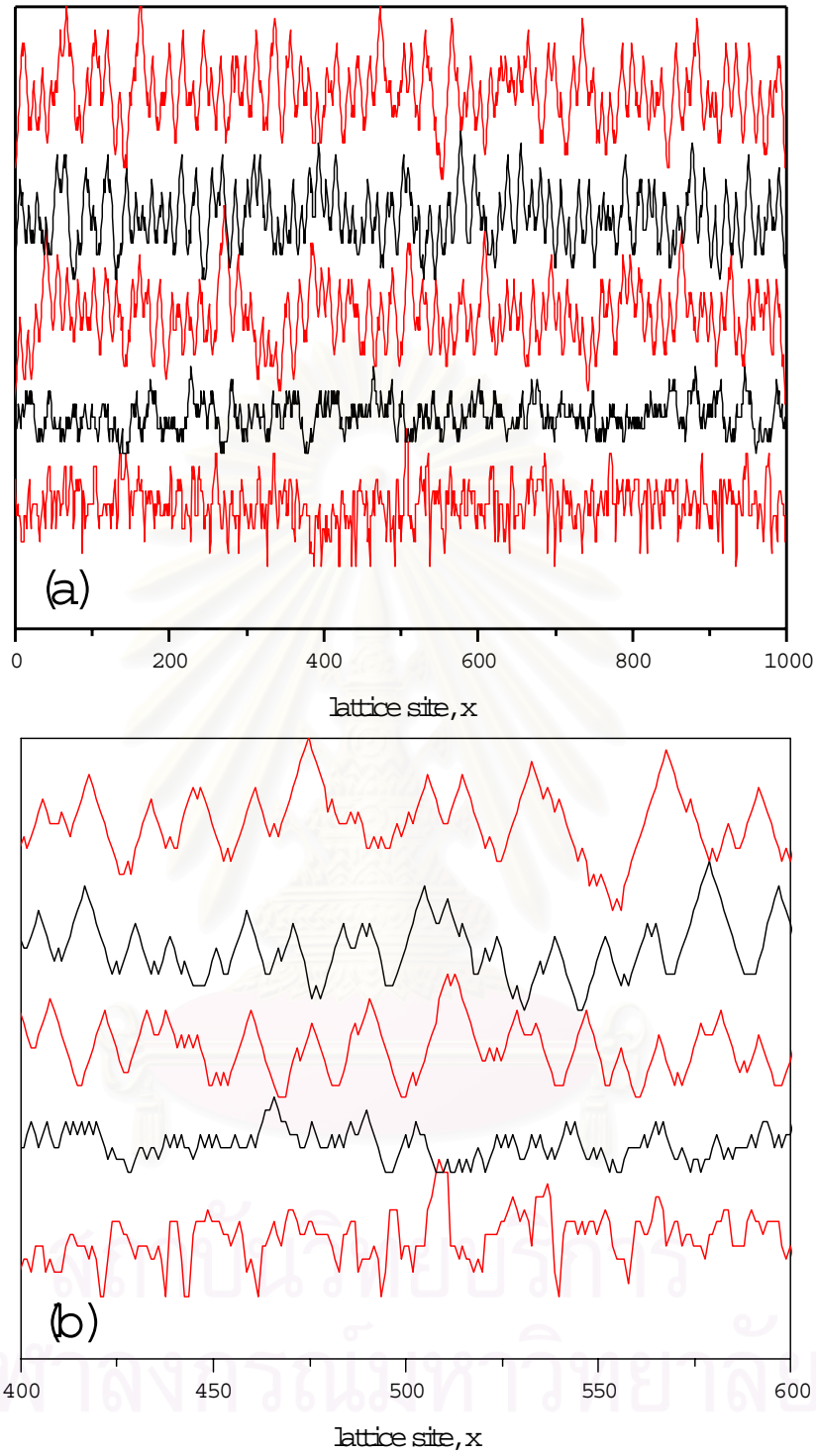

Figure 3.6: The surface morphologies of lattice mismatch model for T = 550 K, substrate site = 1000 at 10 ML when strain energy increase. Strain energy = 0, 0.8, 1.2, 1.6, 2.0 eV from bottom to top. a) Show the morphology entire substrate and zoom in to show morphology of 200 lattice sites(400-600) in b).

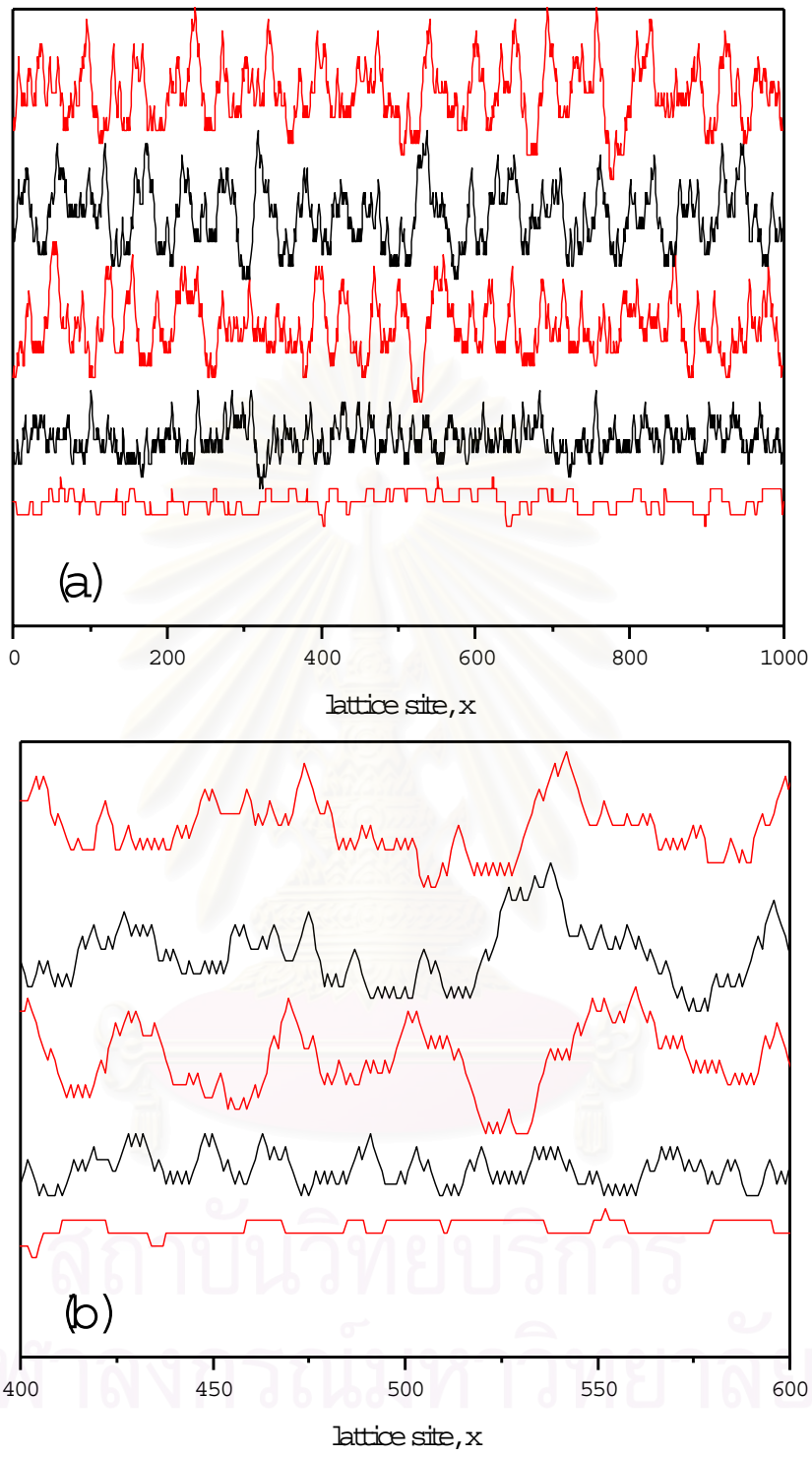

Figure 3.7: The surface morphologies of lattice mismatch model for T = 650 K, substrate site = 1000 at 10 ML when strain energy increase. Strain energy = 0, 0.8, 1.2, 1.6, 2.0 eV from bottom to top. a) Show the morphology entire substrate and zoom in to show morphology of 200 lattice sites(400-600) in b).

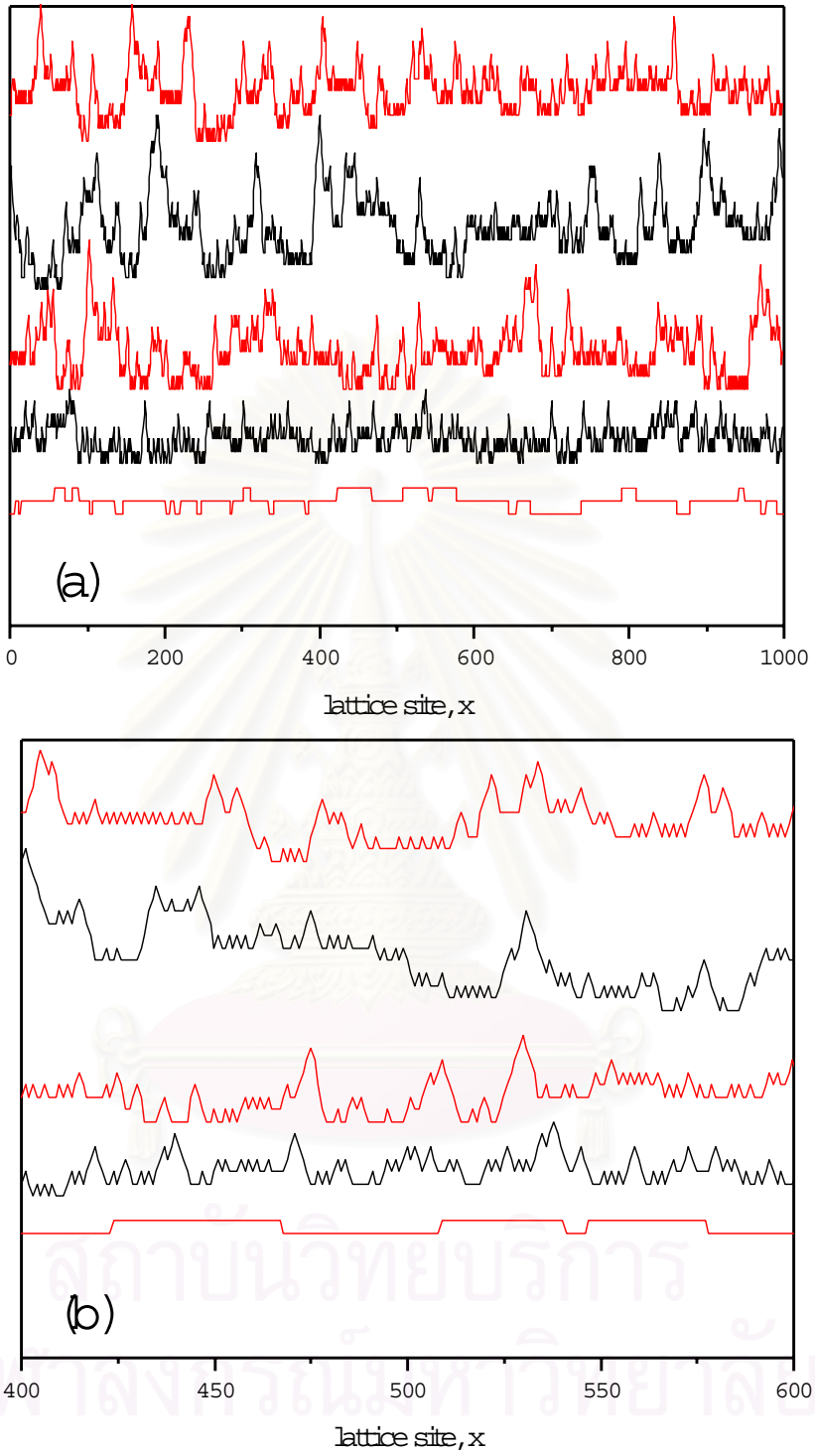

Figure 3.8: The surface morphologies of lattice mismatch model for T = 750 K, substrate site = 1000 at 10 ML when strain energy increase. Strain energy = 0, 0.8, 1.2, 1.6, 2.0 eV from bottom to top. a) Show the morphology entire substrate and zoom in to show morphology of 200 lattice sites(400-600) in b).

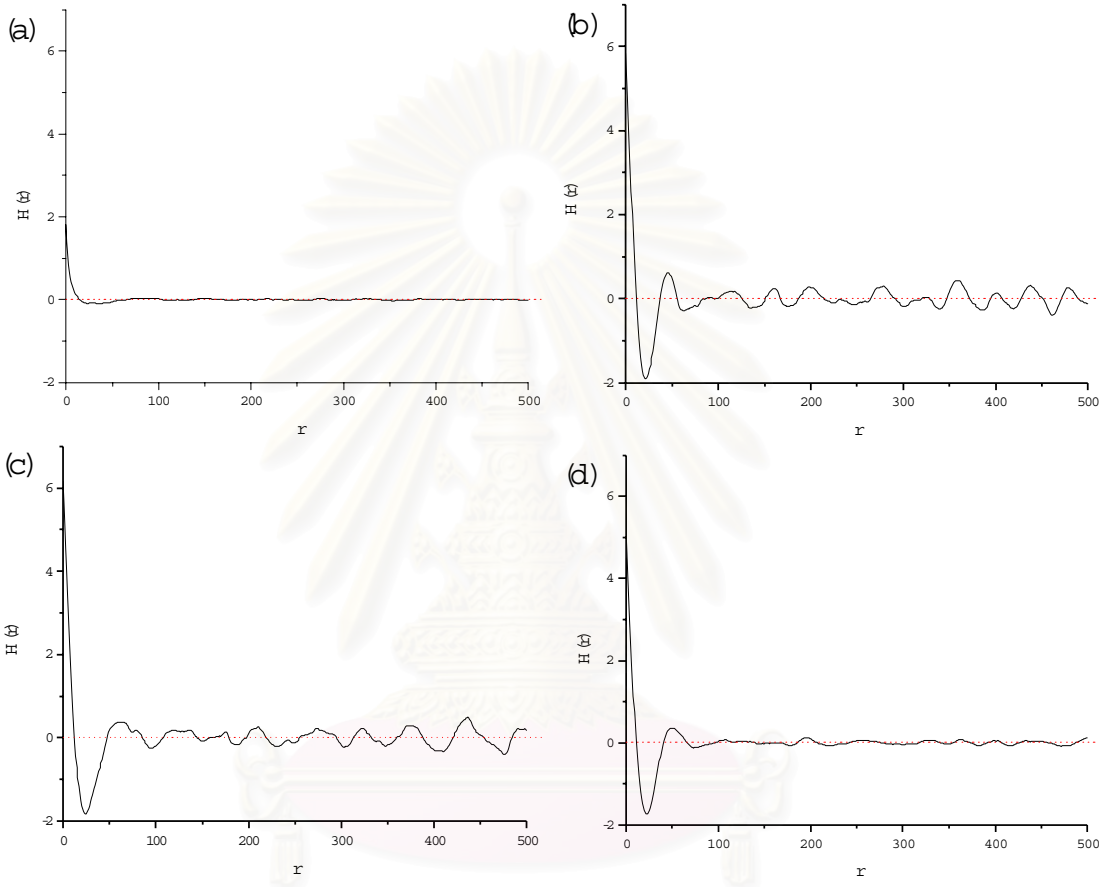

Figure 3.9: The height-height correlation function $H(r)$ of lattice mismatch model for T = 650 K, substrate site = 1000 at 10 ML when strain energy increase . Strain energy = (a) 0.8 eV, (b) 1.2 eV, (c) 1.6 eV , (d) 2.0 eV.

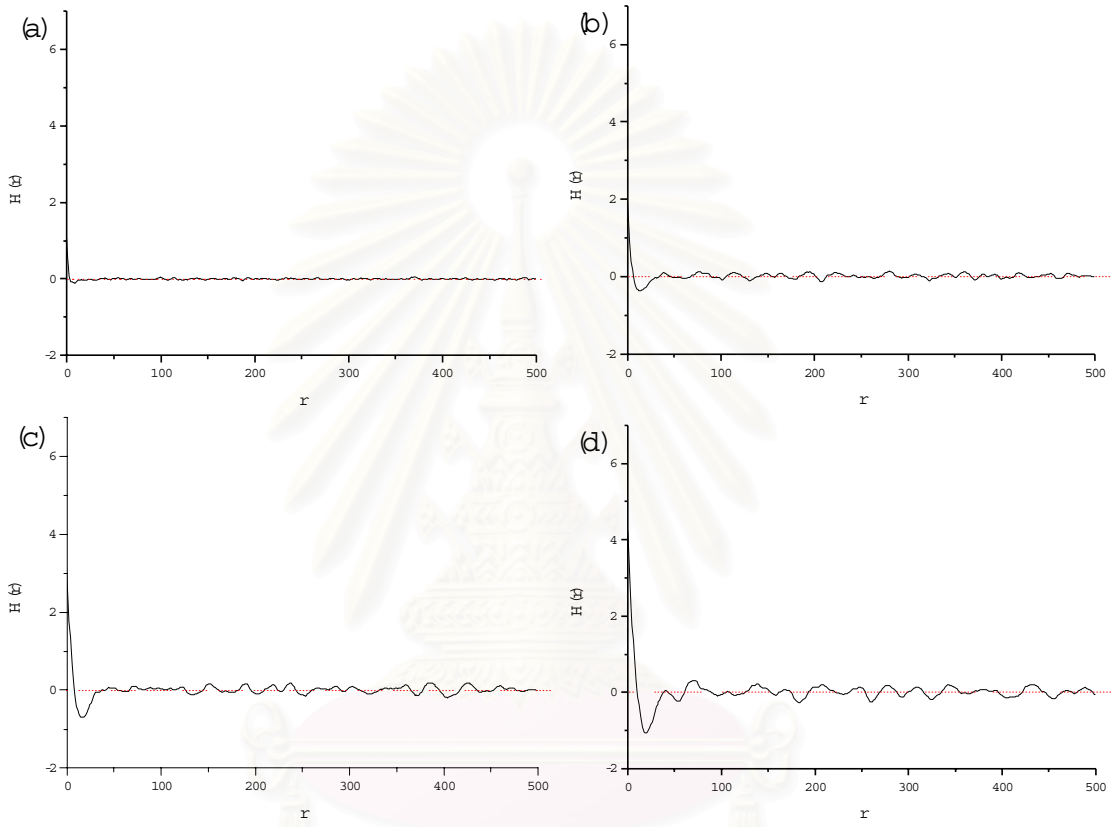

Figure 3.10: The height-height correlation function $H(r)$ of lattice mismatch model for T = 650 K, substrate site = 1000 at strain energy = 1.6 eV. Thickness = (a) 1 ML, (b) 2 ML, (c) 3 ML , (d) 5 ML.

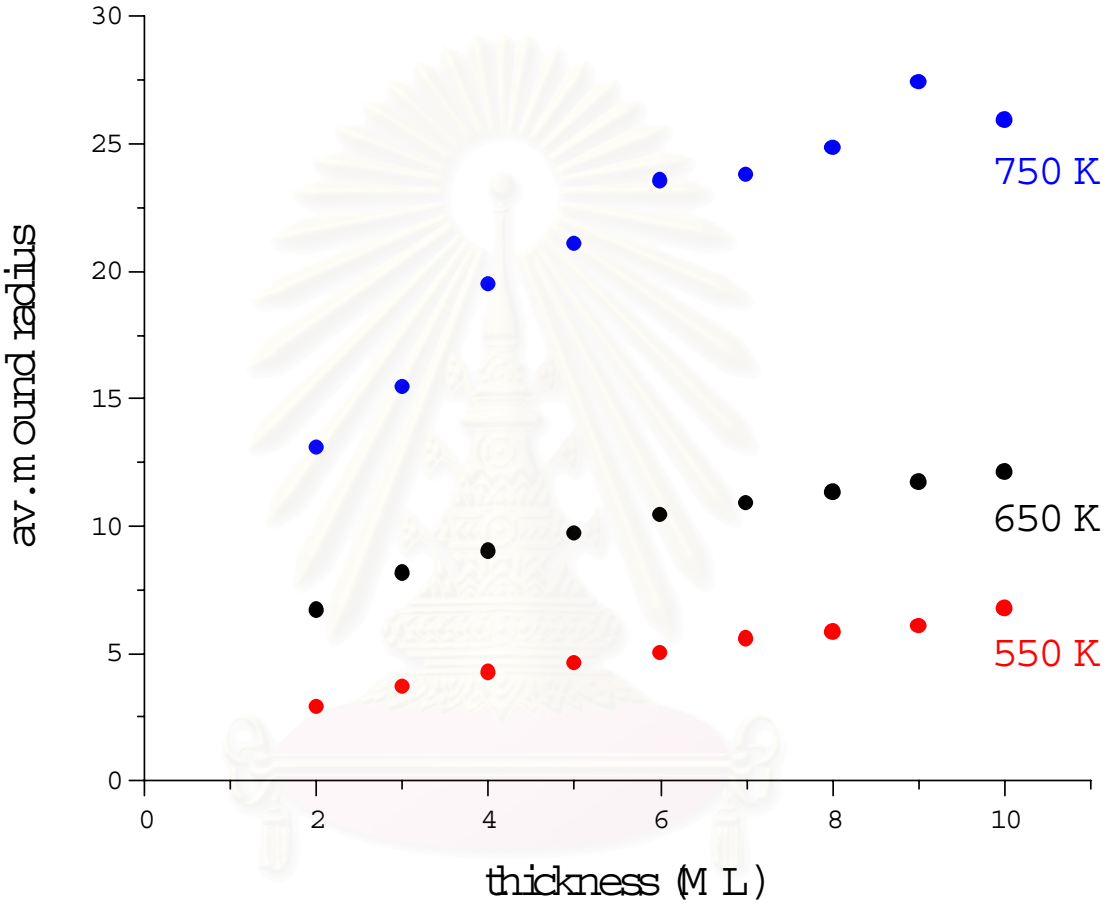

Figure 3.11: The plot of average mound radius versus thichness at strain energy = 2.0 eV for substrate temperature T = 550 K, 650 K, and 750 K.

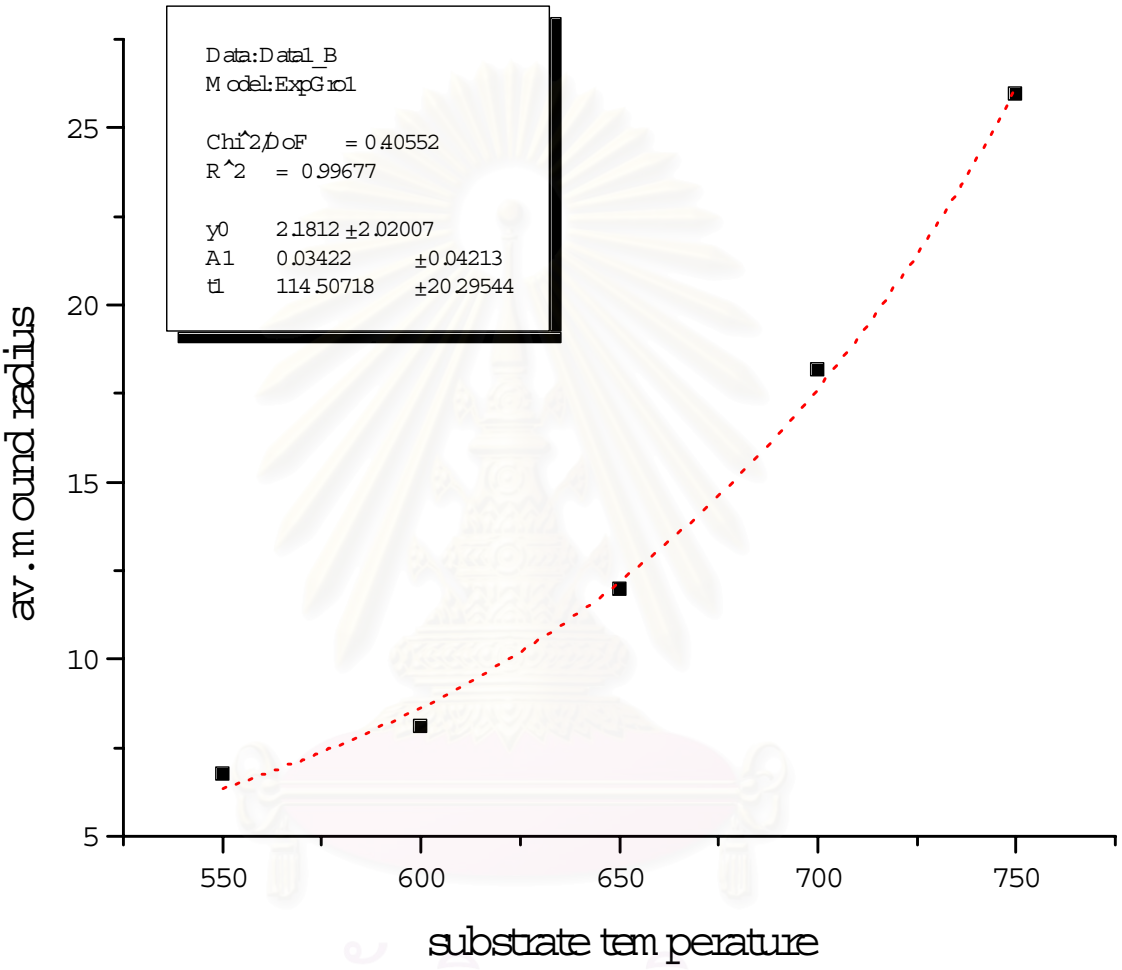

Figure 3.12: The plot of average mound radius versus substrate temperature for strain energy = 2.0 eV at 10 ML.

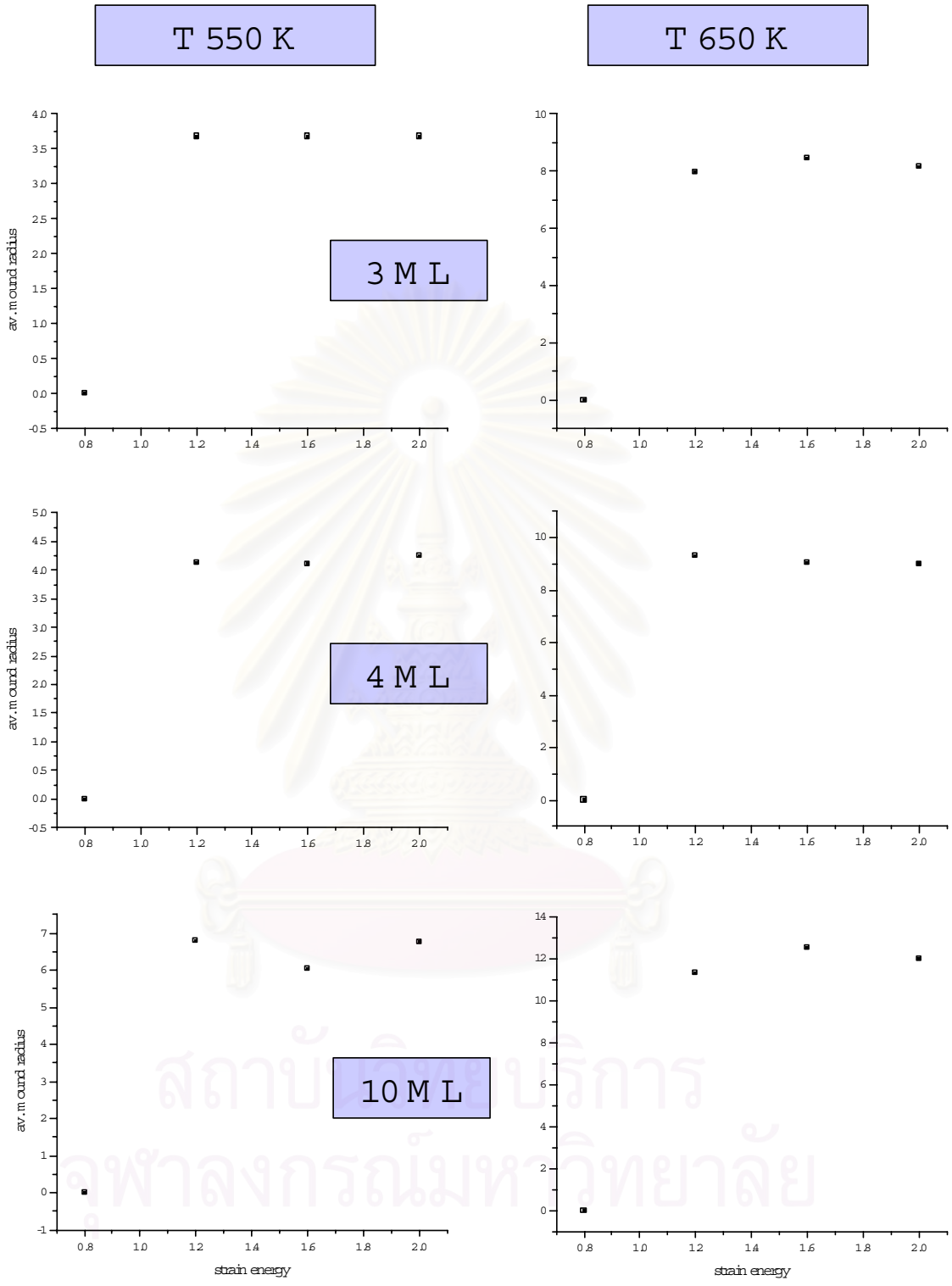

Figure 3.13: The plot of average mound radius versus strain energy for T = 550 K and 650 K at 3, 4, 10 ML.

Chapter 4

Conclusions

We have studied homoepitaxial MBE growth system, a system without strain, using computer simulation of the MBE model. We, then, modified the original MBE model for the study of heteroepitaxial MBE growth system which is a system with different material in the substrate and thin film layer. Our modified model is also know as the Lattice Mismatch model. It was modified in the part of the activation energy of the Arrhenius hopping rate by adding the effect of strain that resulted from the mismatch of the lattice constant between the substrate and the thin film material in the heteroepitaxial growth system. We looked into the effect of the substrate temperature, which was the energy source for the surface atoms to diffuse, for both types of MBE systems. We investigated the influence of strain on the characteristic of the surfaces especially for the heteroepitaxial growth system. The characteristic of surface we studied are the dynamic of morphological evolutions, interface width that is used to measure the roughness of the surface, and the height-height correlation function used to determine the mound formation and study mound properties.

For the MBE model, we found that when the substrate temperature is low in the range of 400 K to 600 K, the surface morphologies are very rough. When considering the plot of interface width as a function of time, the slope β for both temperatures are 0.5 corresponding to the Random Deposotion model, i.e. a model with no diffusion. This means for these temperatures, atoms in the MBE model cannot move or diffuse at all. This is because deposited atoms which are dropped

randomly do not have enough energy to overcome the bond originally formed. This is the cause of very rough surfaces for 400 K and 600 K. For higher temperatures, the surfaces become smoother and the growing rate of roughness decreases. When the substrate temperature is increased, the energy of the deposited atoms also increase until they have enough energy to overcome the bonding energy. The atoms begin to break their original bonds and are free to diffuse on the surface filling up the gaps or empty sites on the surface. For very high substrate temperature, for example at 900 K, the surface morphology is very smooth and the interface width oscillates in the w-t plot, which is the chatracteristic of a very smooth layer-by-layer growth.

For the Lattice mismatch model, firstly we carried out simulation of the model without strain i.e. set the strain energy to zero and compared to the MBE model. We found that the transition of surface morpholgies depends on the substrate temperature in the same way as in the MBE model. Then, we added the effect of strain to study the heteroepitaxial growth. At 550 K, the surface morphologies changed its shape and became a pyramid type. For 650 K and 750 K, the effect of the strain is more obvious on the surface morphologies. The smooth surfaces became kinetically rough with mound formations. The mound formation can be detected from the oscillation in the height-height correlation function $H(r)$. The critical strength of the strain that leads to mound formation is between 0.8 and 1.2 eV. for all substrate temperatures. In other words, the lattice mismatch between the substrate and the thin film needs to be large enough so that the mounds can be formed. Futhermore, we found that we begin to observe the formation of the mounds at 2 ML and the average mound radius increased as a function of the film thickness. It implied that the critical thickness leading to the mound formation on the surface should be between 1 ML and 2 ML. In other words, the critical thickness for mound formation in heteroepitaxial growth should be between 1 ML and 2 ML. Moreover, the average mound radius exponentially increased when the substrate temperature is increased as in the experiment[23, 24].

This is because when the substrate temperature increases, atoms can diffuse for a longer distance corresponding to higher probablity for the atoms to continue hopping until they assembled with other atoms or mounds. Then we studied the influence of the strength of the strain on the time evolution of average mound radius. At a constant substrate temperature, the evolution of average mound radius for every film thickness shows the same trend. We can detect the mound formation at the strain energy of 1.2 eV and the average mound radius does not significantly change when the strain energy increases. According to the previous result, the strain effect leads to the jump of the diffusing atom up to the upper terrace. Thus, we propose that the effect of the strain should effect on the vertical enlargement of the mound size. Therefore, we cannot find a relationship between the increase of the strain energy and the average mound radius. Moreover, we cannot see a relationship between the increase of the strain energy and the average mound height because the thickness used in the simulation is not enough. That reults in the average mound height not being obviously different for all systems with different strain energies, substrate temperatures, and thicknesses. It can be summarized that the lateral and vertical enlargement depend on the substrate temperature and the strength of the strain, respectively.

In the future, we intend to continue to improve our model to accommodate real experiment. For example, the substrate dimension should be extended to 2 dimensions in order for the simulation to be comparable with experiments. The decrease of strain strength increasing film thickness can be added to make the model more realistic.

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APPENDIX

Appendix A

Computer Facilities

Generally, the performance of a computer is an important factor that affects the simulation time. In this work, our simulations are carried out on the computer based on Intel Pentium 4 Hyper-theading running at 3.2 GHz with base-memory of 1 GB. The system is running on Linux using a re-compiled kernel version 2.4.24 to accommodate symmetric multi-processing (SMP). The codes for the simulation were written on C language using gcc-lib version 2.95.3.

For example, running time for the MBE model at T = 900 K, substrate size (L) = 1000 and thickness (t) = 1000 ML is approximately 2 days. For Lattice Mismatch model at T = 750 K, L = 1000, t = 10 ML and strain energy (E_s) = 2.0 eV, it takes 2 days to complete the run. All the previous examples are simulation time for one run. These are used to simulate the morphology that does not need to average. But the height-height correlation function, $H(r)$, must be averaged. For this work, the running time to calculate $H(r)$ at the condition of T = 750 K, L = 1000, t = 10 ML and strain energy (E_s) = 2.0 eV for 10 runs is approximately 18 days.

Vitae

Mr. Piti Panichayunon was born on 5 August 1978 in Songkla, Thailand. He received his bacherlor degree of Science in Physics from Prince of Songkla University in 1999.

Conference Presentations :

2004 P. Panichayunon, P. Chatraphorn and S. Chatraphorn, "A realistic model for molecular beam epitaxy growth with strain effects", *The* 12^{th} *Science Seminar 2004*, Faculty of Science, Chulalongkorn University (March 18-19, 2004): PH-6

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