การจำลองการปลูกฟิล์มบางโดยใช้เทคนิคการลดการรบกวนในระบบพื้นผิวแบบ (2+1) มิติ

นางสาวปราณี ช้างแก้ว

วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิทยาศาสตรมหาบัณฑิต
สาขาวิชาฟิสิกส์ ภาควิชาฟิสิกส์
คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย
ปีการศึกษา 2550

THIN FILM GROWTH SIMULATION WITH NOISE REDUCTION TECHNIQUES IN (2+1) DIMENSIONAL SUBSTRATE SYSTEMS

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A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Science Program in Physics
Department of Physics
Faculty of Science
Chulalongkorn University
Academic Year 2007

Thesis Title	THIN FILM GROWTH SIMULATION WITH NOISE REDUCTION TECHNIQUES IN (2+1) DIMENSIONAL SUBSTRATE SYSTEMS
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Field of Study	Physics
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ปราณี ช้างแก้ว : การจำลองการปลูกฟิล์มบางโดยใช้เทคนิคการลดการรบกวนในระบบพื้นผิวแบบ (2+1) มิติ. (THIN FILM GROWTH SIMULATION WITH NOISE REDUCTION TECHNIQUES IN (2+1) DIMENSIONAL SUBSTRATE SYSTEMS) อ.ที่ปรึกษา : ผศ.ดร. ปัจฉา ฉัตราภรณ์, 57 หน้า.

เทคนิคการลดการรบกวนสองแบบได้แก่ เทคนิคการเพิ่มระยะการแพร่บนพื้นผิว (long surface diffusion length technique) และเทคนิคมัลติเพิลฮิต (multiple hit technique) ได้ถูกนำมาใช้ในการจำลองการปลูกฟิล์มบางเพื่อให้ได้ฟิล์มที่เรียบ เทคนิคการเพิ่มระยะการแพร่บนพื้นผิวเทียบเท่ากับการเพิ่มอุณหภูมิในการปลูกฟิล์มจริงในขณะที่เทคนิคมัลติเพิลฮิตเป็นเทคนิคทางคอมพิวเตอร์เท่านั้น เราทำการจำลองปลูกฟิล์มด้วยแบบจำลอง Das Sarma-Temborenea (DT) ร่วมกับเทคนิคการลดการรบกวนทั้งสองแบบบนแผ่นรองรับแบบ 2 มิติ เพื่อเปรียบเทียบว่าเทคนิคมัลติเพิลฮิตให้ผลที่เทียบเท่ากับเทคนิคการเพิ่มระยะการแพร่บนพื้นผิวหรือไม่ ผลการศึกษาพบว่า ทั้งสองเทคนิคให้ผลเทียบเท่ากันสำหรับการศึกษาเรื่องการปลูกฟิล์มแบบชั้นต่อชั้น (layer-by-layer growth) ซึ่งเป็นการปลูกที่ทำให้ได้ฟิล์มที่เรียบ ลักษณะที่แสดงว่าเป็นการปลูกฟิล์มแบบชั้นต่อชั้นดูจากการแกว่งของค่าเบี่ยงเบนมาตรฐานของผิวฟิล์ม (Interface width) นอกจากนี้ยังพบว่าเวลาที่การปลูกฟิล์มแบบชั้นต่อชั้นหยุด (t_c) เป็นไปตามความสัมพันธ์ $t_c \sim (\ell/L)^{\delta}$ เมื่อ L คือขนาดของแผ่นรองรับ ℓ คือระยะการแพร่บนพื้นผิวและ $\delta = 1.5$ สำหรับเทคนิคการเพิ่มระยะการแพร่บนพื้นผิว และเป็นไปตามความสัมพันธ์ $t_c \sim m^{\mu}$ เมื่อ m คือ มัลติเพิลฮิตพารามิเตอร์และ $\mu = 2.5$ สำหรับเทคนิคมัลติเปิลฮิต เราได้ศึกษาผลของเทคนิคทั้งสองที่มีต่อค่าของ Growth exponent (β) ของแบบจำลอง DT บนพื้นผิวแบบ 2 มิติด้วย ผลการศึกษาแสดงให้เห็นว่าค่า Growth exponent ลดลงเมื่อ ℓ และ m เพิ่มขึ้น โดยเมื่อ m มีค่ามากๆ β ลู่เข้าสู่ค่าประมาณ 0.07 ขณะที่เมื่อ ℓ มีค่ามากๆ β จะแกว่งรอบๆ ค่าประมาณ 0.12 - 0.13

นอกจากนี้เราได้ศึกษาผลของขนาดแผ่นรองรับที่มีค่าจำกัดของแบบจำลอง DT แบบ 2 มิติด้วย ผลการศึกษาพบว่า ขนาดของแผ่นรองรับที่จำกัดไม่มีผลต่อค่า Growth exponent แต่มีผลอย่างมากกับค่า Roughness exponent (α) จากการศึกษาด้วยวิธีการประมาณค่าแบบนอกช่วงพบว่าที่ขนาดแผ่นรองรับเป็นอนันต์ α มีค่าประมาณ 0.005

ภาควิชา..... ฟิสิกส์..... ลายมือชื่อนิสิต.....

สาขาวิชา..... ฟิสิกส์..... ลายมือชื่ออาจารย์ที่ปรึกษา.....

ปีการศึกษา.....2550.....

487 23635 23 : MAJOR PHYSICS

KEY WORD : LONG SURFACE DIFFUSION LENGTH TECHNIQUE / MULTIPLE HIT NOISE REDUCTION TECHNIQUE / FINITE SIZE EFFECTS / TWO-DIMENSIONAL DT MODEL / LAYER-BY-LAYER GROWTH

PRANEE CHANGKAEW: THIN FILM GROWTH SIMULATION WITH NOISE REDUCTION TECHNIQUES IN (2+1) DIMENSIONAL SUBSTRATE SYSTEMS. THESIS ADVISOR: ASSISTANT PROFESSOR PATCHA CHATRAPHORN, Ph.D., 57 pp.

Two noise reduction techniques: the long surface diffusion length noise reduction technique and multiple hit noise reduction technique are used to produce smooth film surface in thin film growth simulation. The long surface diffusion length technique is equivalent to the increase in growth temperature while the multiple hit technique is a computational technique. We have simulated thin film growth by using Das Sarma-Temborenea (DT) model with the two noise-reduction techniques in two-dimensional substrates to compare whether the multiple hit noise reduction technique is equivalent to the long surface diffusion length noise reduction technique. Our simulation results show that both techniques are equivalent for the study of layer-by-layer growth which is very smooth film surface growth indicated by oscillations in surface roughness during early growth time. Both techniques produce a smoother film surfaces. Additionally, we find that the damping time t_c, the time when the layer-by-layer damps out, depends on the noise reduction parameters with power law relations: $t_c \sim (\ell/L)^{\delta}$ for the long surface diffusion length technique when L is the substrate size, ℓ is surface diffusion length and $\delta = 1.5$, and $t_c \sim m^{\mu}$, for the multiple hit technique when m is multiple hit parameter and $\mu = 2.5$. We also study effects of the two noise reduction techniques on the growth exponent β of the DT model in two-dimensions. Our results show that the growth exponent decreases as parameter ℓ and m are increased. At large m, the growth exponent converges to $\beta \approx 0.07$ while at large ℓ, the growth exponent fluctuates and around $\beta \approx$ 0.12-0.13. In addition, Finite size effects on the growth exponent and the roughness exponent of (2+1)-dimensional DT model are studied as well. We found that the growth exponent is not significantly affected by the substrate size while the roughness exponent is affected greatly. Extrapolation technique shows that the roughness exponent decreases to $\alpha \approx 0.005$ when the substrate size approaches $L \to \infty$.

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

Field of study... Physics..... Advisor's signature.....

Academic year...2007.....

ACKNOWLEDGEMENTS

This thesis can be completed with the extensive support and assistance from my advisor, Asst. Prof. Dr. Patcha Chatraphorn. I am grateful to my advisor for her valuable advice and guidance on this work.

I wish to thank Asst. Prof. Dr. Sojiphong Chatraphorn for his guidance and for the facility such as high-efficiency computer. I wish to thank Asst. Prof. Dr. Kajornyod Yoodee for his suggestion from the time when I was a new graduate student at Chulalongkorn University. I wish to thank Dr. Nuttakorn Thubthong for his help in solving problems in my programming.

I would like to thank the students in Semiconductor Physics Research Laboratory (SPRL) for all the help and ideas during this work. Especially, I want to thank Mr. Chalasai Chaisorn for his suggestions.

I would like to thank my thesis committee, Dr. Ahpisit Ungkitchanukit, Assoc. Prof. Udomsilp Pinsook and Dr. Satreerat Hodak. Their comments on this thesis are also greatly appreciated.

I would like to thank Mahidolwittayunusorn School for supporting a scholarship during my study. I wish to thank the staffs of Physics Department of Mahidolwittayanusorn School for hard working when I am a graduate student.

Finally, I thank my mother and my brother for love and everything. I wish to thank especially Mr. Jarupat Disrattakit for his ideas on everything. I am thankful for all the teachers who have taught me.

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CHAPTER I

INTRODUCTION

Thin film growth technology is an important technology used widely in many applications. A well-known technological process used to produce high quality thin films is Molecular Beam Epitaxy (MBE). In this technique, atoms from vapor or molecular beam are deposited and then are grown on a substrate under epitaxy condition, i.e. atomic structure of the film can be controlled by the structure of the substrate. The conditions for the ideal MBE are considered with no evaporation from the surface, no vacancy in the film, and overhanging at the growth process is not allowed. Usually, an aggregation or a deposition process produces quite a rough surface (a kinetically rough interface)[1]. Surface diffusion process activates a smoother interface. A high temperature MBE growth enables one to produce smooth thin films, since a high substrate temperature yields higher surface diffusion that gives rise to layer-by-layer growth.

In experiments, a smooth layer-by-layer growth is identified by Reflection High Energy Electron Diffraction (RHEED) intensity oscillations [2–3]. Usually, the RHEED intensity oscillates with a period of one monolayer. In reality the layer-by-layer growth is not “absolute”: the next layer is produced before the previous layer is completely filled so the RHEED intensity oscillation eventually damps out. The damping time, the time that the layer-by-layer dies out, depends on the substrate temperature.

Simulation technique is utilized to study growth mechanism such as atom aggregation and surface diffusion. In simulation, the layer-by-layer is identified by oscillations observed in the plot of interface width W (root mean square fluctuation of the surface height of simulated films) versus deposition time (deposition time unit: the time

interval of one monolayer means that number of deposited particles during that time equals number of lattice site on the substrate). The layer-by-layer growth is only a temporary growth mode because the oscillation of W eventually damps and crosses over to a power law behavior associated with kinetic surface roughening. In the case of perfect layer-by-layer growth, interface width fluctuates between 0 (flat interface or complete filled layer) and 1 (a half filled layer) whereas in a kinetically rough growth, the interface width increases as power law with time (films thickness). In growth simulations, two noise-reduction techniques - long surface diffusion length [4 - 6] and multiple hit [4, 6 - 10] noised-reductions - are used to reduce stochastic noise and enhance the layer-by-layer growth. The long surface diffusion length is equivalent to the increase of the growth temperature in experiments while the multiple hit noise-reduction is only a computational technique. Interesting issues are whether the multiple hit noise-reduction is equivalent to the long surface diffusion length technique, and how scaling relations between the damping time and noise-reduction parameters are.

In 1998, Brende, Kallabis and Wolf [7] investigated another limited mobility growth model on one-dimensional substrates using the multiple hit noise reduction technique. They found that the layer-by-layer growth was visible when the noise was reduced and the damping time depended on the parameter m with a power law relation when m is a parameter that tells how much noise reduction was done. In 2002, Punyindu Chatraphorn and Das Sarma [4] studied one-dimensional solid-on-solid limited mobility growth models using the long surface diffusion length and the multiple hit noise-reductions. Their results show that these two noise reductions are equivalent and the damping time is proportional to m^{μ} and $(\ell/L)^{\delta}$ when ℓ is the diffusion length, L is substrate size, μ and δ are constant. But in the two-dimensional substrates, only the multiple hit technique was used (no result for the long surface diffusions length technique). In our work, we use both of the two noise-reduction techniques in the two-dimensional substrates to confirm that the multiple hit noise reduction equivalents to the long surface diffusion length, and that the damping time $t_c \sim (\ell/L)^{\delta}$ and $t_c \sim m^{\mu}$ in the two-dimensional substrate systems as well.

Furthermore, in studies of a discrete growth model, one of the goals is to find universality class of the model. This can be done via a calculation of critical exponents

such as growth exponent (β), roughness exponent (α) and dynamical exponent (z), of the growth model. Estimation of the critical exponents helps in the finding of the continuum growth equation that describes each model. In some models, however, there are crossovers of the critical exponents that make it difficult to define the universality class. In these cases, finding asymptotic exponents are necessary. One technique used to obtain the asymptotic exponents is the noise reduction technique. The multiple hit noise reduction is applied to attain correct asymptotic critical exponents in some growth models [6, 10-11]. The noise reduction technique dose not changes the universality class of the model [9-12]. It only reduces high surface steps and deep wells in the surface morphology. This suppression leads to the success of the noise reduction technique in acquiring asymptotically correct universality class of the growth model [6, 11]. For example, in 1998, Punyindu and Das Sarma [11] used the multiple hit noise reduction technique with (1+1)-dimensional Das Sarma-Tamburenea (DT) model and showed that this model belonged to the nonlinear fourth-order universality class whereas the original DT model without the noise reduction technique indicated the linear forth-order universality class with complications on the symmetry of the morphologies [6-11]. For (2+1)-dimensional growth, the multiple hit noised reduction technique is used to prove that the (2+1)-dimensional DT model belongs to the linear second-order universality class, EW universality class, [6]. In 1993, Tamborenea and Das Sarmar [5] showed that the long surface diffusion length is also effective on finding asymptotic values of the critical exponents in (1+1)-dimensional kink diffusion model (KD) model, random deposition with relaxation (RDR) model. However, the long surface diffusion length noised reduction technique was not used to find asymptotic critical exponents in (2+1)-dimensional growth. In our thesis, we study a critical exponent (the growth exponent β) both the long surface diffusions length technique and the multiple hit noise reduction technique. Our results are compared to see whether these techniques have similar effects on the critical exponent.

To obtain correct asymptotic exponents, there is another method presented in the literature. In this method, correction-to-scaling terms are studied to reduce finite size effects on a growth model [13-15]. Finite size of the substrate length has strong effects on behavior of the critical exponents and the method aims to extrapolate results from finite

size substrates to the infinitely large substrate [13-15]. In 2003, Aarão Reis and coworkers [14] showed that the (1+1)-dimensional DT model belonged to the nonlinear forth-order universality class which is the same as results from the noise reduced DT model done earlier [11]. However, in some models, this technique yields unreliable asymptotic estimation [14]. In our work, we study the finite size effects in (2+1)-dimensions of a growth model without the noise reduction techniques to obtain the correct asymptotic critical exponents.

Overview of our thesis

In our work, we simulate films using the DT model with two noise reductions techniques: the long surface diffusion length and the multiple hit noise reduction technique, on two-dimensional substrates ((2+1)-dimensional substrate systems). In chapter 2, we talk about theory and model such as growth process (deposition, desorption, and diffusion process), discrete model (Random Deposition (RD) model and DT model), universality class (scaling and continuum growth equations), and noise reduction techniques. For chapter 3, we present result and discussion on the DT model with noise reduction techniques in (2+1)-dimensions to confirm *whether the multiple hit noise reductions is equivalent to the long surface diffusion length*. Both interface width and morphologies are compared, we also try to find relationship for the damping time and noise reduction parameters. In chapter 4, we show the result and discussion on the study of the finite size effects on the (2+1)-dimensional DT model without the noise reduction techniques. The results are extrapolated to find the asymptotic growth exponent and roughness exponent in an attempt *to predict the correction-to-scaling terms of those exponents*. Finally, Chapter 5 is the conclusion of our study.

CHAPTER II

THEORY AND MODEL

In thin film growth, there are many processes that occur on the film surface. In this chapter, we will talk about these processes, growth simulation techniques, discrete growth models, and noised reduction techniques. Furthermore, we will introduce theories and equations used to analyze simulation results such as the scaling concept and continuum growth equations.

2.1 Growth Process

Microscopic growth processes on the surface consist of three interplayed processes: deposition, desorption and surface diffusion processes [1]. These processes have strong effects on the properties of a grown film.

2.1.1 Deposition process

The deposition process is the process that an atom from atomic vapor or electron beam reaches a random position on surface and then forms bonds with neighboring atoms. It is incorporated at that random site and becomes a part of the growing film. These nearly incorporated atoms may not stay at the deposition sites permanently because the bonds may be broken again and the atoms may continue with the desorption or the diffusion process.

2.2.2 Desorption process

The desorption is a procedure that deposited atoms on the surface evaporate from the interface. Probability of desorption depends on the strength of bonds between the atom and neighboring atoms. This strength of bonds indicates amount of energy needed to destroy the bond. Desorption rate can be calculated from

$$R^{ev} = R_0^{ev} \exp(-E_B / k_B T), \tag{2.1}$$

where R_o^{ev} is the attempt frequency for the desorption process (in the order of $10^{13} s^{-1}$ [16]), E_B is binding energy of the atom on the surface, k_B is Bolthzmann's constant and T is substrate temperature [16]. At low substrate temperature in MBE growth, the desoption process can be neglected from the study [1, 16]. Growth process under the condition that there is no evaporation of atoms on the surface is called *conserved growth*.

2.2.3 Diffusion Process

When an atom arrives at a random position on the interface, it forms bonds with neighboring atoms. However, if the atom has enough energy to break these bonds, it can move to other sites. This is called "diffusion process" which becomes important when the temperature of the substrate is high enough. When an atom diffuses on the surface, it tries to search for the energetically most favorable site. This means the diffusing atom tries to move to a site that it can form many bonds. High substrate temperature leads to high mobility and the atoms can diffuse to sites far from the deposition sites. The distance that an atom can diffuse is the "diffusion length" which, obviously, depends on the substrate temperature.

2.2 Discrete Growth Model

Discrete growth models are used to study growth process in the atomic scale. The simplest discrete growth model is the Random deposition (RD) model [1]. For our work, we simulate the thin film growth using the Das Sarma and Tamborenea (DT) model [17].

2.2.1 Random Deposition (RD) model

Natural interface growth process is a random process. In simulation technique, the RD model is used to simulate the random process and study deposition mechanisms and statistical properties of the growth process.

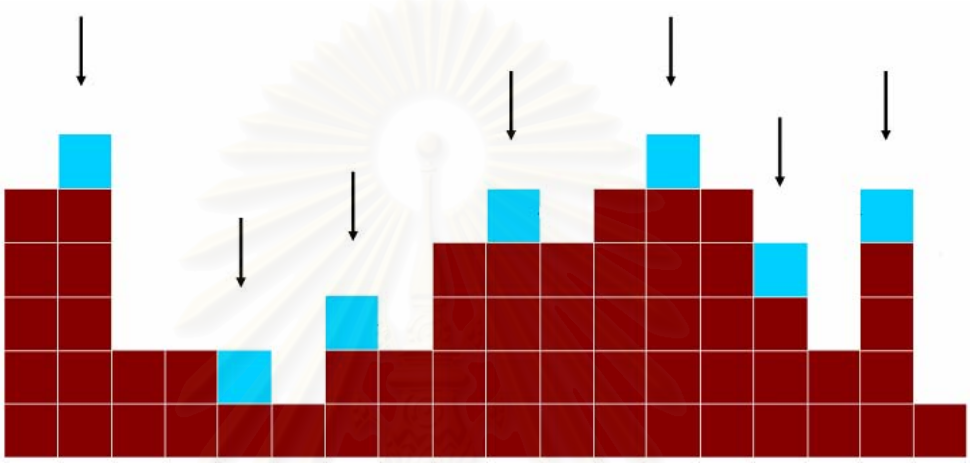

Fig.2.1 Illustration of the aggregation of (1+1) dimensional Random Deposition (RD) model with L = 18. The atoms fall from random positions, indicated by arrows.

In simulation, size of a system is determined by number of lattice sites on the substrate. Most simulations are on either one- or two- dimensional substrates. Convention notation is (d+1) when d is the dimension of the substrate. For a (1+1) dimensional simulation, the substrate is a straight line. In this case, the substrate size (L) is defined as number of lattice sites on the line. For example, Fig. 2.1 is a diagram of a (1+1) dimensional RD model with the substrate size L = 18. More realistic simulations are done on two-dimensional substrates which can be denoted as (2+1) dimensional simulations. In this case, the system size is defined as number of sites on each side of the substrate. In our work, all simulations are done on square substrates so the size of a system is denoted by L when actually the substrate has $L \times L$ sites.

For the RD model, the diffusion and desorption processes are not included. As shown in Fig. 2.1, an incident atom is released from a random position above the substrate. It travels down vertically until it reaches the top of that column and sticks there. The height of that column is increased by one. A new atom is then released from another randomly chosen position. And the process continues until the simulated film reaches the desired thickness.

2.2.2 Das Sarma-Tamborenea (DT) model

In our work, we use the Das Sarma-Tamborenea (DT) model [17] with two noise reduction techniques: long surface diffusion length [4-7] and multiple hit techniques [4, 6-11]. All simulations are done on (2+1)-dimensions. The DT model is a solid-on-solid limited mobility growth model. The solid-on-solid conditions exclude overhangs, evaporation, and vacancy. Those correspond to the ideal MBE growth.

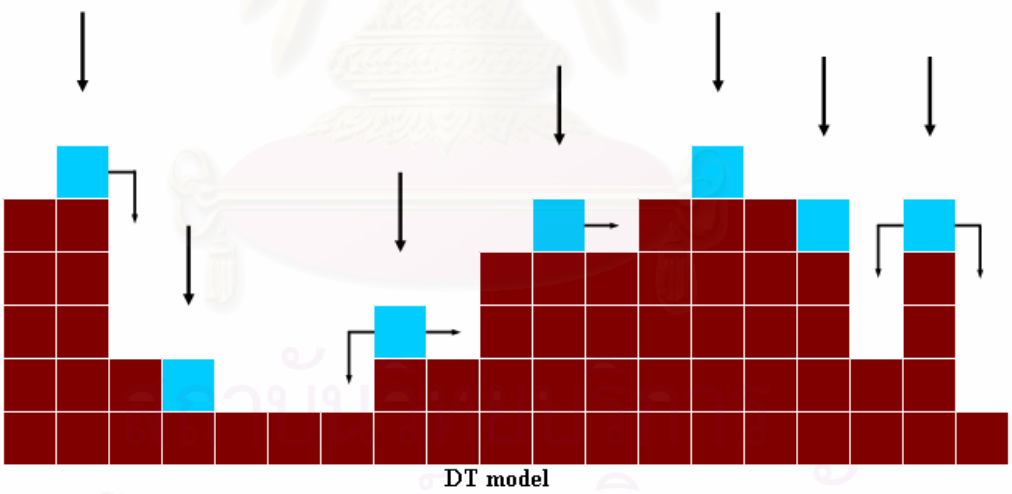

Fig.2.2 Illustration of deposition and diffusion rules in the DT model on (1+1) dimensional systems with $L = 19$, large arrows show the column of incident atoms and small arrows indicate directions that atoms can diffuse.

In this model (see Fig.2.2), an atom is released from a randomly chosen site above a surface. Large vertical arrows indicate the falling atoms above the interface. After the deposition, each atom moves according to the model diffusion rules as shown with small arrows. It can move only to its nearest neighbors (diffusion length $\ell = 1$) to find the final site where it can *increase* number of bonds. If more than one neighbor provides higher bonding number, one of them is randomly chosen. The exception is when the original site provides one or more lateral bones (total of two or more bonds) then the deposited atom is not allowed to move. These aggregation rules are equivalent to low temperature MBE growth, a deposited atom has enough energy to break only one bone, but not enough to break two or more bonds.

2.3 Universality class

Generally, standard tools to study surface growth are experiments, a discrete growth models, scaling concept and continuum growth equations. For our thesis, we mainly use the scaling concepts and the discrete growth model. We study the scaling concept to define the universality class of growth model. The universality class is a product of modern statistical mechanics [1].

2.3.1 Scaling Concept

In a study of surface properties, the quantities of interest are interface width (W) and the critical exponents such as the growth exponent (β), the roughness exponent (α) and the dynamical exponent (z).

For the interface width which is a standard deviation of surface height, it is defined as

$$W(L,t) = \left\langle \left[\frac{1}{L^d} \sum_{i=1}^{L} \left[h(i,t) - \bar{h}(t) \right]^2 \right]^{1/2} \right\rangle . \qquad (2.2)$$

Here, $h(i,t)$ is the height of column i at time t, $\bar{h}(t)$ is the mean height of the surface at t defined by

$$\bar{h}(t) = \frac{1}{L}\sum_{i=1}^{L} h_i \ , \tag{2.3}$$

and *d* is the dimension of the substrate. If the deposition rate is constant, the average height increases linearly with time. The bracket, $\langle\ \rangle$, denotes a configurational average over many different runs. The surface width has two regions separated by a crossover time or saturation time (t_{sat}). At early time of growth ($t << t_{sat}$), interface width increases as a power of time

$$W(L,t) \sim t^{\beta}, \tag{2.4}$$

where β is called the *growth exponent*. For long time, ($t >> t_{sat}$), interface width reaches a saturated value (W_{sat}) that depends on the substrate size as power laws,

$$W_{sat}(L) \sim L^{\alpha}, \tag{2.5}$$

where α is called the *roughness exponent*. Furthermore, the crossover time or saturation time depends on the substrate size,

$$t_{sat} \sim L^{z}, \tag{2.6}$$

where z is called the *dynamical exponent*. These three critical exponents obey scaling relation,

$$z = \frac{\alpha}{\beta}. \tag{2.7}$$

A typically interface width versus time plot is illustrated in Fig.2.3. The dot line indicates the saturation time. Usually, time unit is monolayer (deposition time unit: the time interval of one monolayer means that number of deposited particles during that time equals number of lattice sites on the substrate). In the growth regime, surface width grows linearly on a log-log plot and the slope of the best linear fit is the growth exponent β. In the saturation regime, surface width becomes constant. This constant value, W_{sat}, depends on the system size as shown in Fig.2.4. If we plot W_{sat} versus L on a log-log scale. The data should fall on a straight line with the slope being the roughness exponent α.

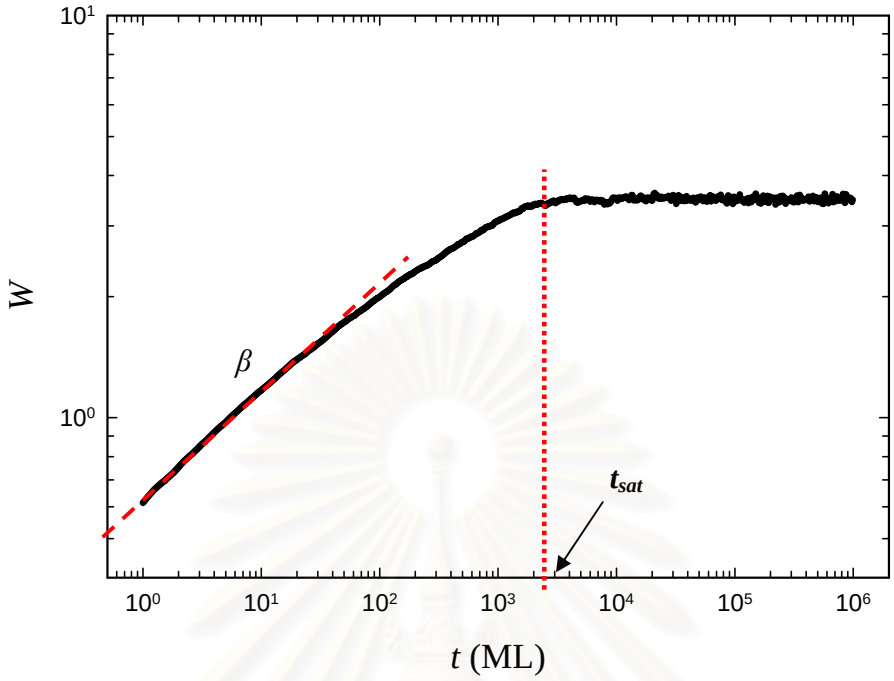

Fig.2.3 Illustration of the log-log plot of the interface width growth for the DT model in (2+1) dimensions with $L \times L = 900 \times 900$. The vertical dot line indicates the saturation time and slope of the dashed line is β.

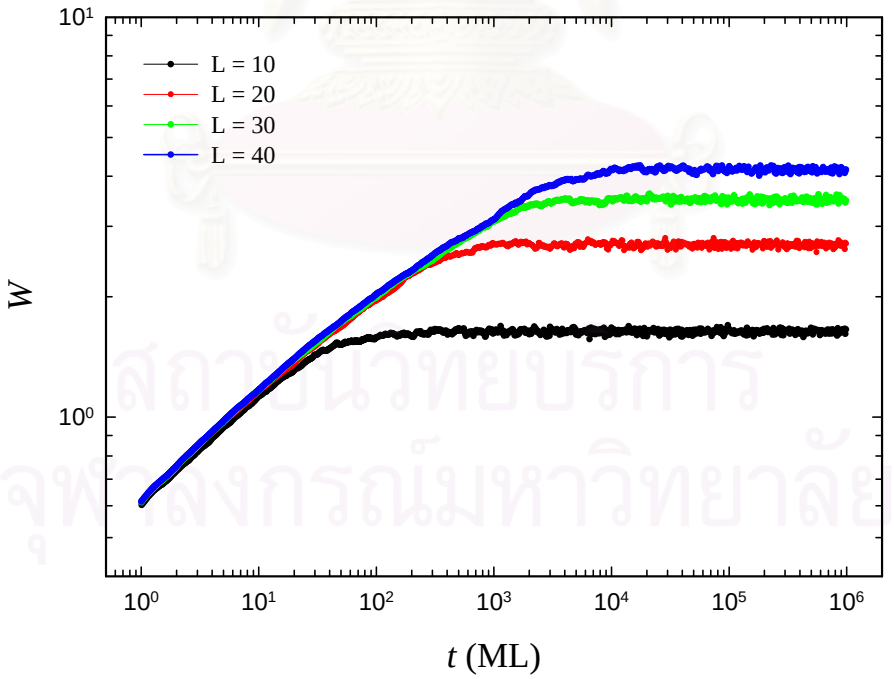

Fig.2.4 Illustration of the log-log plot of the interface width growth for the DT model in (2+1)-dimensions. The different curves indicate results from different substrate sizes.

2.4.2 Continuum growth equations

Continuum growth equations, stochastic are used to study behavior of the interface in large length scale, Details in small scale are neglected and the focus is on asymptotic coarse-grained properties [1]. These continuum equations are derived from symmetry principles [1]. The critical exponents investigated from a discrete growth model should be consistent with the corresponding continuum growth equation describing that model.

Symmetry principles used in creating continuum growth equations are as follows.

1. Invariance under translation in time: $t \to t + \delta t$. It should not matter when the time is set as zero so the equation should not change when $t \to t + \delta t$ so terms with direct-time-dependent must be excluded. Example, $\frac{\partial h}{\partial t}$ obeys this symmetry [1].
2. Translation invariance along growth direction, invariance under the translation: $h \to h + \delta h$. It should not matter when the height is set as zero so the equation should not change when $h \to h + \delta h$. Example, ∇h , $\nabla^2 h, \ldots \nabla^n h$ survive this condition [1].
3. Translation invariance in direction perpendicular to the growth direction: $x \to x + \delta x$. It should be independent of x, having the symmetry when $x \to x + \delta x$ so terms x-dependent must be excluded. Example, $\frac{\partial^n h}{\partial^n x}$ with $n > 0$ include this symmetry [1].
4. Rotation and inversion symmetry about the growth direction ***n,*** invariance under the translation: $x \to -x$. Example, $(\nabla h)^2$ and $\nabla^2 h$ respond this condition but ∇h and $\nabla(\nabla^2 h)$ not exist this symmetry [1]. In some model, there are other system such as
5. up-down symmetry for h , invariance under the translation: $h \to -h$. Example, $\nabla^2 h$ assent this symmetry while $(\nabla h)^2$ and $(\nabla h)^4$ exclude this transformation [1].

Those arguments are used to construct the continuum growth equations. If condition 5th is obeyed, the equation will be linear and the model that can be described by those linear equations are consistent with linear them. Otherwise, the equations are nonlinear and the models follow nonlinear theory.

The simplest growth equation describes fluctuation of interface is the second-order linear growth equations called *Edwards-Wilkinson* (EW) equation [1, 5-6, 18-20]

$$\frac{\partial h(x,t)}{\partial t} = \nu_2 \nabla^2 h + \eta(x,t). \tag{2.10}$$

Here, $h(x,t)$ is the interface height at position *x* and time *t.* $\eta(x,t)$ is noise term and ν_2 is a constant. The scaling exponents of the EW equation [1] are

$$\alpha = \frac{2-d}{2}, \qquad \beta = \frac{2-d}{4}, \qquad z = 2, \tag{2.11}$$

when *d* is the dimensional substrate. If the discrete growth model has asymptotic scaling exponents that agree with equation (2.11), that model belongs to the EW universality class. Some models have lateral growth thus a nonlinear term $(\nabla h)^2$ can be included to in the EW growth equation and a new continuum equation can be written as [1]

$$\frac{\partial h(x,t)}{\partial t} = \nu_2 \nabla^2 h + \lambda_2 (\nabla h)^2 + \eta(x,t), \tag{2.12}$$

which is called *Kardar-Parisi-Zang* (KPZ) equation [1, 20]. And give the scaling exponents that are α = 1/2, β = 1/3 and *z* = 3/2 in (1+1)-dimensional substrate.

When we consider the surface diffusion process, the growth equation described diffusion is the forth-order linear term [1, 21] expressed by

$$\frac{\partial h(x,t)}{\partial t} = -\nu_4 \nabla^4 h + \eta(x,t),. \tag{2.13}$$

When ν_4 is constant. This term provides the scaling exponents as

$$\alpha = \frac{4-d}{2}, \qquad \beta = \frac{4-d}{8}, \qquad z = 4. \tag{2.14}$$

Villain, Lai and Das Sarma [22, 23] proposed the fourth-order nonlinear equation,

$$\frac{\partial h(x,t)}{\partial t} = -\nu_4 \nabla^4 h + \lambda_1 \nabla^2 (\nabla h)^2 + \eta(x,t), \tag{2.15}$$

when λ_1 is constant. The equation (2.15) is called *Villain-Lai-Das Sarma* (VLDS) equation [14, 19, 22, 23]. The scaling exponents of equation (2.15) [1] are

$$\alpha = \frac{4-d}{3}, \qquad \beta = \frac{4-d}{8+d}, \qquad z = \frac{8+d}{3}. \tag{2.16}$$

Equation (2.15) is also frequency called a conserved KPZ equation [1, 22]. The asymptotic critical exponents of each dominant term from the continuum growth equation for (1+1)- and (2+1)-dimensions [21] are shown in Table 2.1.

Table 2.1. The asymptotic critical exponents of dominant terms in continuum growth equation for one-dimensional substrate (d =1) and two-dimensional substrates (d = 2) growth models.

Universality class	α		β		z	
	$d=1$	$d=2$	$d=1$	$d=2$	$d=1$	$d=2$
2nd order linear equation (EW)	0.5	0	0.25	0	2	2
4th order linear equation	1.5	1	0.375	0.25	4	4
4th order nonlinear equation (VLDS)	1	0.667	0.333	0.2	3	3.333

2.5 Noise Reduction Techniques

In simulations, stochastic noise can be very strong. Two noise reduction techniques are introduced to help reduce effect of the noise.

2.5.1 Long surface diffusion length technique

For the *long surface diffusion length technique* ($\ell > 1$) [4-6], we increase the diffusion length (ℓ), which is the lateral length that an atom can diffuse. In experiments, it is found that higher substrate temperature promotes the diffusion of surface atoms. So this $\ell > 1$ technique in simulations is equivalent to increasing substrate temperature in experiments. For our work, we define the parameter ℓ as a maximum number of times an atom can hop to find the final site under diffusion rules of the DT model. This mean an atom can hop up to ℓ times to find a site with at least two bonds. Note that, with this technique, we simulate the DT Model with a large diffusion length that is equivalent to the increase in the substrate temperature. However, the desorption process is neglected from the model which implies temperature that is not very high. So our model is valid for only a range of temperature that is high enough for atoms to have large diffusion length but not high enough for desorption.

2.5.2 Multiple hit noise reduction technique

For the *multiple hit noise reduction* ($m > 1$) [4, 6-11], a multiple hit parameter m is defined as a number of the time a site must be selected before actual incorporation can happen. In this technique, the diffusion rules are the same as the original model ($\ell = 1$). After an adatom chooses its final site, the incorporation does not immediately occur. Each surface site has its own counter. When a site is selected, the counter of that site is increased by one but the height of that site remains the same until the counter reaches the multiple hit parameter (m), which is an integer ($m = 1$ for the original model), then the height of that site is increased by one (one atom) and the counter is reset to zero (see Fig.2.5).

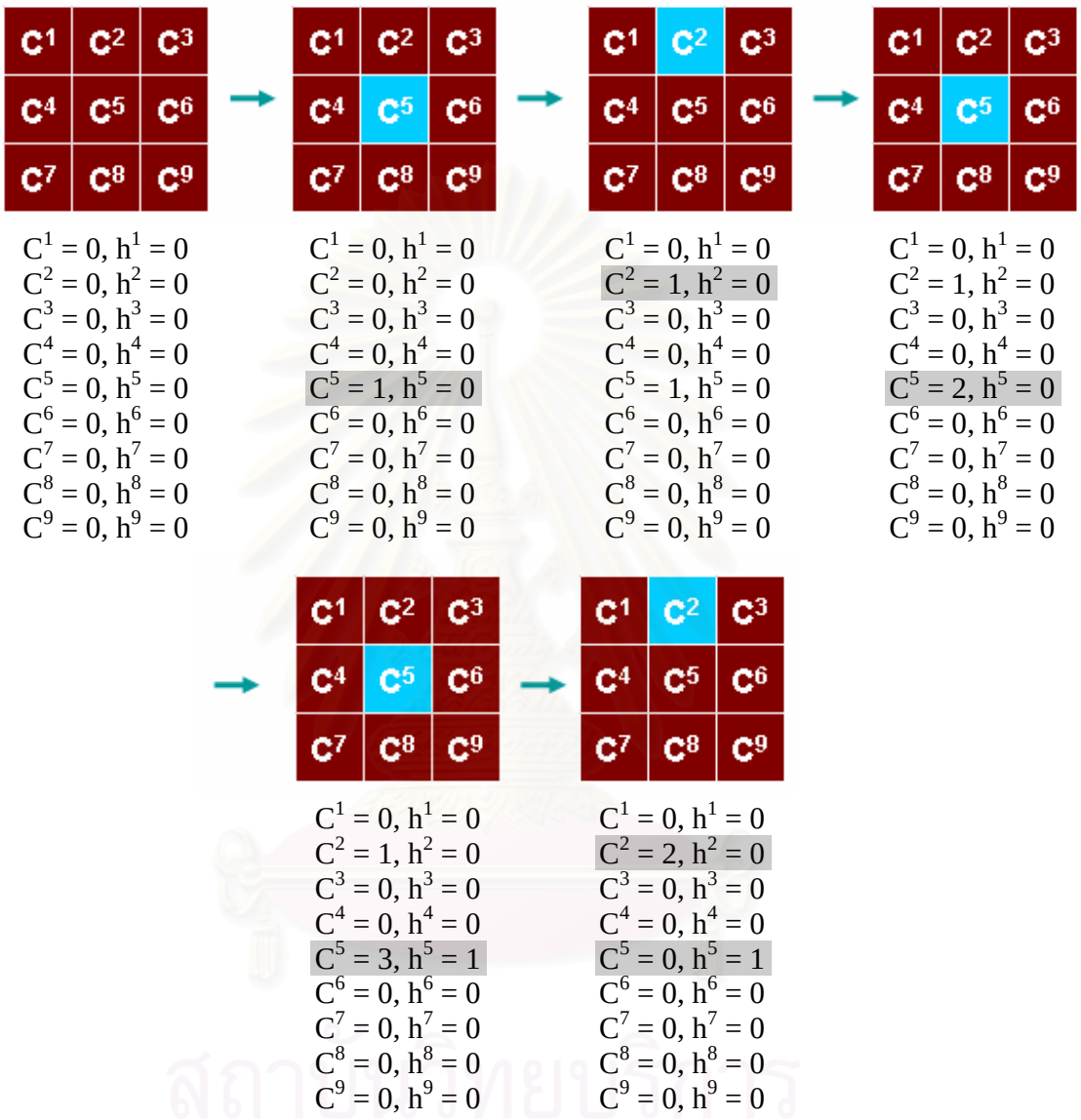

Fig. 2.5 Illustrations of the multiple hit noise reduction in case m = 3 on (2+1)-dimensional flat substrates, after deposited atom chooses its final site the counter of that site is increased by one but its height not change until the counter equal to 3.

CHAPTER III

RESULT AND DISCUSSIONS: DT MODEL WITH NOISE REDUCTION TECHNIQUES IN (2+1) DIMENSIONS

In this chapter, we present our results from simulations of the DT model with both the long surface diffusion noise reduction technique and the multiple hit noise reduction technique. The time evolution of the interface width and the surface morphologies are presented in the first section. In the second section, effects of the noise reduction parameters on the growth exponent are discussed.

3.1 DT model with the long surface diffusion length and the multiple hit noise reduction techniques

3.1.1 The interface width

We simulate thin film growth with the DT model in (2+1) dimensions using the noise reduction techniques: the long surface diffusion length and the multiple hit techniques. Now we present our results simulations. In Fig. 3.1, we present *W*-*t* oscillations of the DT model with $L \times L = 1000 \times 1000$ with an average over many different configurations using the long surface diffusion length noise reduction technique, ℓ = 1, 9, 36, 64, 100, and 144. When the growth time is less than 0.5 ML, the interface widths from simulating with all value used for the parameter ℓ are straight. The slope of the straight lines, which is the growth exponent, is approximately 0.5 corresponding to the growth exponent of the random deposition model [1].

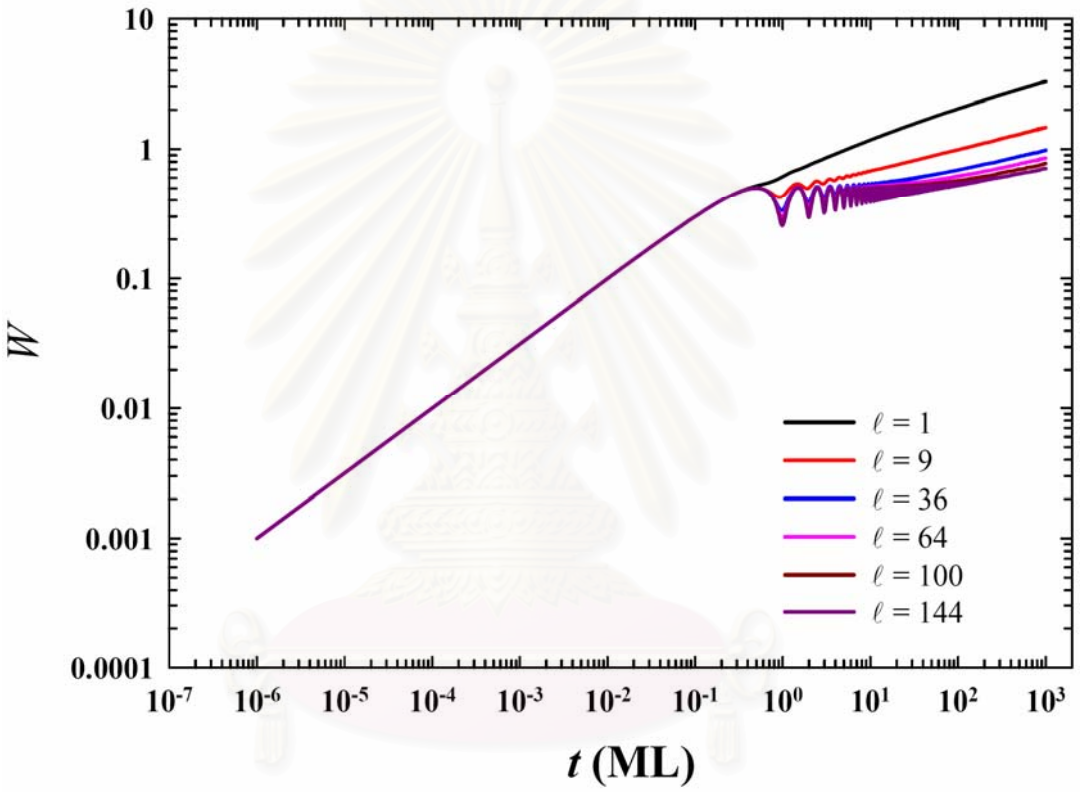

Fig. 3.1 *W*-*t* oscillations of the (2+1)-dimensional DT model with $m = 1$, $L \times L = 1000 \times 1000$, $\ell = 1$, 9, 36, 64, 100 and 144 (top to bottom).

This results show that during 0-0.5 ML, both the DT model and the noise reduced DT model show behavior that obeys the random deposition process. Since at early growth time, surface diffusion of atom is weak yields the diffusion rules of the DT model and the long surface diffusion length technique are smaller than the random deposition process then obtained growth exponent is like the RD model.

Fig. 3.2 is shown *W*-*t* oscillations of the DT model with $L \times L$ = 1000×1000 and a configurationally average over many different runs using the surface diffusion length ℓ = 1, 9, 36, 64, 100, and 144. While Fig. 3.3 is the plots of *W*-*t* oscillations of the DT model using the multiple hit noise reductions, *m* = 1, 3, 5, 8, 10 and 15. From both Fig.3.2 and Fig 3.3, at early time ($t < t_c$), the growth is clearly in layer-by-layer mode when $\ell > 1$ or $m > 1$. This can be seen from the oscillations of the surface with W. *W*-*t* oscillations indicate that each layer is grown from flat surface then surface width increases until a half filled layer and decreases into flat surface at a completely filled layer before next layer is grown. Thus the interface width fluctuates between the minimum values (a completely filled layer) and the maximum values (a half filled layer) and a period of the oscillations are one monolayer (ML). Note that, for "perfect" layer-by-layer growth, $W(t)$ must fluctuates between 0 (a completely filled layer) and 1 (a half completely filled layer) but from our results, the oscillations damp out. This is because, eventually when the film is thicker, a new layer starts forming before the preceding layer is completely filled. Thus *W* is not turns to zero. This result agrees with Ref. [4, 7, 24]. At large ℓ and *m*, the minimum *W* of each layer is lower than at small ℓ and *m*. This indicates that the layer-by-layer growth is near perfect at larger ℓ and *m*. For long growth time ($t > t_c$), no layer-by-layer oscillations are found. $W(t)$ crosses over to kinetically roughness. Furthermore, our simulations are equivalent to RHEED study of GaAs (331)B at different substrate temperatures in Ref. [3] and RHEED intensity during Ag growth onto Si (111) surface with deposition rate 60ML/min at different substrate temperatures in Ref. [25].

Comparing Fig. 3.2 and Fig 3.3., we can see that the minimum values of *W* at each period from the multiple hit technique are less than the minimum *W* from the long surface diffusion length technique, especially at large *m*. The maximum values of *W* at each layer from both noise reduction techniques, however, are similar.

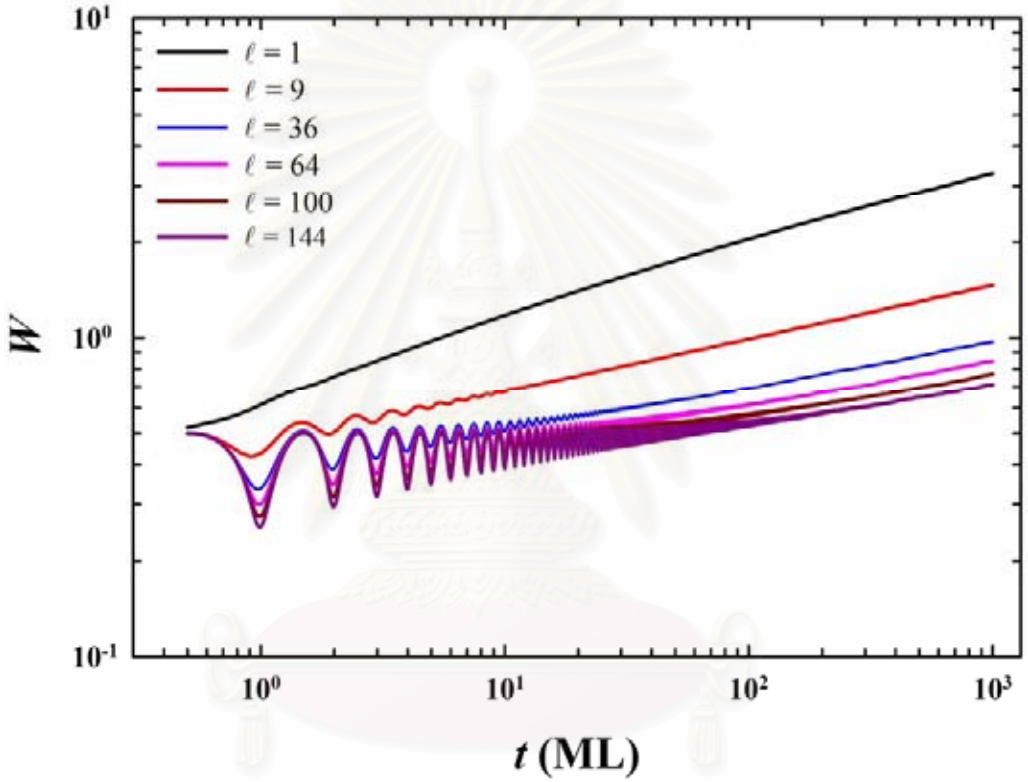

Fig. 3.2 *W-t* oscillations of the (2+1)-dimensional DT model with $m = 1$, $L \times L = 1000 \times 1000$, $\ell = 1$, 9, 36, 64, 100 and 144 (top to bottom).

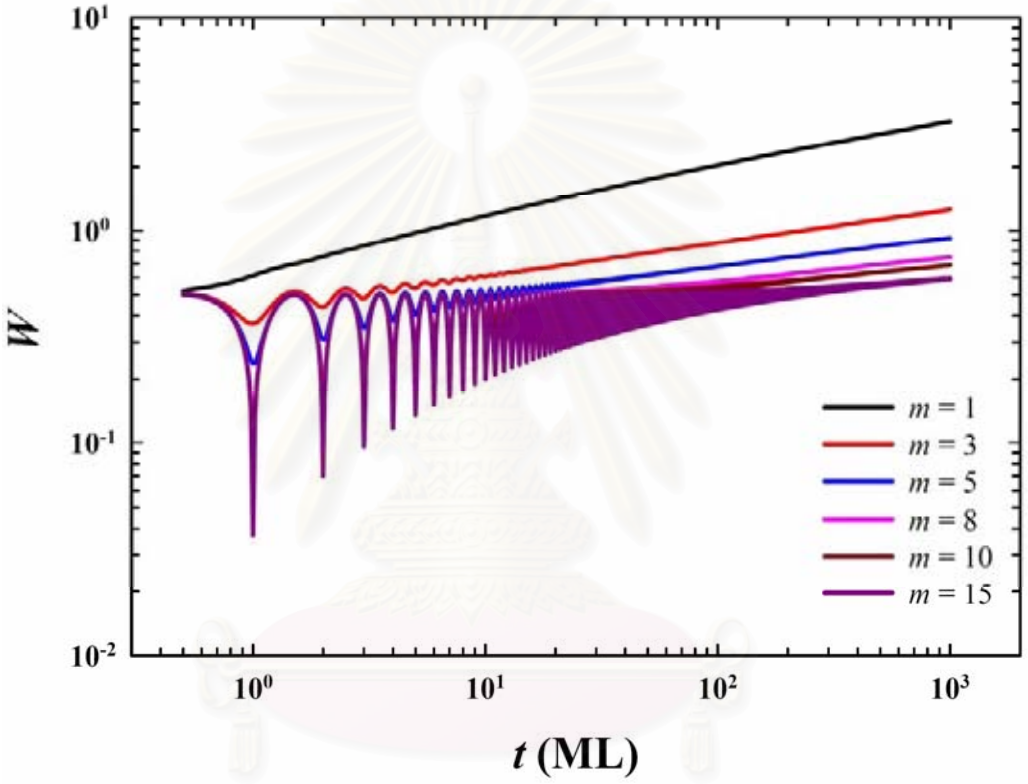

Fig. 3.3 *W*-*t* oscillations of the (2+1)-dimensional DT model with $\ell = 1$, $L \times L = 1000 \times 1000$, $m = 1$, 3, 5, 8, 10 and 15 (top to bottom).

There results show that during the layer-by-layer growth region, the multiple hit technique produces "better" layer-by-layer than the long surface diffusion length technique. After the end of the layer-by-layer growth, the *W*-*t* plots from the two noise reduction techniques are practically undistinguished. Thus, we can confirm that the long surface diffusion length technique and the multiple hit technique enhance layer-by-layer growth in the (2+1)-dimensional systems. From $\ell > 1$ technique (see Fig. 3.2) and $m > 1$ technique (see Fig. 3.3), obvious results are that the damping time t_c is long as ℓ and m increase. We rescale t axis with t_c under assumptions; $t_c \sim m^{\mu}$ and $t_c \sim (\ell/L)^{\delta}$ by plotting W^2 versus t/m^{μ} (see Fig. 3.4) and W^2 versus $t/(\ell/L)^{\delta}$ (see Fig. 3.5) then varying the constants, μ and δ, until the curves are best collapse to find a scaling collapse. Our results show that the graphs are best collapsed at $\mu = 2.5$ for $m > 1$ technique (agree with Ref. [4]) and $\delta = 1.5$ for $\ell > 1$ technique, which prove that the damping time for the (2+1)-dimensional DT model obeys the scaling relations;

$$t_c \sim \begin{cases} m^{\mu} & \text{for the multiple hit techniques,} \\ (\ell/L)^{\delta} & \text{for the long surface diffusion length.} \end{cases}$$

Beside we can confirm that $W(t) \sim f_m (t / m^{\mu})$ or $W(t) \sim f_{\ell} (t / (\ell/L)^{\delta})$ in the layer-by-layer mode. Finally, previous literatures [26, 27] studied about theory for the layer-by-layer growth oscillations by a renormalization group approach. The exponent δ is shown that depend on $\delta = \gamma \frac{zd}{z-d}$ [27], when γ is constant and depends on diffusion process and dimension of islands [24, 26, 27]. Then the exponent is that $\delta = \gamma \frac{4d}{4-d}$ for conserved KPZ equation [24] which is sometime also referred to as the forth-order nonlinear growth equation [4] which obey equation 2.14 [4, 24] and $\delta = \gamma \frac{2d}{2-d}$ for EW equation. When $d = 2$ and $\gamma = 1/2$ [24], the exponent δ should be 2 [4] for the forth-order nonlinear growth equation and equals to ∞ [4] for the EW equation. From our result, the exponent δ equals to 1.5 which is approximately 25 % less than the value of the forth-order nonlinear equation which should be $\delta = 2$.

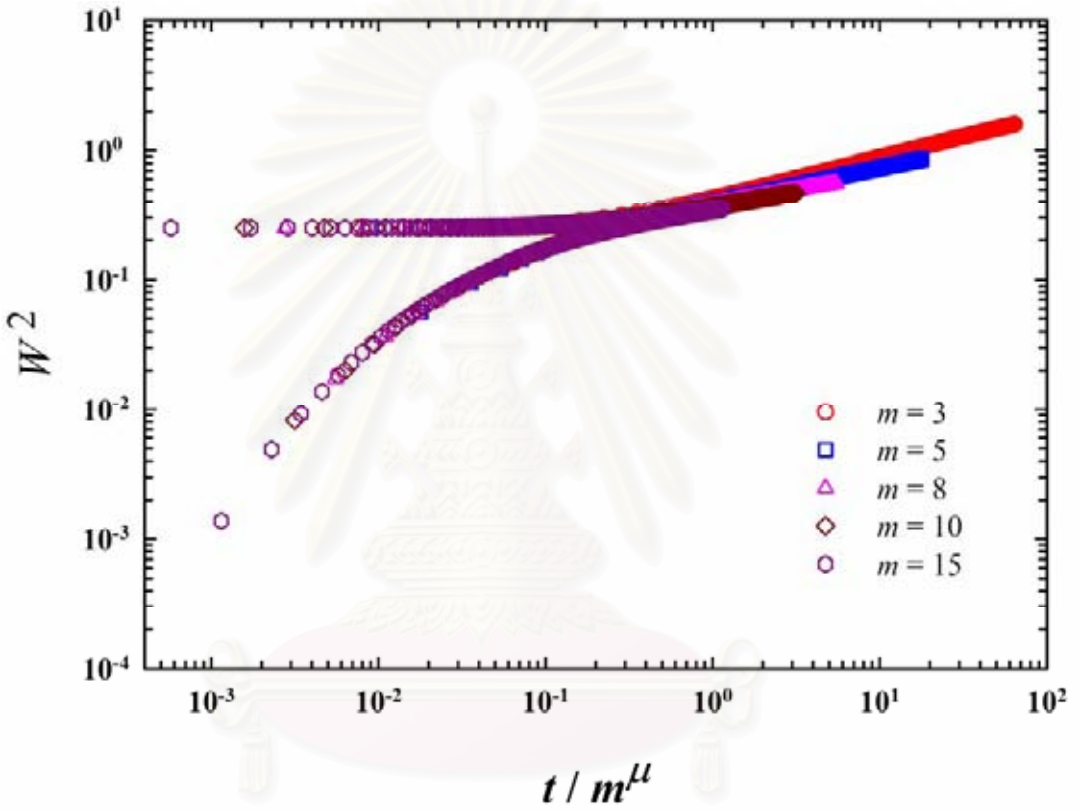

Fig. 3.4 Point plots at every a half ML of W^2 versus t / m^{μ} of the DT model with $\ell = 1$, $L \times L = 1000 \times 1000$, $m = 3, 5, 8, 10$ and 15 that obtains best collapse at $\mu = 2.5$.

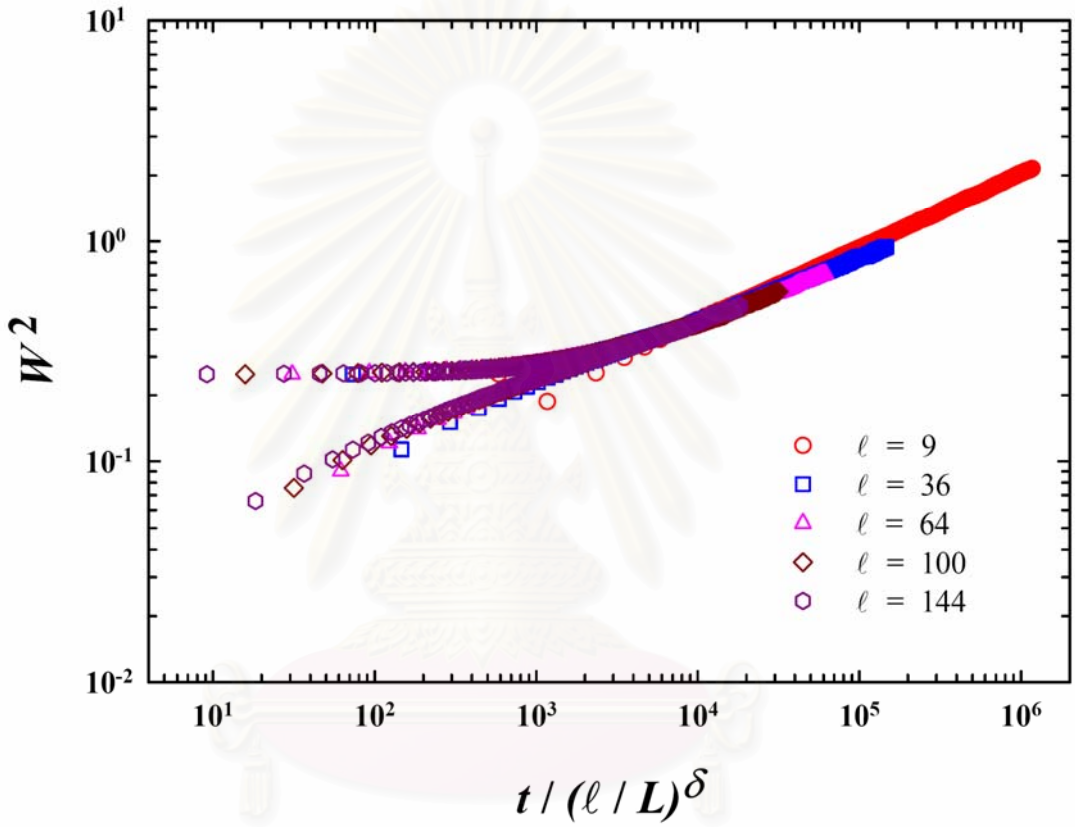

Fig. 3.5 Point plots at every a half ML of W^2 versus $t / (\ell/L)^{\delta}$ of the DT model with m = 1, $L \times L$ = 1000×1000, ℓ = 9, 36, 64, 100 and 144 that obtains best collapse at δ = 1.5.

This difference may arise from the way we define ℓ. Traditionally, ℓ is defined as the distance between the random deposition site and the final incorporation site. But in our case, ℓ is the number of hop allowed. If the diffusing atom goes in one direction only, these two definitions give the same ℓ. However, if the atom changes direction during diffusion, the two definitions give different values for ℓ. And $\delta = 2$ comes from the fact that the parameter γ is chosen as $\gamma = 1/2$ [24] which is from the assumption that the island density $\rho \sim \ell^{-1}$. Obviously, if ℓ is different, γ is not going to be 1/2 and δ will not be 2 as predicted. The value $\gamma = 1/2$, come from assumption that the density of islands (ρ) is related to diffusion length (ℓ) as $\rho \sim \ell^{-1}$ [24].

3.1.2 Surface morphologies

Here we present surface morphologies of both the original DT model and the noise reduced DT model from our simulations. First, in Fig 3.6., morphologies from the DT model with the long surface diffusion length noise reduction technique ($\ell = 144$) at very early time are shown. Each morphology is a section of 100×100 lattice sites from a system of 1000×1000 lattice sites. They are snap shots at t = 0.5 ML, 1 ML, 1.5 ML, 2 ML, 2.5 ML and 3 ML. All of them are from the layer-by-layer growth regime. It is obvious from Fig. 3.6 that morphologies at 0.5 ML, 1.5 ML and 2.5 ML are approximately half-filled. For example, at 0.5 ML, about half of the surface in Fig. 3.6 (a) have $h = 0$ and the other half have $h = 1$. This contributes to a relatively large standard deviation of the h value – relatively large surface width W. On the other hand, morphologies at 1 ML, 2 ML, and 3 ML are almost completely filled. For example, at 1 ML, most of the surface have $h = 1$, while very few columns have $h = 2$ (the new layer starts forming) and very few columns have $h = 0$. In this situation, the values of h from most sites are 1 while very few are 0 or 2. Thus contributes to very small standard deviation of the value of h – relatively small value of W. The alternate between half-filed layers and almost completely filled layers in this manner yields oscillation in W-t plots. The period of oscillation is 1 ML as shown in Fig. 3.2.

Information from Fig. 3.6 confirms that early growth time of the DT model with long surface diffusion length noise reduction technique is, indeed, in layer-by-layer mode

as previously seen in the *W-t* plot (Fig. 3.2). Note that if the layer-by-layer is “perfect”, the morphologies at 1 ML should be perfectly smooth with h of all columns at $h = 1$. Note also that the DT model with multiple hit noise reduction technique shows similar morphologies at these early times.

Morphologies of the DT model with multiple hit noise reduction technique with varies m are shown in Fig. 3.7-3.10. Each morphology is a section of 200 × 200 from a substrate of 1000 × 1000 lattice sites. All morphologies are at 1000 ML and they are all plotted on the same scale for easy comparison. The vertical scale is reset so they are height $\langle h \rangle$ at zero and the plot is actually of the height fluctuation $h - \langle h \rangle$. In Fig. 3.7, we set $m = 1$ which is the original DT model. Because $t = 1000$ ML which is after the *W-t* oscillation already damps out, the morphology here is in the kinetically rough growth region. We can see lots of high surface steps and deep grooves on the surface. When the noise is reduced with $m = 5$, the surface in Fig. 3.8 is much smoother than in Fig. 3.7 with further noise reduction at $m = 10$ and 15 in Fig. 3.9 and Fig. 3.10, the surface became smoother as m increased. This result agrees with the W-t plot in Fig. 3.3 where it can be seen that the surface width of a system with large m is smaller than the system with small m. It should be noted that although the surface with large m are smooth, they still look somewhat like the morphology of the original DT model in Fig. 3.7 but with less high steps and less deep grooves. If we look at the morphologies closely, we can see that the look “rough” in a sense that the height of nearby columns do not correlate much but rather there are a lot of up-down-up-down fluctuation from one column to the next.

In Fig. 3.11 – 3.14, morphologies of the DT model with long surface diffusion length noise reduction technique are shown. In Fig. 3.11, we set $\ell = 1$ which means the model is back to the original DT model (as in Fig. 3.7) for comparison. All morphologies are plot on the same scale as the ones in Fig. 3.7 - 3.10 for easy comparison. These are, again, at $t = 1000$ ML which is already in the kinetically rough growth model. When $\ell = 36$ in Fig. 3.12, the surface becomes smoother because the long surface diffusion length helps reducing the deep grooves by letting diffusing atom search for the grooves and be incorporate there. With large values of ℓ, $\ell = 100$ in Fig. 3.13 and $\ell = 144$ in Fig. 3.14, the morphologies become smoother with increasing ℓ. Thus morphologies are consistent

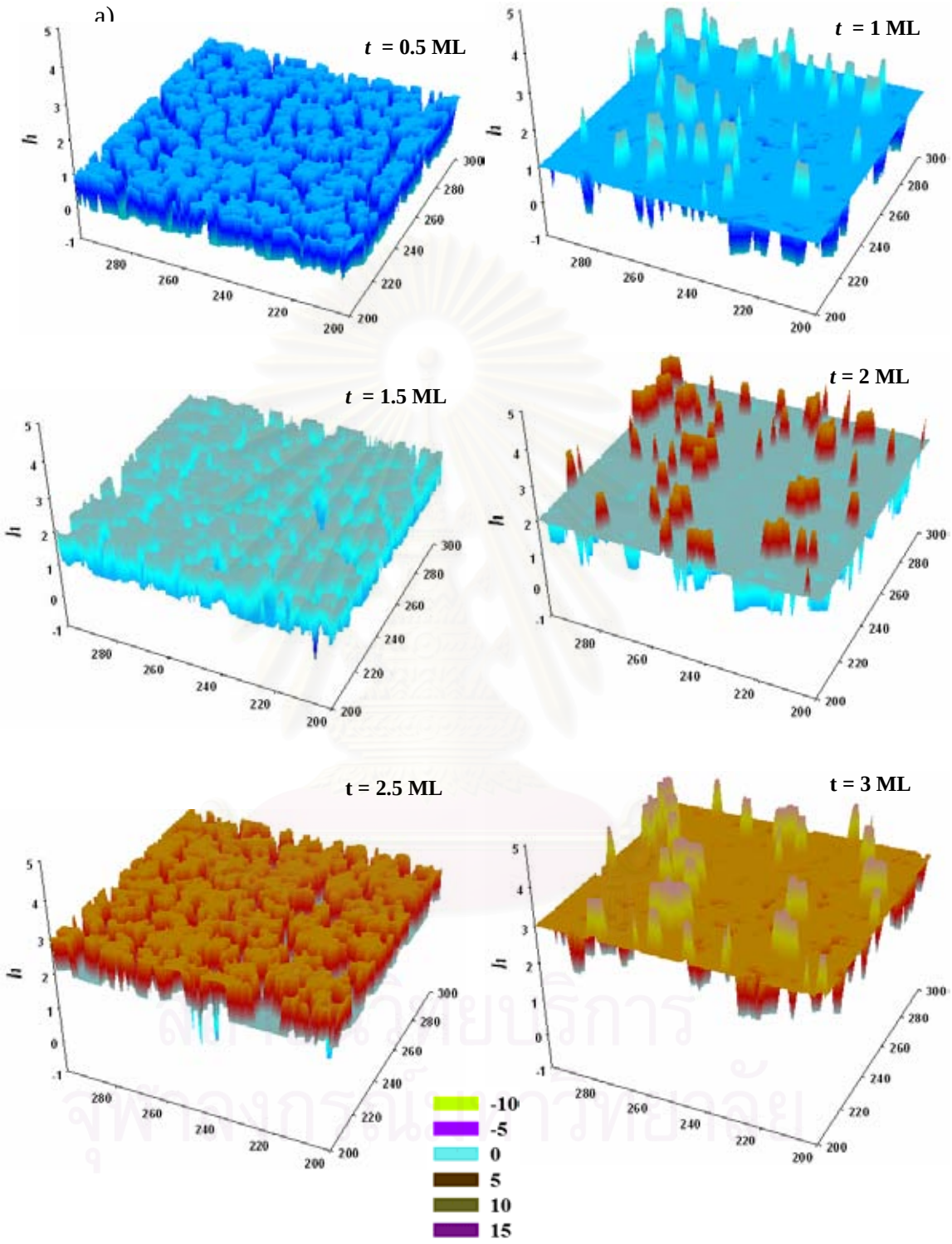

Fig.3.6 Surface morphologies of noise reduced DT model with $\ell = 144$, $m = 1$ and $L \times L = 1000 \times 1000$ (a sections of 100×100 is shown in each plot) at t equals to a) 0.5 ML b) 1ML c) 1.5 ML d) 2ML e) 2.5 ML and f) 3 ML.

with the smaller surface width W with large ℓ in the W-t plot in Fig. 3.2.

Comparing the two noise reduction techniques, we see that both of them can induce layer-by-layer growth during early time and both techniques produce smoother surface up to 1000 ML. However, morphologies from the two techniques are not indistinguishable. For the multiple hit technique, islands on a surface are small and sharp while for the long surface diffusion length technique, there are very few island on a surface and the islands have wide top. This is become behavior of diffusing atom of the multiple hit technique are the same as in original DT model so the shape of islands are similar to islands in the original model but with high surface step and deep grooves being suppressed. However, behavior of diffusing atoms of the long surface diffusion length technique is different from atoms in the original model. With large ℓ, each atom tries to search for a step-edge on the surface which is a site that can provide large bonding number. This mechanism promotes nucleation of small islands so they merge and we are left with few large islands on the surface instead.

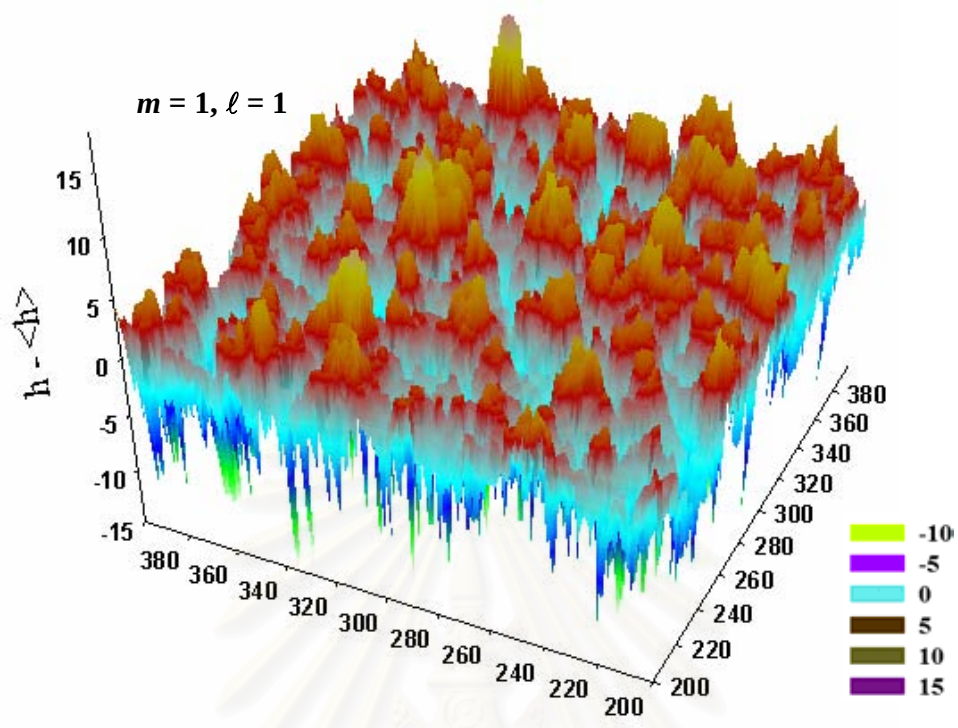

Fig. 3.7 Surface morphology of the original DT model with ℓ = 1, m = 1 and $L \times L$ = 1000 ×1000 (a sections of 200×200) at t = 1000 ML.

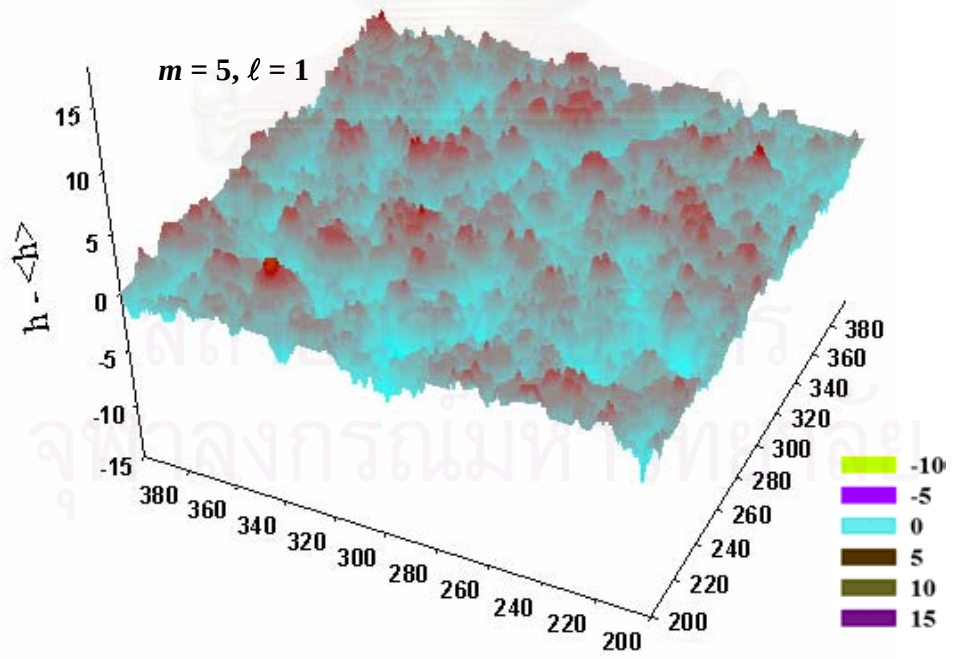

Fig. 3.8 Surface morphology of noise reduced DT model with ℓ = 1, m = 5 and $L \times L$ = 1000 ×1000 (a sections of 200×200) at t = 1000 ML.

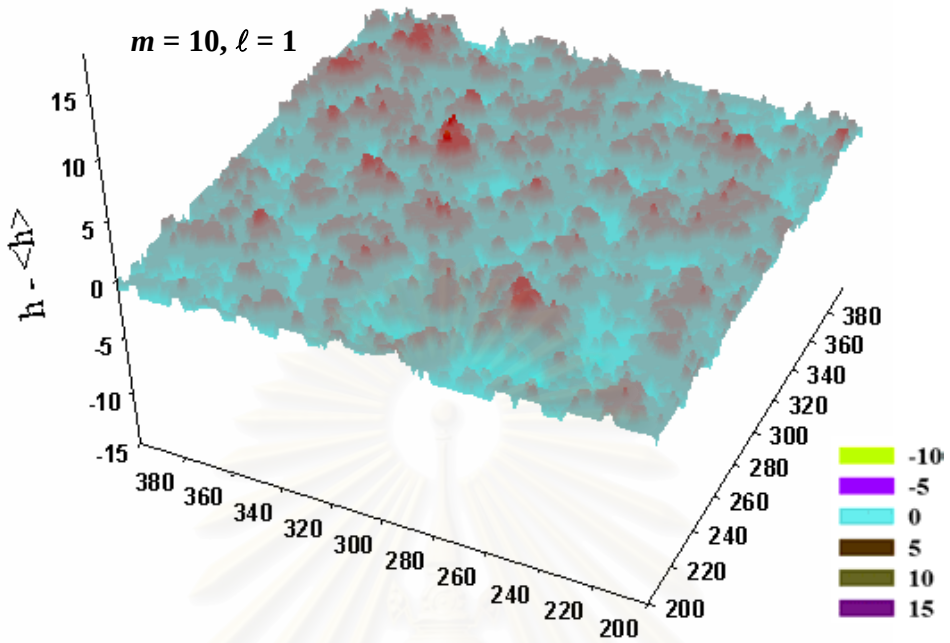

Fig. 3.9 Surface morphology of noise reduced DT model with ℓ = 1, m = 10 and $L \times L$ = 1000 ×1000 (a sections of 200×200) at t = 1000 ML.

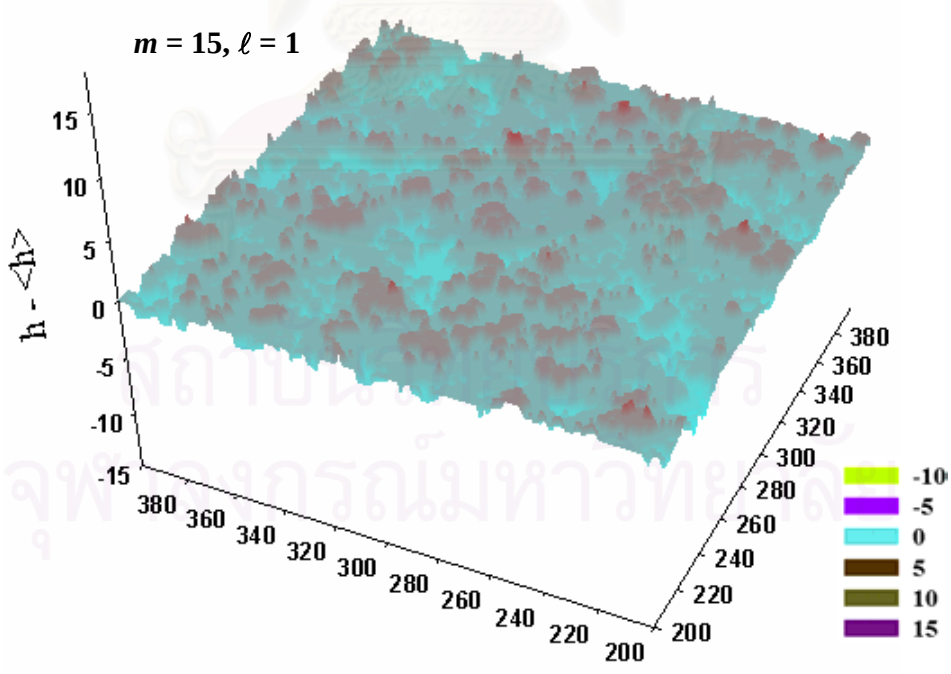

Fig. 3.10 Surface morphology of noise reduced DT model with ℓ = 1, m = 15 and $L \times L$ = 1000 ×1000 (a sections of 200×200) at t = 1000 ML.

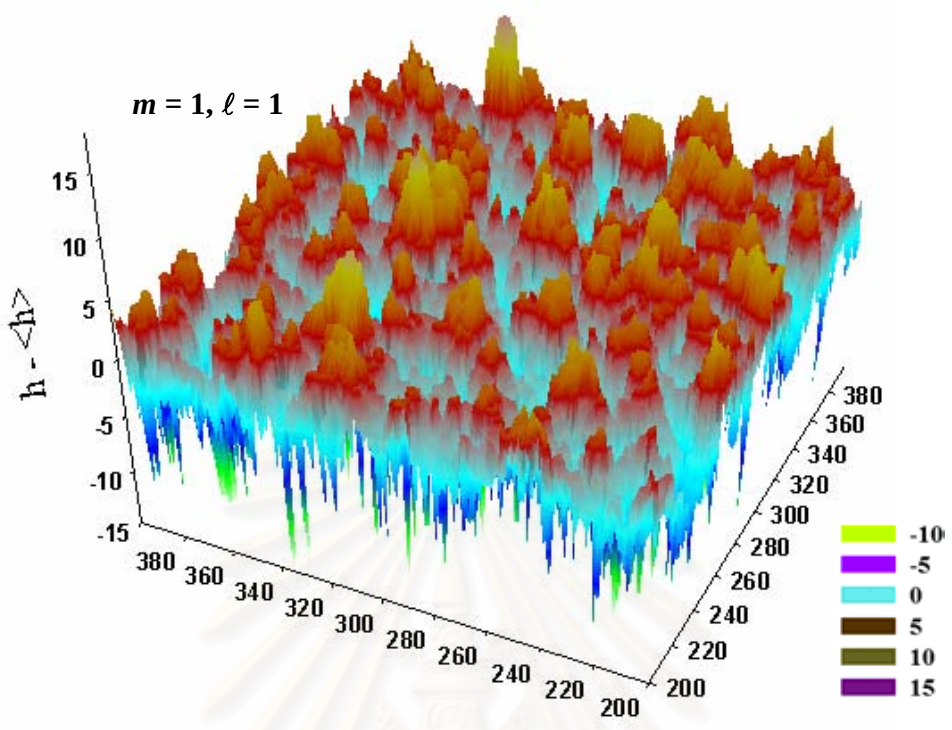

Fig. 3.11 Surface morphology of the original DT model with ℓ = 1, m = 1 and $L \times L$ = 1000 ×1000 (a sections of 200×200) at t = 1000 ML.

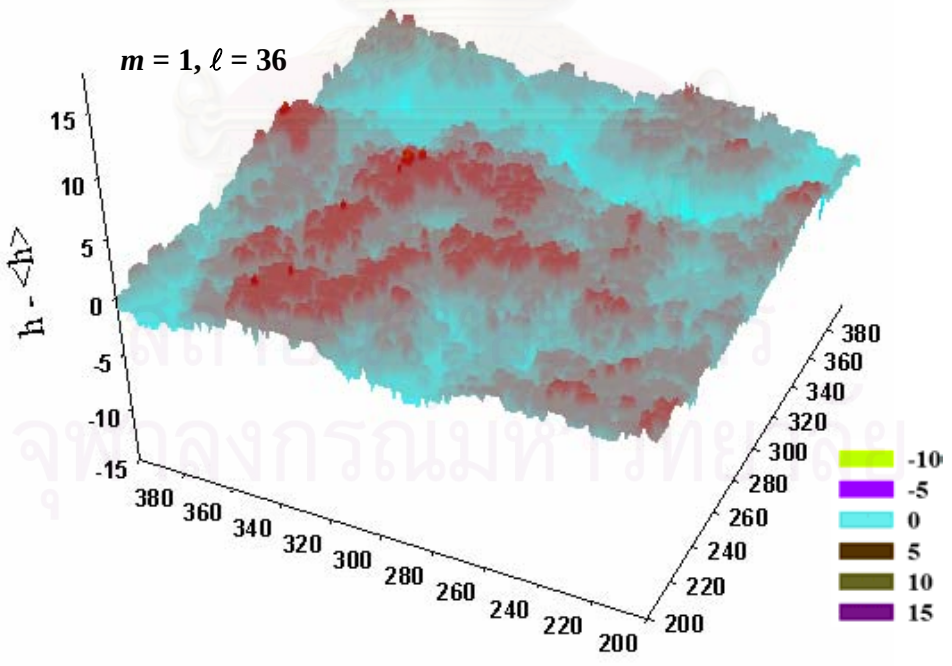

Fig. 3.12 Surface morphology of noise reduced DT model with ℓ = 36, m = 1 and $L \times L$ = 1000 ×1000 (a sections of 200×200) at t = 1000 ML.

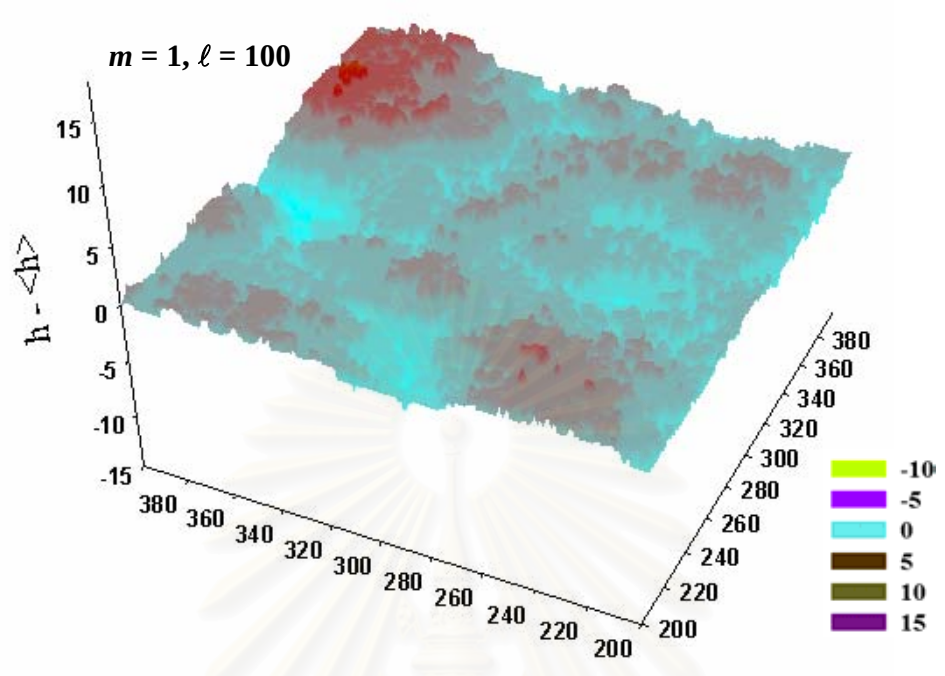

Fig. 3.13 Surface morphology of noise reduced DT model with ℓ = 100, m = 5 and $L \times L$ = 1000 ×1000 (a sections of 200×200) at t = 1000 ML.

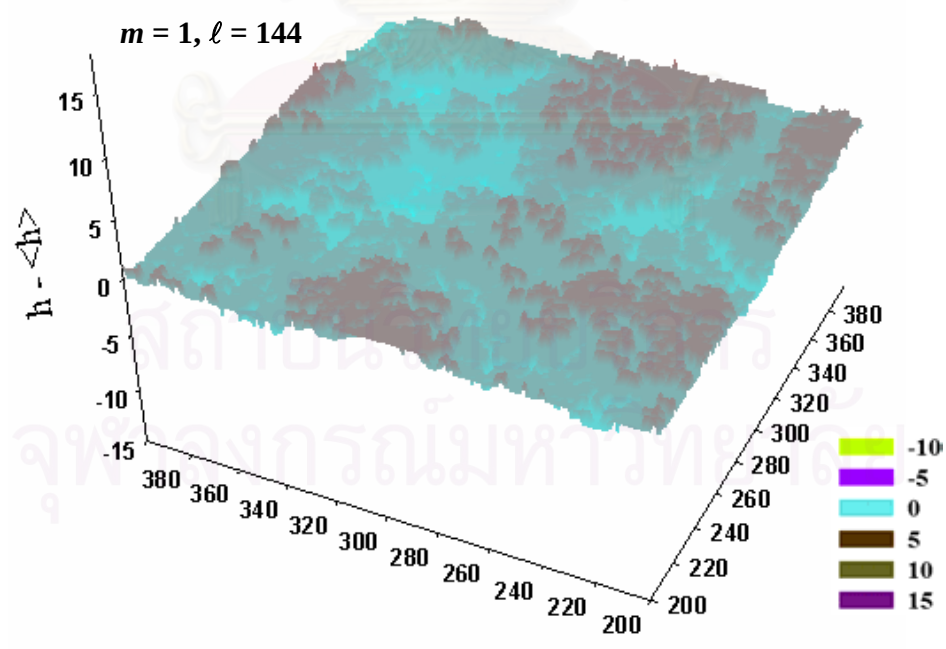

Fig. 3.14 Surface morphology of noise reduced DT model with ℓ = 144, m = 5 and $L \times L$ = 1000 ×1000 (a sections of 200×200) at t = 1000 ML.

3.2 Effects of noise reduction parameter on growth exponent

We are interest to see effects of the noise reduction parameters (ℓ and m) on the growth exponent β. It is clear from both the *W-t* plots and the morphologies that when the value of the noise reduction is large, the growth exponent becomes small. To indicate that the value of the growth exponent in this section may not be the "true" value for the DT model, we call the noise reduction parameter – dependent growth exponent *effective growth exponent* (β_{eff}). The effective growth exponents are calculated from the *W-t* plots of our simulating for the DT model with both the long surface diffusion length noise reduction technique and the multiple hit noise reduction technique.

In Fig 3.15, the surface width from the DT with long surface diffusion length noise reduction technique with various values of ℓ (ℓ = 1, 10, 40 and 100) are plotted as a function of time. Each curve is from a system with $L \times L = 1000 \times 1000$ with an average over different configurations. The top curve with (ℓ = 1), which is the original DT model, does not oscillate for obvious observe. However, it is quite clear that the curve can be separated in two regimes with different slopes. During early time ($t < 10^2$ ML), the best fit yields β_{eff} = 0.261 while in the later time ($t > 10^2$ ML), the best fit yield β_{eff} = 0.199. The first value β_{eff} = 0.261 is close to the theoretical value of β = 0.25 from the linear forth-order continuum growth equation (Equation 2.13. This for can not be the true asymptotic value for the growth exponent for the DT model as the morphologies do not show up-down symmetry indicating that the continuum equation describing the DT model must be a nonlinear equation. The crossover of β_{eff} to β_{eff} = 0.199 during later growth time seems to provide an answer to that problem the value β_{eff} = 0.199, in very close to the theoretical value of β from the nonlinear froth-order condition grave equation (Equation 2.15). This crossover shows that the continuum equation describing the DT model contains both the linear forth-order term $(\nabla^4 h)$ and the nonlinear froth-order term $(\nabla^2 (\nabla h)^2)$.

When the value of ℓ is increased, results in Fig.3.15 show that early time surface width oscillation, as already discussed earlier in section 3.1. However, for $t > 10^2$ ML, all curves can be fitted rather well with a straight line. The slope of the curves decrease as

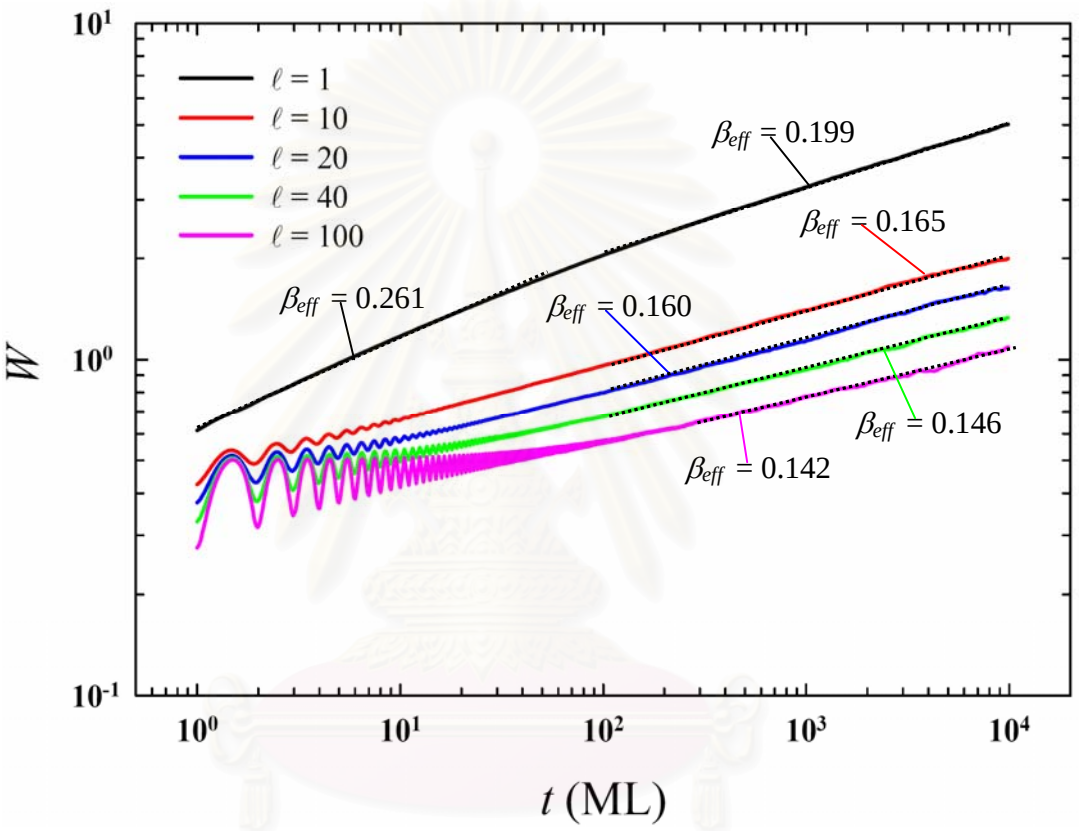

Fig. 3.15 *W*-*t* oscillations of (2+1)-dimensional DT model with $L \times L$ = 1000×1000, m = 1, ℓ = 1, 10, 20, 40 and 100 (top to bottom). The dot straight lines are the best power-law fits which produce the effective growth exponent β_{eff} that decreases as ℓ increases.

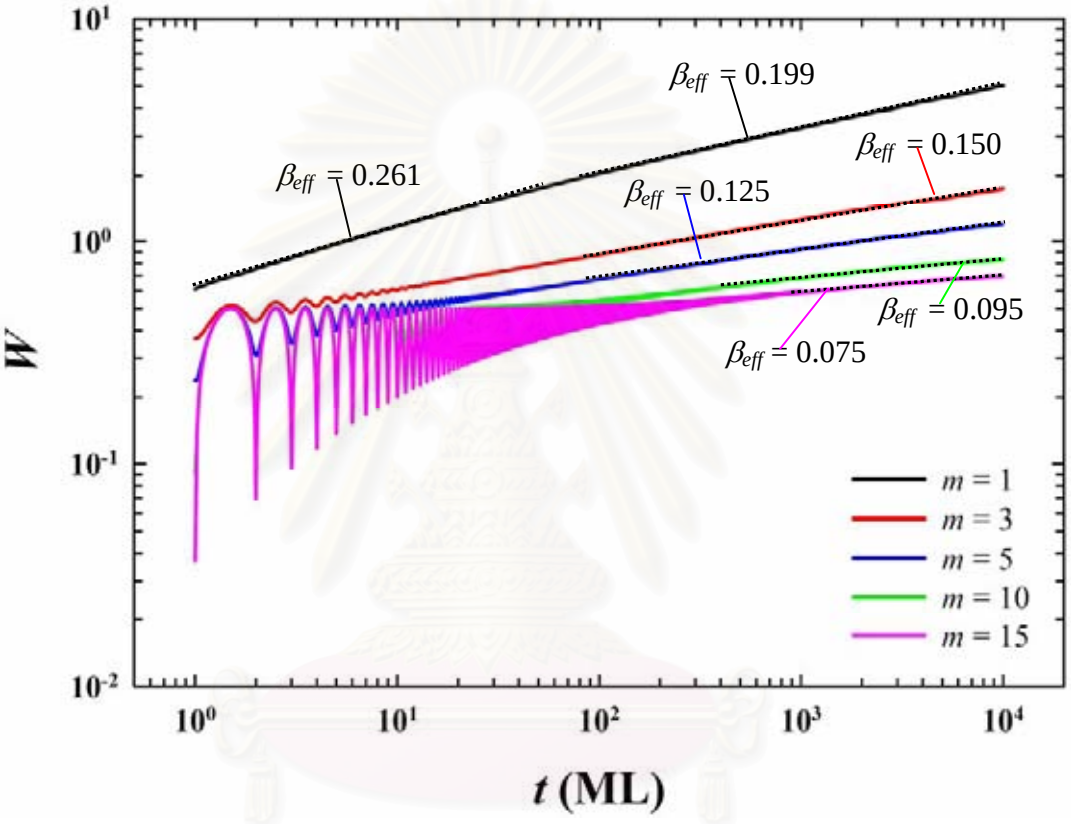

Fig. 3.16 *W*-*t* oscillations of (2+1)-dimensional DT model with $L \times L$ = 1000×1000, m = 1, 3, 5, 10, 15 and ℓ = 1 (top to bottom). The dot straight lines are the best power-law fits which produce the effective growth exponent β_{eff} that decreases as m increases.

ℓ is increased. From β_{eff} = 0.199 for ℓ = 1, the effective growth exponent goes down to β_{eff} = 0.142 for ℓ = 100. This result seems to agree previous works [6, 19] that pointed out that the continuum equation for the DT model should contain the linear second-order term $(\nabla^2 h)$ also the work [6, 19] was done by studying particle diffusion current, which is a completely different approach from our growth exponent study. To our knowledge, the linear second-order term has not been confirmed by exact calculation of the value of β. The confirmation of β the $\nabla^2 h$ term is complicated because the theoretical value of β from the $\nabla^2 h$ term is 0(log) in (2+1)-dimensions. Our results that show decreasing value of β_{eff} is quite encouraging.

Similar produces have been repeated using the DT model with multiple hit noise reduction technique. The results are shown in Fig. 3.16. Here, we obtain similar results-increasing m yield decreasing β_{eff}. With the multiple hit noised reduction technique, we are able to reduce value of the effective growth exponent to β_{eff} = 0.075 with m = 15.

Table 3.1 Effective growth exponent β_{eff} in $d = 2$, obtained from the growth region (no layer-by-layer growth and very good power-law fits used least square fit) of log-log plots of $W(t)$.

m	β_{eff}	r^2	ℓ	β_{eff}	r^2
1	0.199	0.9994	1	0.199	0.9994
3	0.150	0.9987	10	0.165	0.9988
5	0.125	0.9963	20	0.160	0.9985
7	0.110	0.9962	30	0.155	0.9992
9	0.096	0.9975	40	0.146	0.9975
11	0.088	0.9958	50	0.152	0.9992
13	0.082	0.9929	60	0.146	0.9973
15	0.075	0.9922	70	0.149	0.9983
17	0.071	0.9935	100	0.142	0.9970
19	0.064	0.9924	200	0.149	0.9899
21	0.068	0.9954	300	0.130	0.9984
			400	0.140	0.9882
			500	0.122	0.9948

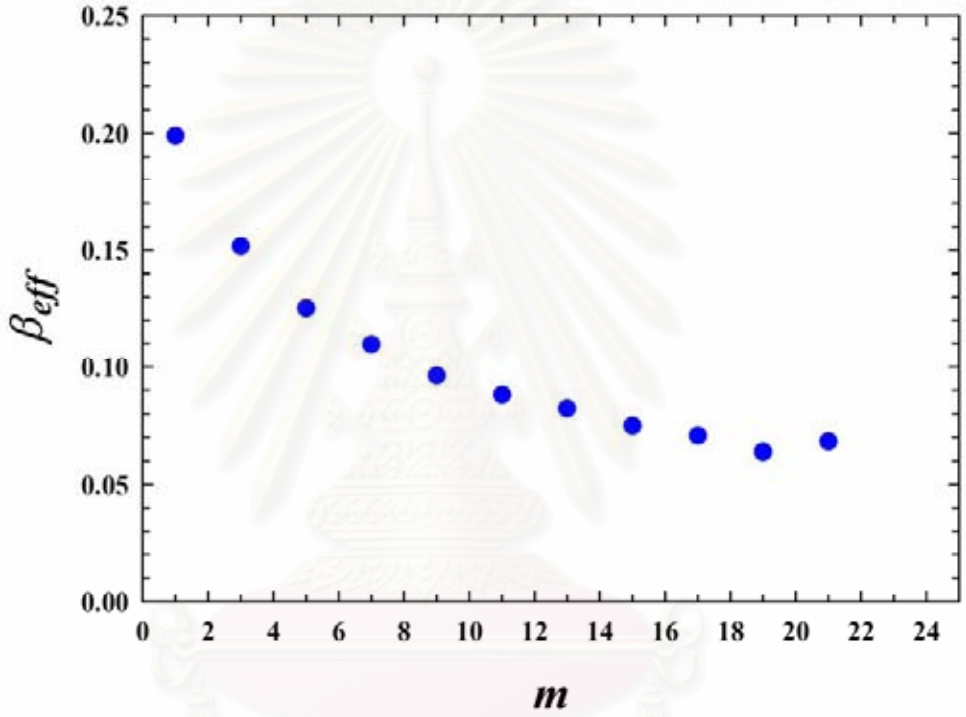

Fig 3.17 The effective growth exponent β_{eff} versus noise reduction parameter m for the DT model with the multiple hit technique in (2+1) dimensions.

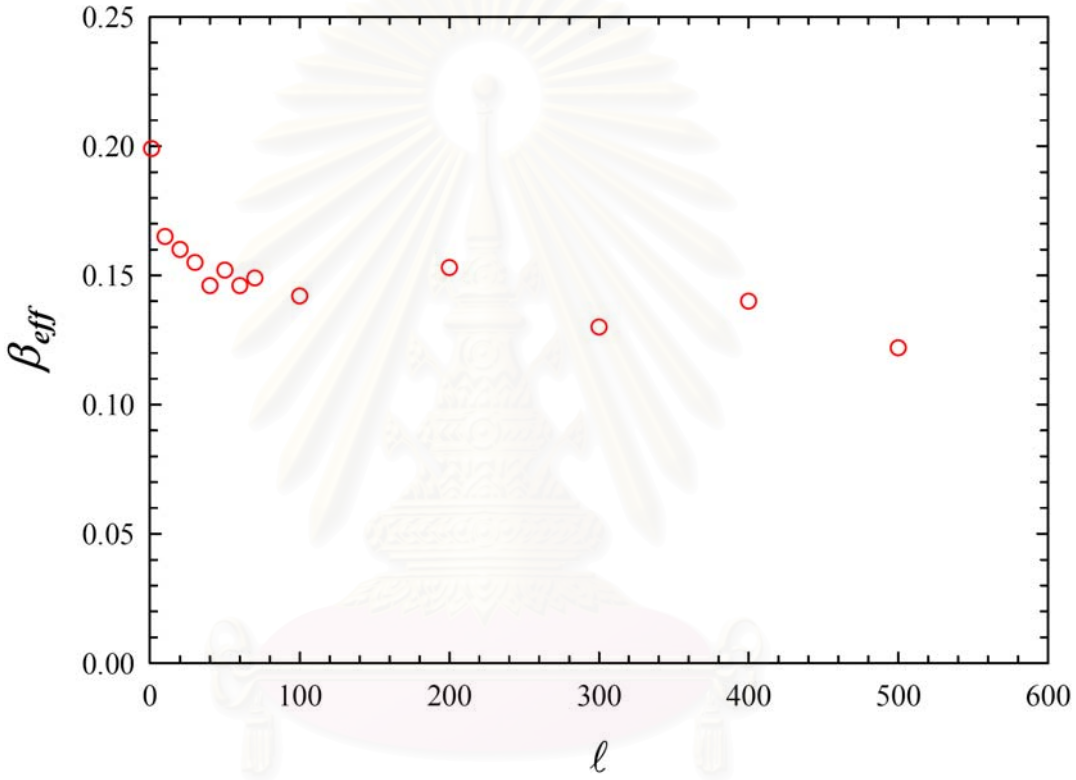

Fig. 3.18 The effective exponent β_{eff} versus noise reduction parameter ℓ for the DT model with the long surface diffusion length in (2+1) dimensions.

CHAPTER IV

RESULT AND DISCUSSIONS: FINITE SIZE EFFECTS ON THE DT MODEL IN (2+1) DIMENSIONS

In chapter III, the noise reduced models suggest that asymptotic behavior of the (2+1)-dimensional DT model may belong to linear second-order continuum growth equation which corresponds to the EW universality class this is in agreement with previous literature [6] which used a diffusion approach (particle diffusion current) to study the model. Another approach was done the (1+1)-dimensional DT model. Previous works [14, 15] studied the finite size effects on scaling exponents and found that results after correction term for finite size effects were added agree with results from the noise reduction technique studies. In this chapter we present our results from the study of finite size effects on the DT model in (2+1) dimensions. We simulated the original DT model (ℓ =1 and m = 1) on two-dimensional substrates. The substrate size $L \times L$ is varied with L = 10, 20, 30, 40, 50, 60, 80, 100, 200, and 1000. Periodic boundary conditions are used. Number of the configurationally average are set to be 200 to 500 for small substrate size (L = 10, 20, 30, 40, 50, 60 and 80), 30 for L = 100, and 5 for L = 200 and 1000. For system with $L \leq 100$, the simulations were done up to time long enough to observe clear saturation of the surface width.

4.1 The growth exponent

The interface width W as a function of deposition time t (films thickness) for several substrate sizes are shown in Fig. 4.1. In the early growth region (typically, 1 ML $\leq t \leq$ 20 ML), W rapidly increases and then gradually crossover to a saturated value in a steady-state region. Note that when the substrate size is large the linear increase of log W as a function of log t continues for longer time. The crossover from the growth region to the steady-state region happens at later time for a system with large L. It can also be seen from the figure that the surface width in a large L system substrates to a large value.

First, we consider the growth exponent which describes the time evolution of the surface roughness. We tried to calculate the slope in the growth region which would yield β, but there is a problem of how to define the growth region. For this work, we choose the growth region by the least square method on log W-log t plots. It is still difficult to determine when the growth region begins and ends because there are slowly crossovers in the interface widths curves. We choose to fit our log W-log t data with a straight line (which yields $W \sim t^{\beta}$) with r-squared $\geq$ 0.999 (r-squared (r^2) is a parameter used to determine how well the data can be fitted to a straight line. The closer to the value of r^2 = 1, the better). The growth region was separated into two parts as Fig. 4.2. The first growth region, stars at an initial time to in the range $2 < t_0 < 4$ ML to a final time t_1 that still provides r-squared = 0.999, Produces effective growth exponent $\beta_L^{(1)}$ for each curve. The second growth region is in the interval [t_1, t_2] that gives r-square = 0.999. Slopes from this region provide $\beta_L^{(2)}$ for each curve. Table 4.1 shows the effective growth exponents $\beta_L^{(1)}$ and $\beta_L^{(2)}$ for several systems of various substrate size. $\beta_L^{(2)}$ was observed only when the substrate L is larger than 30. Our results in Table 4.1 show that growth exponents from the early time region for all substrate size are approximately the same $\beta_L^{(1)} \approx 0.25$. This value of β is consistent with the forth-order linear equation. One the other hand, the growth exponents from the second part of the growth region for all substrate size also have approximately the same value at $\beta_L^{(2)} \approx 0.20$. This value corresponds to the forth-order nonlinear equation.

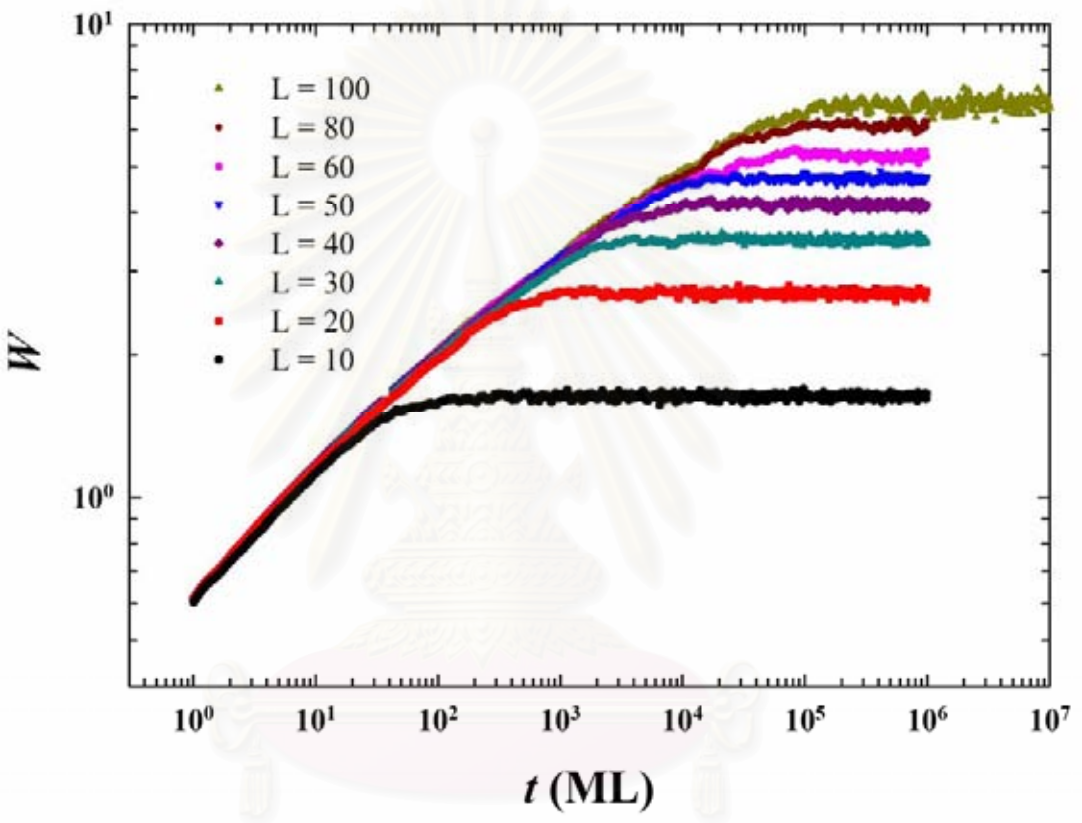

Fig 4.1 *W*-*t* of the (2+1)-dimensional DT model with m = 1 and ℓ = 1. When vary substrate sizes, $L \times L$ here L = 10, 20, 30, 40, 50, 60, 80 and 100. The saturation times increase as substrate sizes increase.

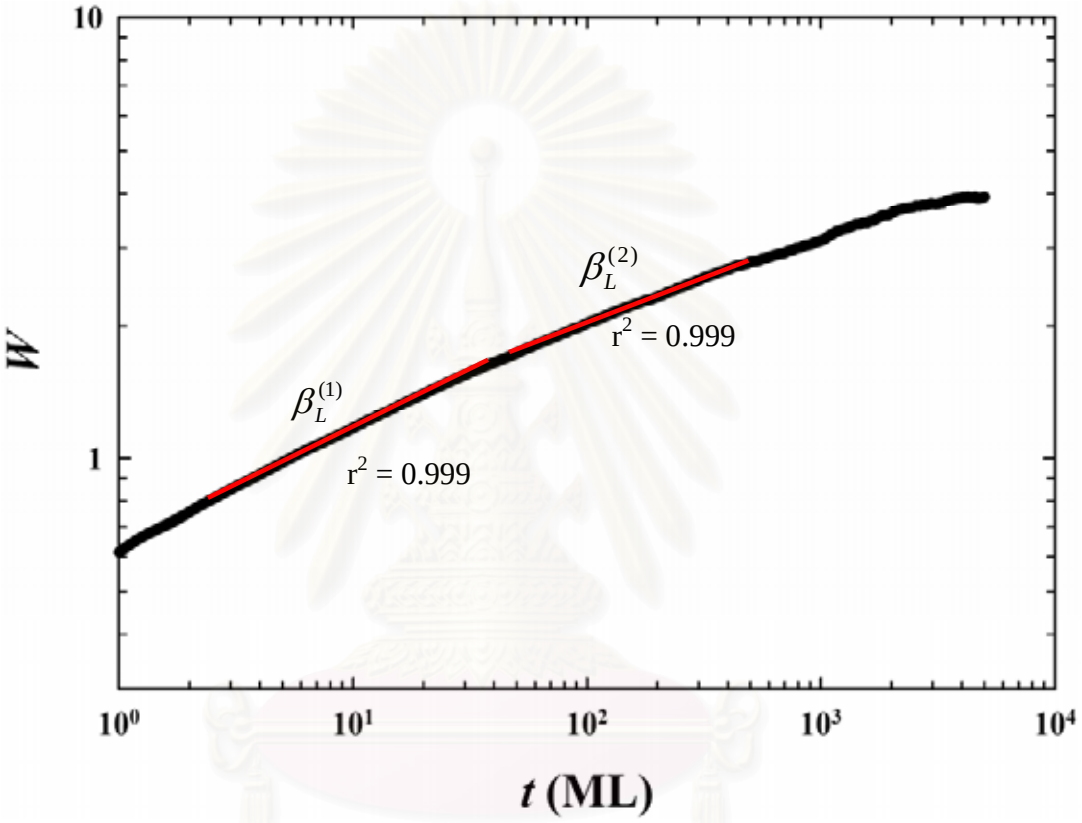

Fig. 4.2 Illustration of definition of growth regions for the (2+1)-dimensional DT model for each substrate size, first and second growth regions are indicated $\beta_L^{(1)}$ and $\beta_L^{(1)}$ respectively. R-squared of data in each growth region is also shown.

Table 4.1 Effective exponents $\beta_L^{(1)}$ and $\beta_L^{(2)}$ obtained from log *W*- log *t* plots of the (2+1)-dimensional DT model using least square fits to define the approximated growth regions

Substrate length (*L*)	**R^2 = 0.999** $\beta_L^{(1)}$	t_1 **(ML)**	**R^2 = 0.999** $\beta_L^{(2)}$	t_2 **(ML)**
10	0.251	18	-	-
20	0.248	48	-	-
30	0.250	58	-	-
40	0.250	72	0.200	546
50	0.249	85	0.198	1340
60	0.247	122	0.199	650
80	0.250	75	0.198	1860
100	0.250	144	0.194	2207
200	0.249	72	0.203	2931
1000	0.249	124	0.196	1000

From our results, the growth exponents from all substrate sizes have a crossover from the forth-order linear equation to the forth-order nonlinear equation. This implies that both the $\nabla^4 h$ and the $\nabla^2(\nabla h)^2$ terms are included in the continuum growth equation for the (2+1)-dimensional DT model, i.e. $\frac{\partial h}{\partial t} = \nu_4 \nabla^4 h + \lambda_1 \nabla^2 (\nabla h)^2 + \eta(x,t)$. The coefficient ν_4 must be larger than the coefficient λ_1, so effects of the $\nabla^4 h$ term shows through in the value of the growth exponent from early time. To see effects of the substrate size on the value of $\beta_L^{(1)}$ and $\beta_L^{(2)}$, we plot $\beta_L^{(1)}$ and $\beta_L^{(2)}$ versus $1/L$ as shown in Fig. 4.3. This method was used in (1+1)-dimensional DT model [14, 15] to find the "asymptotic" β which is the value of the growth exponent in the ideal case of $L \to \infty$. From the β_L versus $1/L$ plot, the curve can be extrapolated back to find the Y-intercept of the curve which is the value of β_L with $1/L = 0$ or $L \to \infty$. However, from our results, the value of $\beta_L^{(1)}$ and $\beta_L^{(2)}$ do not seems to depend on L because, as can be seen in Fig.4.3, the values of $\beta_L^{(1)}$ are practically 0.25 for all values of L while $\beta_L^{(2)}$ fluctuates very closely around the value of 0.20. If we insist on extrapolating the curve, we would surely obtain $\beta_L^{(1)} \approx 0.25$ and $\beta_L^{(2)} \approx 0.20$. This shows that finite size substrates do not have any strong effect on the growth exponents β for the (2+1) dimensional DT model. This method that work so well in the (1+1)-dimension DT model [14, 15] does not help in obtaining the "true" asymptotic β in our case. On the other hand, this is quit consistent with experiments. As we mentioned before, the growth exponent gives information about time evolution of the roughness of the surface. Large β means the film roughness increases rapidly in time. Experimentally, one should see that this time evolution of film roughness depends on growth conditions and material of the film, but does not depend on the size of the film substrate. So the substrate size L should not have much effect on the value of the growth exponent.

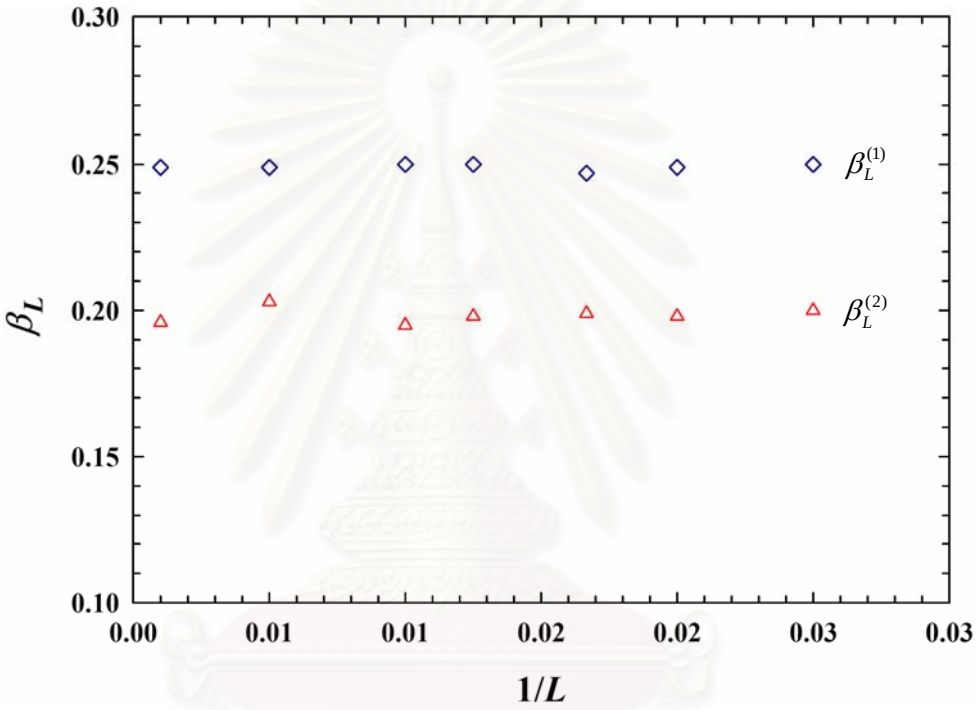

Fig. 4.3 Effective growth exponent $\beta_L^{(1)}$ and $\beta_L^{(2)}$ of the DT model in (2+1) dimensions, obtained from plots of W versus $1/L$ with L = 30, 40, 50, 60, 80, 100, 200 and 1000.

4.1 The roughness exponent

Although the extrapolation method to eliminate finite size effects do not work for the estimation of asymptotic growth exponent of the (2+1)-dimensional DT model, we repeat the procedure to try to calculate the asymptotic roughness exponent α. Traditionally, the roughness exponent α is obtained from a log – log plot of saturation value of W versus the substrate size L. From scaling relation, $W_{sat} \sim t^{\alpha}$, the plot should yield a straight line with the slope being the value of α. That means data from all substrate sizes combined will give just one value of α. In Fig. 4.4, our results from L = 10, 20, 30, 40, 50, 60, 80, and 100 are plotted using the method. The dot line represents the best fit to a straight line which has a slope of 0.616. So our calculated roughness exponent from the traditional method is α = 0.616. But in this study, we also want to have value of the roughness exponent α as a function of the substrate size L. Obviously, the traditional method does not work in our case so we follow another approach to extract α [13, 14, 15]

The effective roughness exponent α_L for each value of L can be calculated with a relation [13, 14]:

$$\alpha_L = \frac{\ln[W_{sat}(L)/W_{sat}(L/2)]}{\ln 2} \ .$$

Here, $W_{sat}(L)$ and $W_{sat}(L/2)$ are the saturation values of the surface width for the substrate size L and L/2 respectively. The value of $W_{sat}(L)$ is obtained from an average of the surface width in the stead-state region (the constant width for each L in Fig.4.1). $W_{sat}(L)$, $W_{sat}(L/2)$ and α_L from our calculation are shown in Table 4.2. The effective roughness exponents were then plotted as a function of $L^{-\Delta}$. The constant Δ that provides the best linear fit (r^2 = 0.987) is 0.2 as shown in Fig 4.5. From Fig 4.5, the results indicate that when $L \to \infty$ the effective roughness exponent α_L converts to 0.005 that suggests the linear second-order $\nabla^2 h$ term (α = 0). This seems to imply that the asymptotic universality class of the (2+1) dimensional DT model is the EW universality class and correction-to-scaling term for the roughness exponent is

$$\alpha_L \approx AL^{-0.2} + \alpha \ ,$$

A is a constant and α is the asymptotic roughness which is $\alpha = 0.005$ in this work.

We note, however, that the data we use here are from small substrate size ($L \leq 100$). The asymptotic value of $\alpha_{L\to\infty} = 0.005$ that we obtain from the extrapolation may not be correct. This is because when the system size is large ($L >> 100$), it is possible that the α_L versus $L^{-\Delta}$ curve may crossover to other behavior and the values of both Δ and $\alpha_{L\to\infty}$ may change. To improve this result, saturation values of surface width from large system sizes are needed. But with the limitation in computer speed, this is difficult to do because surface width from a larger system will saturate at a much later time. So with the resource we have, we still believe that $\Delta = 0.2$ and $\alpha_{L\to\infty} = 0.005$ are the best estimate we can obtain although we acknowledge that $\alpha = 0.005$ may not be the true asymptotic value of the roughness exponent for the (2+1)-dimensional DT model.

Table 4.2 The value of α_L and $W_{sat}(L)$ obtained from large saturation regions of the DT model in (2+1) dimensions.

L	$W_{sat}(L)$	α_L
10	1.63 ± 0.02	-
20	2.69 ± 0.03	0.724 ± 0.02
30	3.49 ± 0.04	-
40	4.15 ± 0.05	0.621 ± 0.02
50	4.72 ± 0.05	-
60	5.25 ± 0.06	0.590 ± 0.02
80	6.10 ± 0.10	0.558 ± 0.03
100	6.74 ± 0.20	0.515 ± 0.04

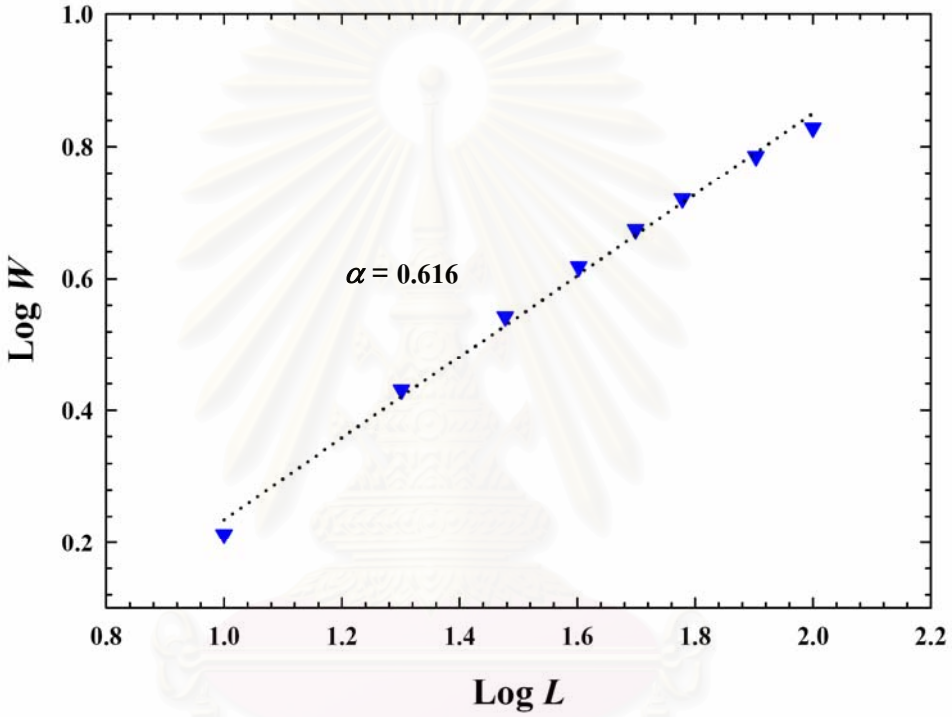

Fig. 4.4 Log W_{sat} versus log L for (2+1)-dimensional DT model with $L \times L$ when L = 10, 20, 30, 40, 50, 60, 80 and 100 (bottom to top). The dot line shows the best linear fits that gives $\alpha = 0.616$.

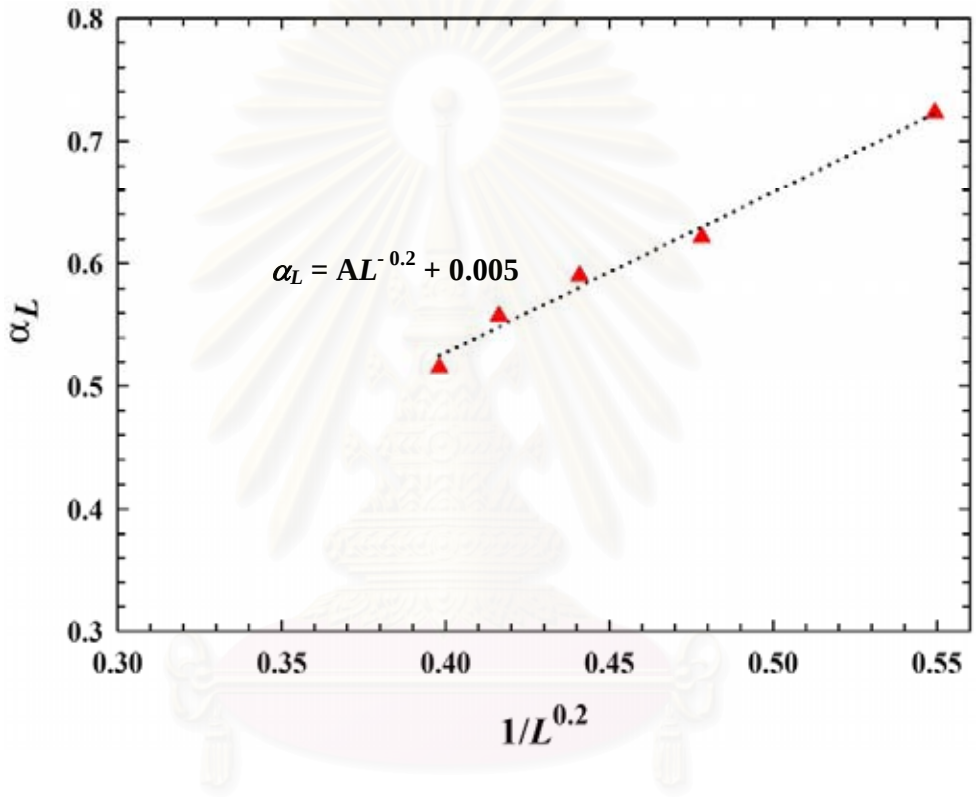

Fig. 4.5 The effective roughness exponents α_L versus $L^{-\Delta}$ in (2+1)-dimensional DT model. The straight dot line is a good linear fit with $\Delta = 0.2$ and A is constant. L = 20, 40, 60, 80 and 100 (top to bottom).

CHAPTER V

CONCLUSIONS

We study the noise reduced DT model in (2+1) dimensional substrates. Two noise reduction techniques - long surface diffusion length and multiple hit - are used. The DT model is a solid-on-solid limited mobility growth model. Aggregation rules of the DT are equivalent to low temperature MBE growth. For The DT model, after an atom is released from a randomly chosen site above the surface, it can move only to its nearest neighbors to find the final site where it can *increase* number of bonds. A deposited atom has enough energy to break only one bond, but not enough to break two or more bonds. The long surface diffusion length technique (ℓ>1) is equivalent to the increase in the substrate temperature that encourage the diffusion of surface atoms while the multiple hit noise reduction technique ($m > 1$) is a computational technique. Parameter ℓ is a maximum length to diffuse under the aggregation rules of the DT model while parameter m is a number of attempts to stick at the chosen final site on the substrate before a deposition occurs.

Our investigations show that the long surface diffusion length noise reduction technique and the multiple hit noise reduction technique can enhance the layer-by-layer growth indicated by oscillation in surface roughness - oscillation of interface width versus time - during early growth time. The layer-by-layer damps out when growth time is longer than the damping time t_c. We find that the damping time depends on the noise reduction parameters with power laws relations: $t_c \sim (\ell/L)^{\delta}$ when L is substrate size and $t_c \sim m^{\mu}$. We found that for the (2+1)-dimensional DT model, $\delta = 1.5$ and $\mu = 2.5$ for the long surface diffusion length and the multiple hit techniques respectively.

Our surface morphologies when $t < t_c$ confirm that these two noise reduction techniques produce smooth film surfaces which is equivalent to increasing substrate temperature in experiments. In fact, the noise reduced films from the long surface diffusion length technique and the multiple hit noise reduction technique are practically indistinguishable. So we can conclude that the two noise reduction techniques are indeed equivalent for the study of the layer-by-layer growth.

After the damping time, surface roughness shows kinetically rough growth and interface width increases with time as a power law, $W \sim t^{\beta}$. For the original DT model (ℓ = 1 and m = 1), there is a slow crossover of the growth exponent from β = 0.26 (that belongs to the linear forth-order equation) to β = 0.2 (that belongs to the nonlinear forth-order equation). In addition, our results show that the two noise reduction techniques have effects on the growth exponent β. For the multiple hit technique, the effective growth exponent β_{eff} decreases as parameter m is increased and it becomes close to zero (that belongs to the EW universality class) at large m. For the long surface diffusion length technique, β_{eff} decreases as parameter ℓ is increased. At large ℓ, β_{eff} fluctuates and does not converge to zero. So we conclude that the long surface diffusion length noise reduction technique is not strong enough to find the asymptotic value of the DT model.

Furthermore, we study finite size effects on the DT model in (2+1) dimensional substrates. We simulated the (2+1) dimensional DT model without the two noise reduction techniques (ℓ = 1 and m = 1) and varied the size of the substrate. We found that the finite size effects are not strong on the calculation of the growth exponent of (2+1)-dimensional DT model. It is, however, so strong that it effects the value of the roughness exponent. Effective roughness exponent α_L of each substrate size is calculated from $\alpha_L = \frac{\ln[W_{sat}(L)/W_{sat}(L/2)]}{\ln 2}$ [13,14]. The effective roughness exponents α_L versus $L^{-\Delta}$ plots are fitted to a linear curve with $\Delta = 0.2$ that gives correction-to-scaling term $\alpha_L \approx AL^{-0.2} + \alpha$, when A is a constant and α is the asymptotic roughness exponent. We found that our results of the (2+1)-dimensional DT model yield the asymptotic roughness

exponent α = 0.005. That indicates the model asymptotically belongs to the EW universality class.

From our work, we belief that the continuum growth equation describing the (2+1)-dimensional DT model consists of the second-order linear term $\nu_2\nabla^2 h$, the forth-order linear term $\nu_4\nabla^4 h$, the froth-order nonlinear term $\lambda_1\nabla^2(\nabla h)^2$ and the noise term $\eta(x,t)$. At early growth time, the simulation results show behavior of the froth-order linear term so it means the coefficient ν_4 is the strongest. However, because λ_1 and ν_2 are not zero, behaviors of the nonlinear forth-order term and the linear second-order appear at later time. With the behavior of the linear second-order term so difficult to see, the coefficient ν_2 must have a very small value. In addition we can confirm that the multiple hit noise reduction technique can reduce noise until the asymptotic behavior of growth model appears. But the long surface diffusion length technique does not work to find the asymptotic growth exponent of the (2+1) DT Model.

Finally, values of the growth exponent (β) and the roughness exponent (α) of the (2+1)-dimensional DT model obtained from different methods in our work are concluded in Table. 5.1.

Table 5.1 The growth exponent (β) and the asymptotic roughness (α) of the (2+1)-dimensional DT model obtained from difference methods.

Methods	β	α
Noise reduction techniques - Multiple hit technique - Long surface diffusion length	 0.005 0.12-0.13	 - -
Traditional scaling	$\beta^{(1)} \approx 0.25$ crossover to $\beta^{(2)} \approx 0.20$	0.616
Finite size effects	$\beta^{(1)} \approx 0.25$ crossover to $\beta^{(2)} \approx 0.20$	0.005

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2007 *Pranee Changkaew and Patcha Chatraphorn. Layer-by-Layer Epitaxy in Noise-Reduced Das Sarma-Tamborenea Model of Surface Growth.* 2nd Siam Physics congress 2007.