Chapter III

Simulation Results and Discussions

As described in the previous chapter, our study is based on WV growth on one dimensional substrate (d = 1+1) which is flat at initial time. In fact, the one-dimensional substrate growth has never been seen [2] in experimental laboratories. But the studies of one dimensional growth systems are still important. This is because we can still gain some insight in the dynamical properties of MBE growth models while using less time in the simulations. Besides, although not an MBE growth, there exist some one dimensional interface roughening processes in real phenomena such as the snowflakes falling on the car windshield, waves clashing on the shoreline, etc. Here we study characteristic of the surface of the growing films, i.e. the *morphology.* Then we calculate the surface width W and find the exponents (α, β, z) to identify the asymptotic universality class of the WV model. Furthermore, we are interested in studying the effect of the potential barrier (ES barrier [6, 7, 8]) in WV model, the WV-ES model. The results from our simulations are shown and discussed in this chapter.

3.1 Morphologies and Scaling Exponents

In this section, we begin with our results of the simplest model (the RD model) and then focus on results of the more complicated WV model and WV-ES model later.

3.1.1 Random Deposition Model

The RD model [1] is the simplest model under the SOS constraints. In the RD model, there is no diffusion at all. The morphology and the surface width of the RD model are shown in Fig. 3.1. In Fig. 3.1(a), the morphology after depositing 10^6 ML is very rough due to the fact that each site x of the surface grows independently and the surface is uncorrelated. The surface width W plot versus time t in Fig. 3.1(b) shows that W increases indefinitely in time. The slope of this plot is the growth exponent according to Eq. (1.4). Here we have $\beta = 0.5$. The growth exponent from our simulation is in agreement with the exact solution calculated in the literature [1].

3.1.2 Wolf-Villain Model

The WV model [3] is a discrete model with very simple diffusion rules but its morphologies and scaling properties are not simple [2]. We begin by investigating the surface width of the WV model. In Fig. 3.2, we show the surface width W plot as a function of time t for a system with $L = 20{,}000$ lattice sites. We found the growth exponent $\beta \approx 0.37$, agreeing with previous works [2, 3, 26]. Since L is very large, we do not see any saturation in this plot.

The roughness exponent α is obtained from the plot of saturated surface width (W_{sat}) as a function of substrate size L. In Fig. 3.3, we plot the saturated width (W_{sat}) at time $t = 10^7$ ML versus the size of the substrate L, with L varying from $L = 10$ to $L = 100$. We obtained the value of the roughness exponent in one-dimensional WV model to be $\alpha \approx 1.40$. Then we calculated the third critical exponent (the dynamical exponent) z by following Eq. (1.14), $z = \alpha/\beta$. The value of the dynamical exponent z of the WV model is $z \approx 1.40/0.37 \approx 4$. All of the critical exponents (α, β, z) we obtained agree well with previous work [3] and these values correspond to the Mullins-Herring (MH) universality [14, 15] listed in Table 1.1. However, we note that many works [20, 26, 27, 28, 29] have shown that this is only a crossover behavior of the WV model. Krug *et al.* [20]

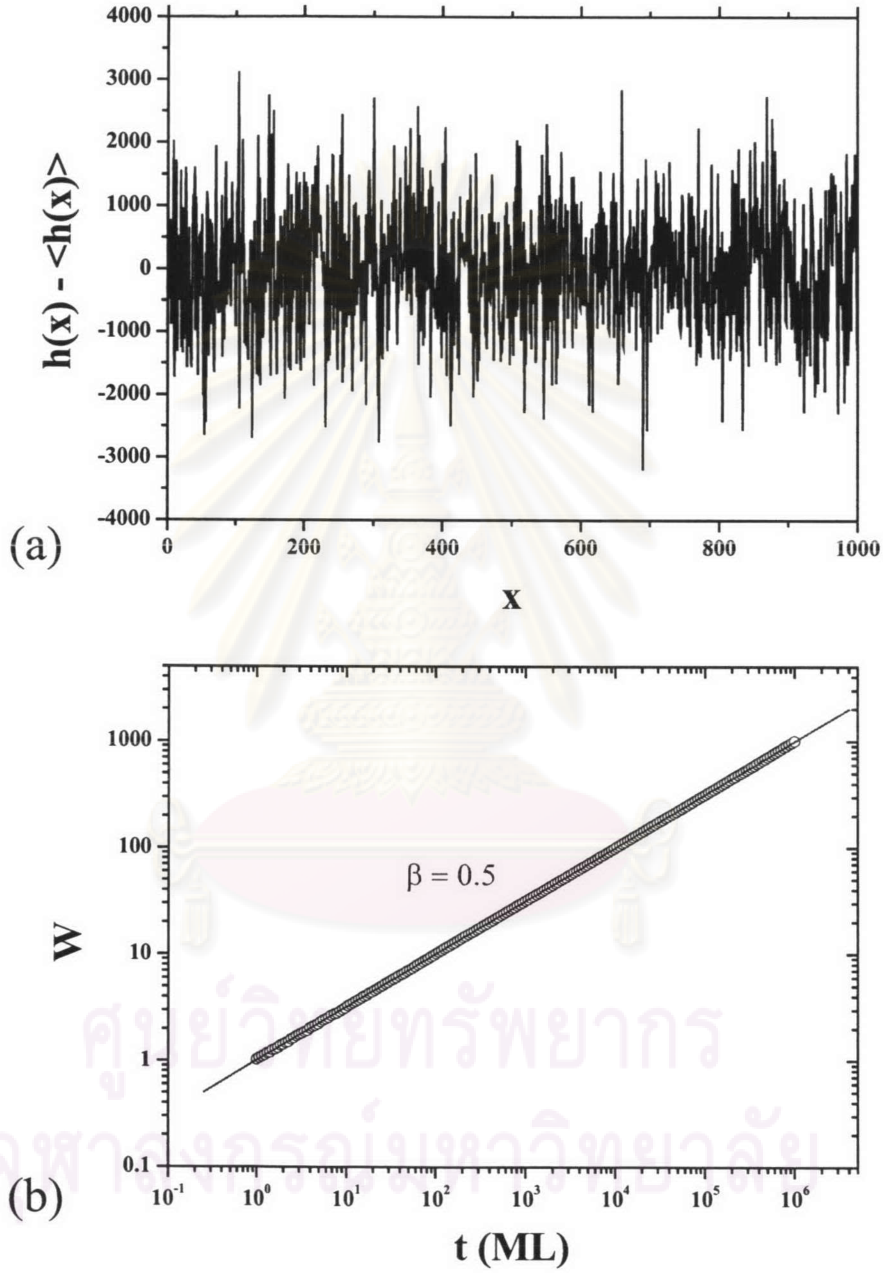

Figure 3.1: (a) The morphology and (b) the surface width of the Random Deposition (RD) model after depositing 10^6 ML on a substrate of size $L = 1000$.

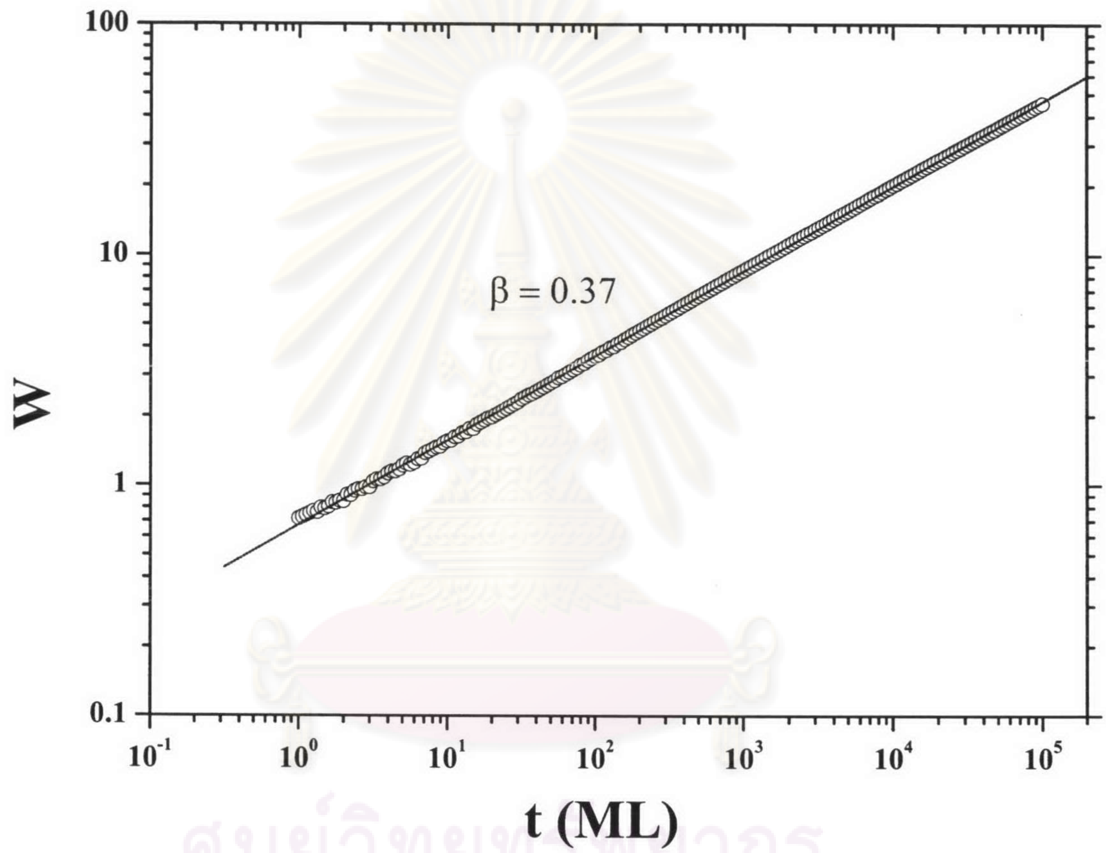

Figure 3.2: The surface width W of the WV model plot versus time t in log-log scale from the system of substrate size L = 20,000 at time $t = 10^5$ ML. We obtain the growth exponent $\beta \approx 0.37$ from the slope of this plot.

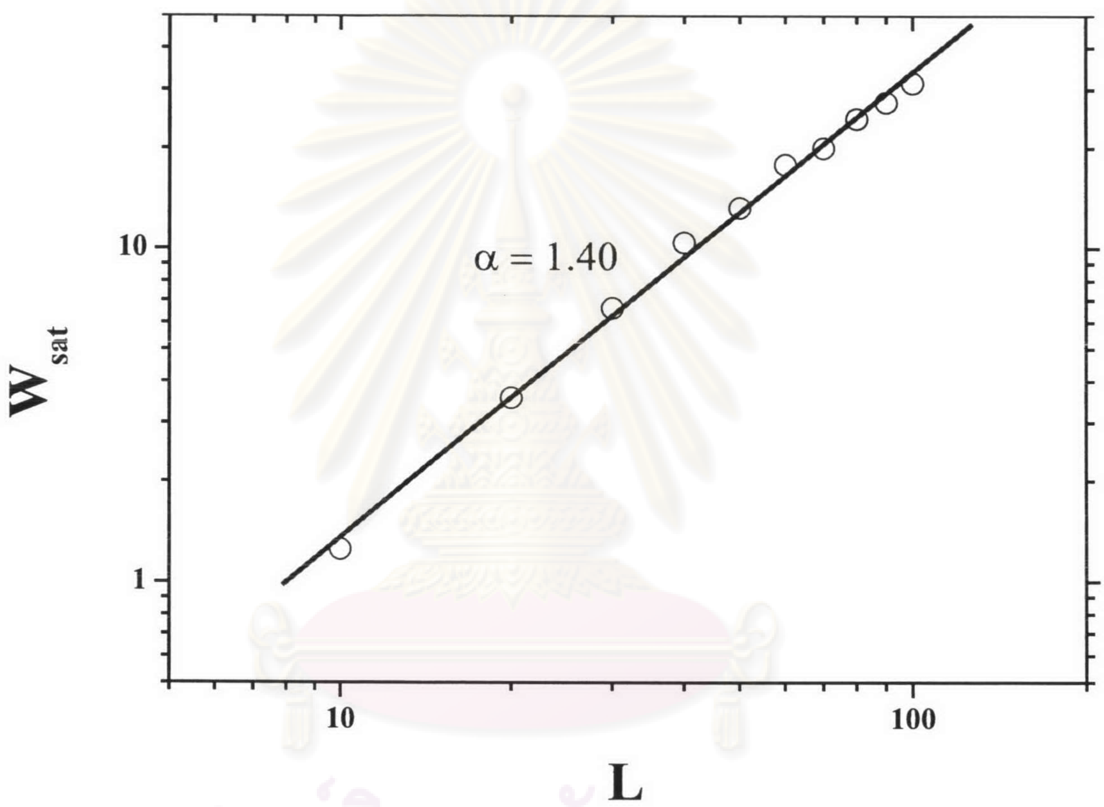

Figure 3.3: The saturate width (W_{sat}) of the WV model plot as a function of substrate size L. We simulate the systems of the substrate size $L = 10$ to $L = 100$ at time $t = 10^7$ ML. The slope of this plot is the roughness exponent $\alpha \approx 1.40$.

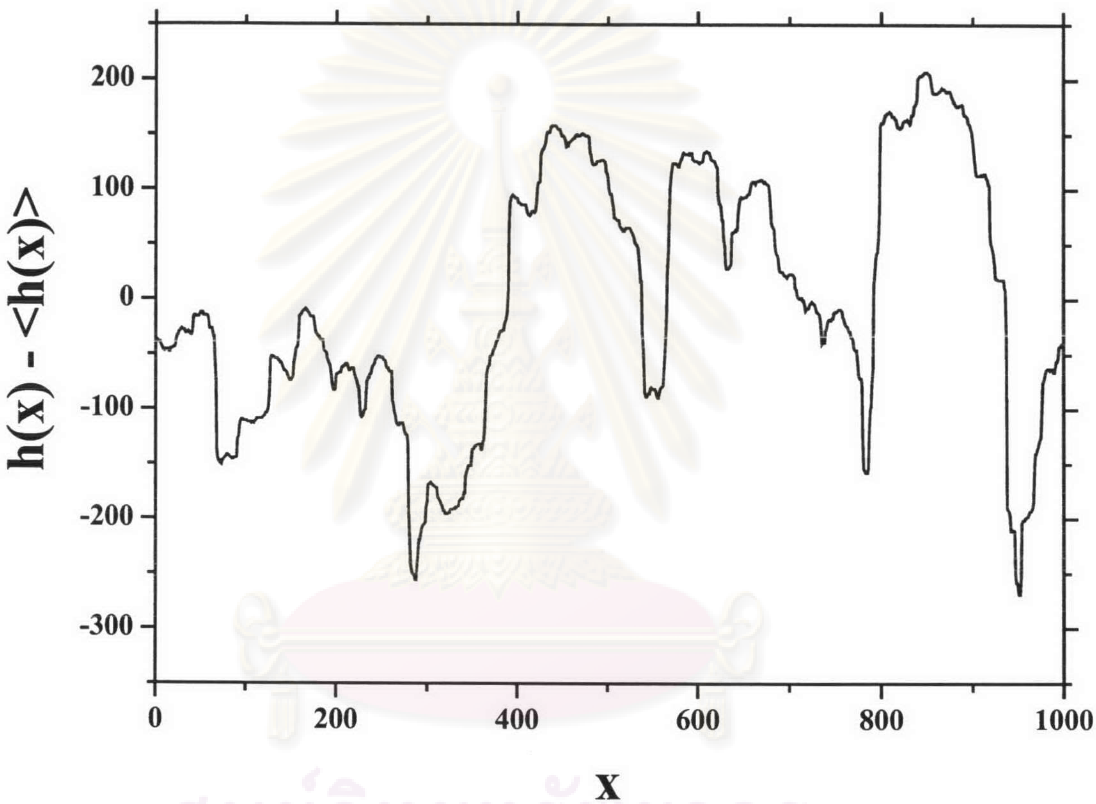

Figure 3.4: The snapshots of the morphology created by the WV model. This morphology comes from the system of substrate size $L = 1000$ and time $t = 10^6$ ML.

suggested that the true asymptotic universality class of the WV model should be the Edward-Wilkinson (EW) universality class [13]. They prove it by using the particle diffusion current calculation [20] (we will discuss this in section 3.3). In principle, if we can grow large films ($L \to \infty$) for long enough time ($t \to \infty$) we can see the crossover to the true asymptotic universality. In practical, however, due to the limitation of computers, that asymptotic time cannot be reached. So from results of the scaling exponents (α, β, z) alone, it seems to lead to the conclusion that the WV model belong to the MH universality class or the linear fourth order equation as in Eq. (1.21).

After we study the scaling behavior, we investigate the surface morphologies of this model. In Fig 3.4, we show a snapshot of the growing interface after 10^6 ML deposition. Although this is not as rough as the RD morphology (compare the minimum and maximum scales on the two plots), it seems that the WV morphology is still quite rough with deep grooves and relatively flat tops. Looking closely at this morphology we see that if we flip it upside down, the surface becomes very different from the original morphology. The new one under the $h \to$ -h transformation will have spiky peaks with shallow valleys. In other words, the up-down symmetry in the system is broken [2, 3, 19] in Fig. 3.4. This information tells us that a linear equation, such as Eq. (1.21), is not the right equation for the WV model. There must be some nonlinear terms in the equation as well. This issue will be addressed in section 3.4.

3.1.3 WV-ES Model

From the original WV model [3], we applied the effect of an ES barrier [6, 7, 8] to the original WV model by defining two probabilities P_U and P_D for adatoms attached to an upper and a lower terraces, as described in the previous chapter. The effect of the ES barrier can be seen when we set $P_D < P_U$ ($0 \leq P_D < P_U \leq 1$). In Fig 3.5 we show the time evolution of the 1+1 dimensional simulated morphology of the WV-ES model with $P_U = 1.0$ and $P_D = 0.5$. The mound formation on the surface comes from the effect of an ES barrier that deposited adatoms cannot come down from upper to lower terraces. The mounding in the growth morphology starts after approximately 10^4 ML as can be seen in Fig. 3.5. These mound formation on the surface is sometimes referred to as an instability [2].

When we fixed $P_U = 1.0$ and vary the strength of the barrier by varying the probability P_D, we found that the surface morphologies have deeper grooves and shaper peaks in systems with stronger barrier (decreasing P_D), as in Fig. 3.6. This is due to the fact that adatoms have less chance to hop down to the lower terraces when P_D is smaller, which corresponds to stronger barrier in this situation. The average size of each mound also seems to be smaller when the barrier is stronger. When the values of P_D and P_U are equal, we found that the morphologies of the WV-ES model (Fig. 3.7) become dynamical rough (no mound formation) surfaces as found in the original WV model. This may be puzzling but it can be explained that when adatoms have equal chance to hop to upper or lower terraces, there is no bias in the model and the model reduces back to the original WV model even through P_D, $P_U < 1$. This can be confirmed by the W-t plot as shown in Fig. 3.8. Of course, if we set the probabilities to be too small, it becomes difficult for atoms to hop and the morphologies in these cases are more rough, such as the system with $P_U = P_D = 0.1$ in Fig. 3.7. And when we set $P_U = P_D = 0$, we found that morphology of this case becomes the same as the morphology from the RD model [1] shown earlier in Fig. 3.1, which is totally predictable because when $P_U = P_D = 0$ atoms lose all mobility and cannot diffuse at all.

The last situation is when we set $P_D > P_U$, it was found that the morphologies are much smoother than the original WV model. This is shown in Fig. 3.9. This case corresponds with the *negative* ES barrier [30] which induces very smooth surface because most of the adatoms hop down to lower terraces and fill up the grooves.

To study the scaling behavior of the WV-ES model, we show in Fig. 3.10 the surface width W plot as a function of time t in log-log scale from a system with $L = 10^3$, $P_U = 1.0$ and $P_D = 0.5$. We found that in the early time the

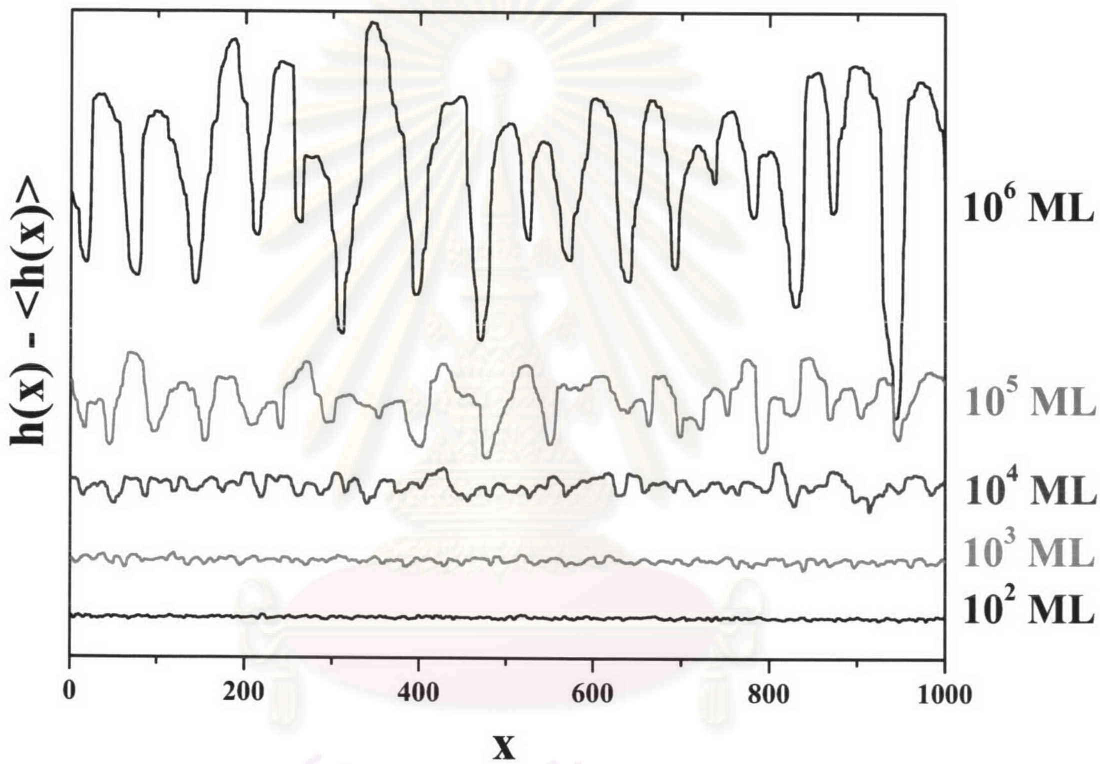

Figure 3.5: The mound evolutions of the WV-ES model in 1+1 dimensions from the systems of substrate size $L = 1000$ at time $t = 10^2$ - 10^6 ML from bottom to top. The systems are simulated with $P_U = 1.0$ and $P_D = 0.5$.

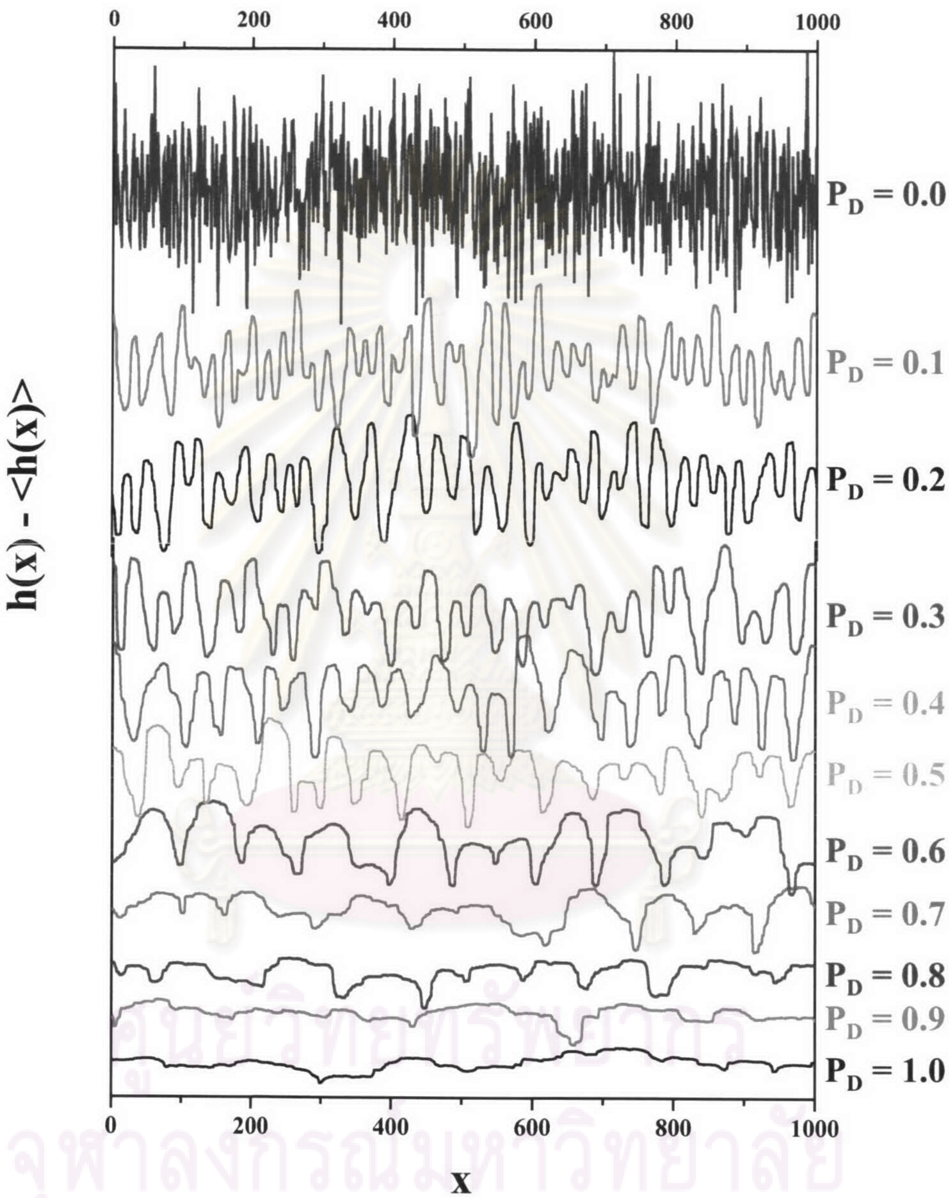

Figure 3.6: The morphologies of the WV-ES model when we vary the values of $P_D = 0.0$ to 1.0 (from top to bottom) by fixed the value of $P_U = 1.0$. We simulate the systems of substrate size $L = 1000$ at time $t = 10^6$ ML.

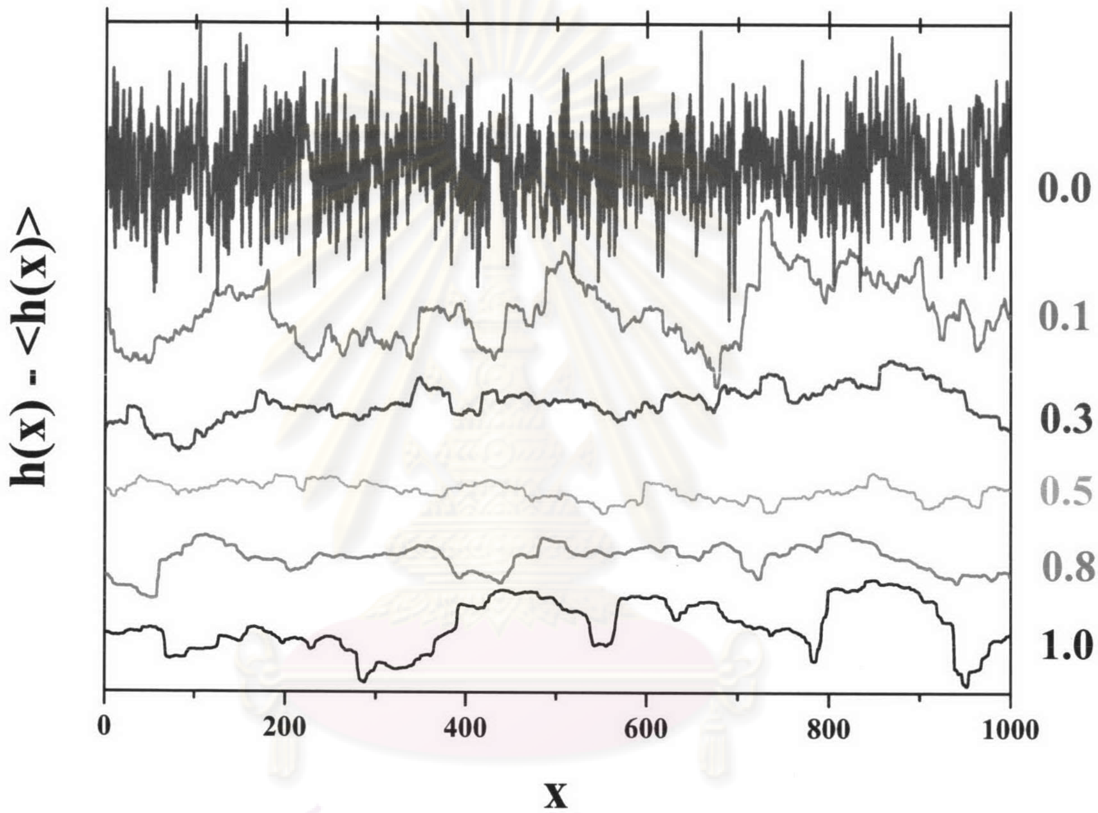

Figure 3.7: The morphologies of the WV-ES model when $P_U = P_D$. We vary the values of P_U and P_D from 1.0 to 0.0 (bottom to top). The values of P_D that equals to 1.0 and 0.0 correspond to the original WV model and RD model respectively. We simulate the systems of substrate size $L = 1000$ at time $t = 10^6$ ML.

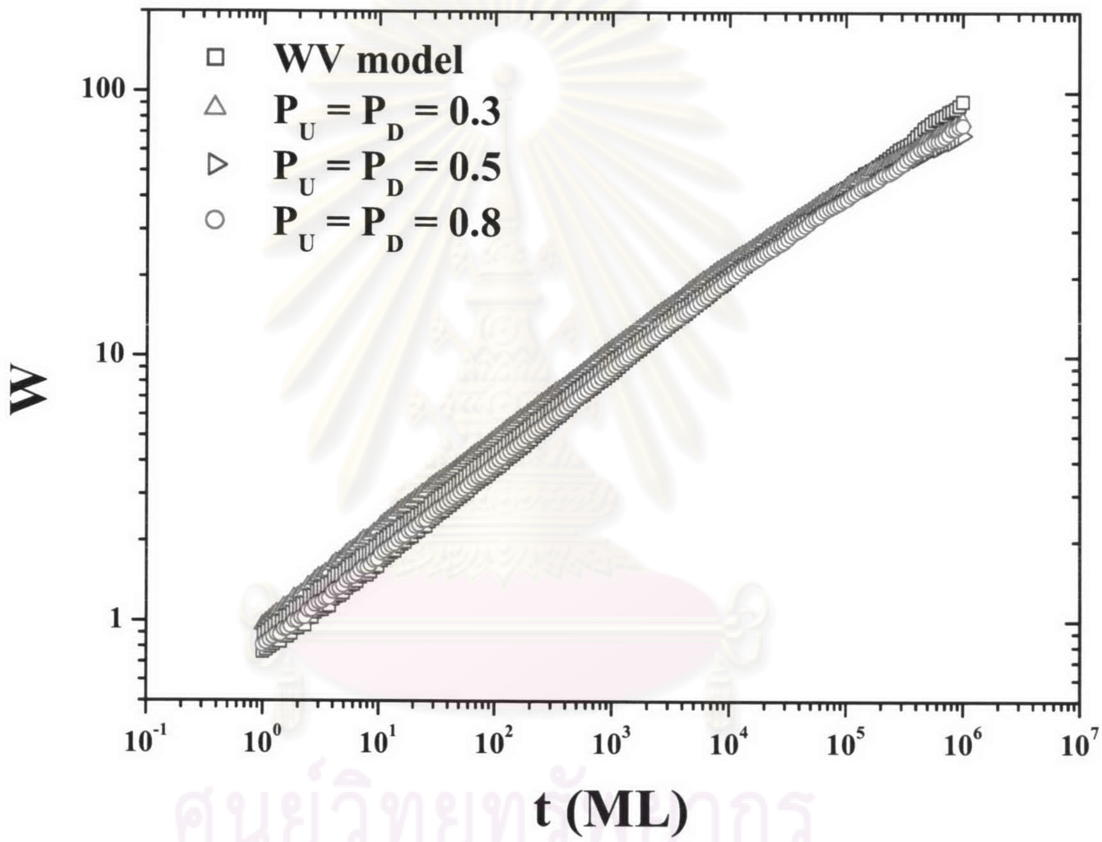

Figure 3.8: The surface width of the WV model and the WV-ES model when P_U = P_U. The results are from systems of substrate size L = 1000.

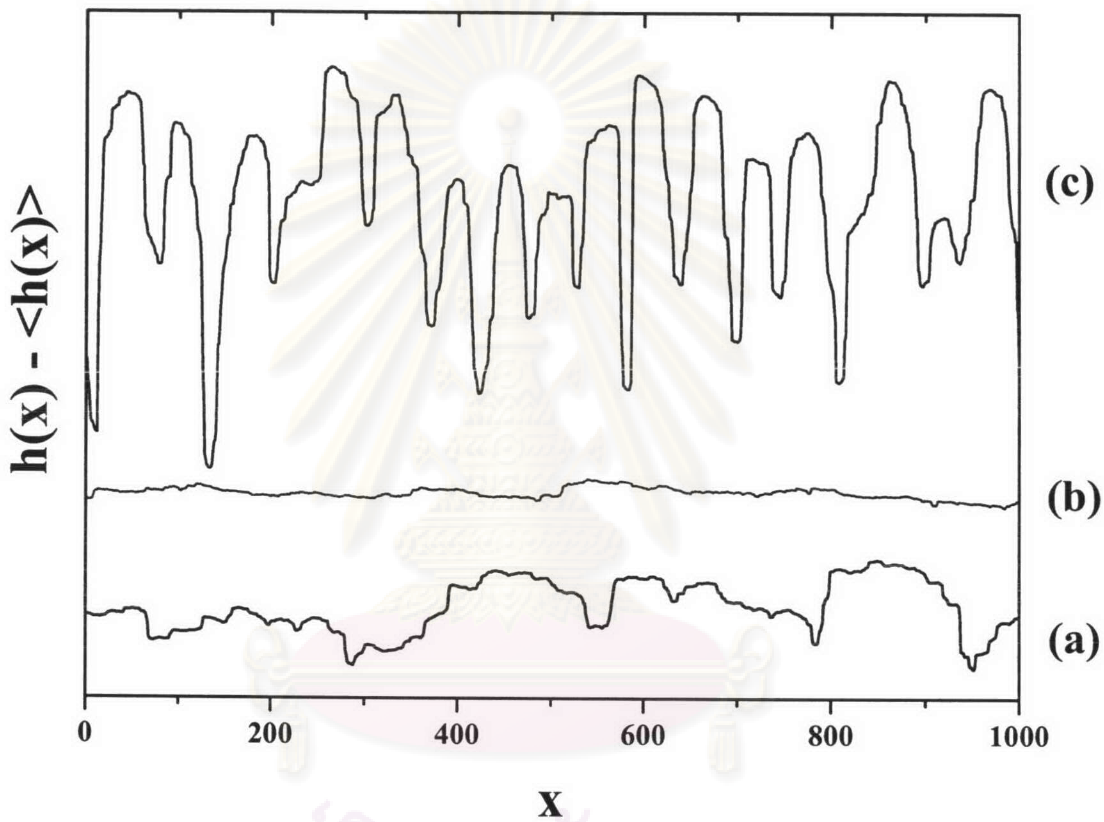

Figure 3.9: The morphologies of the WV-ES model when we set (a) $P_D = 1.0$ and $P_U = 1.0$, (b) $P_U = 0.5$, and $P_D = 1.0$, (c) $P_U = 1.0$ and $P_D = 0.5$. Case (a) corresponds with the original WV model, (b) corresponds with the negative ES barrier, and (c) is the WV-ES model.

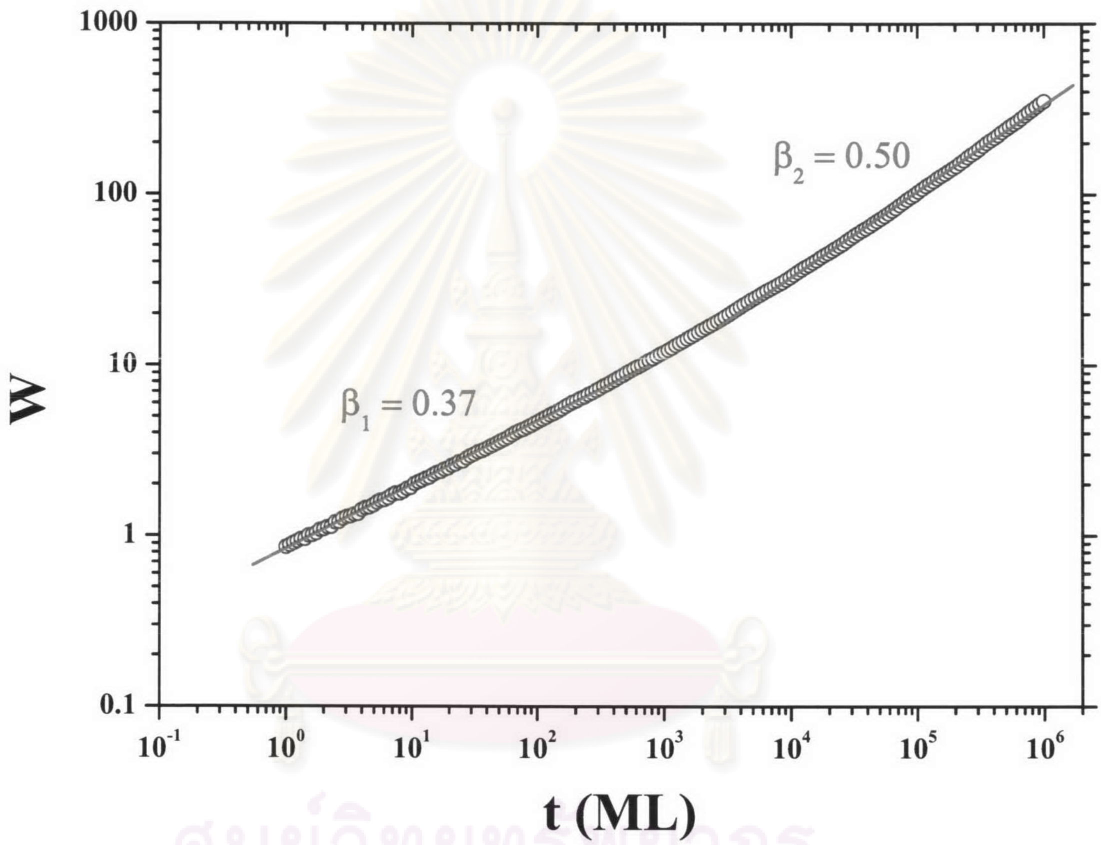

Figure 3.10: The surface width of the system with $L = 1000$, $P_U = 1.0$ and $P_D = 0.5$. We find the growth exponent crossover from $\beta_1 \approx 0.37$ to $\beta_2 \approx 0.50$ after the crossover time $t_c \approx 10^3$ ML.

growth exponent (denoted as β_1 in the figure) is approximately the same as in the original WV model, i.e. $\beta_1 \approx 0.37$. At longer time, however, the growth exponent (denoted as β_2) increases to $\beta_2 \approx 0.5$. From Fig 3.10, the crossover time (t_c) of the growth exponent is approximately at 10^3 ML. The crossover of β from $\beta \approx 0.37$ to $\beta \approx 0.5$ can be explained in the following way. In the early time ($t \ll t_c$) the whole substrate is still connected and the correlation length ξ follows the equation $\xi(\mathrm{t}) \propto t^{1/z}$. During this time, mounds develop and coarsen through the diffusion process. By "coarsen" we mean a few small mounds combine and become one big mound. We can use the correlation function to detect the coarsening of mounds that we will explain in the next section. After the crossover time ($t \gg t_c$), the coarsening process drastically drops and the mounds almost stop growing laterally because grooves become too deep to be filled up. The newly deposited adatoms diffuse mostly on top of each existing mound and the mounds become steeper. At this point, each mound has very little interaction with other mounds on the surface and the correlation length is limited by the size of the mound. The "interaction" of mounds in this situation means each small mounds are coarsen to each other. It is as if in the $t \gg t_c$ regime the substrate is separated into pieces with almost no interaction between these pieces. This causes the growth exponent to increase and eventually $\beta \to 0.5$ just like in the RD model. It is interesting to note that this situation is independent of the strength of the ES barrier as long as the barrier is strong enough to induce mound formation. The difference is that t_c in a system with strong barrier is smaller than t_c in a weaker barrier system. This is shown in Fig. 3.11. In some very weak barrier systems, e.g. $P_D = 0.7$ and $P_D = 0.9$, we do not see the crossover to $\beta \approx 0.5$. It is possible that the barrier is not strong enough to induce mound and there is no such crossover, or there are some mound formation but t_c is larger than 10^6 ML in these cases. This is difficult to judge from the morphologies in Fig. 3.6 but it will be clearer when we discuss the correlation function in the next section.

Note that the value of $\beta \approx 0.5$ in WV-ES model is the same value as we found in the RD model but our WV-ES model behaves very differently from the

RD model (except for the trivial case when $P_U = P_D = 0$). In Fig. 3.12, we show that the saturation steady state exists in WV-ES model and the roughness exponent α, although very large, is still a finite value as shown in Fig. 3.13, while α is infinite in the RD model.

3.2 Correlation Function

Sometimes when we see the morphologies we cannot decide either there is mound formation on the surface or not. There is a tool that can be used to make that decision: the *correlation function* [2, 21, 22, 23], $G(r) = \langle h(\mathbf{x})h(\mathbf{x}+\mathbf{r})\rangle_x$, introduced in Chapter 1. If we find an oscillation in the correlation function, it implies [2, 22, 23] that there are regular mound formation on the surface.

For this thesis, we start from the correlation function of the RD model. In Fig. 3.14, $G(r)$ is zero for all r with a small fluctuation. This means that there is no mound formation on the surface because $G(r)$ does not oscillate. When we calculate correlation function from the WV model, Fig. 3.4, we do not find any oscillation. This is shown in Fig. 3.15. So the WV morphology (Fig. 3.4) is just dynamical rough surface not a mounded surface. In the WV-ES systems, we have shown earlier that we find mounded morphologies when we fix the value of $P_U = 1.0$ and vary the values of P_D. In Fig. 3.16, we vary the values of P_D from 0.9 to 0.1 (where $P_D = 1.0$ corresponds to the original WV model), we find oscillations in the correlation function when $P_D \leq 0.7$, see Figs. 3.16(a)-(i). In Figs. 3.16(a) and (b), $G(r)$ for systems with $P_D \geq 0.8$ do not show any oscillation. We can deduce that there is no mound formation on the surfaces with large P_D (weak barriers). Note that the morphology of the system of $P_D = 0.8$ in Fig. 3.6 shows that mounds start forming however $G(r)$ plot for this system does not show any oscillation. This probably because the mounds seen in Fig. 3.6 when $P_D = 0.8$ are not regular enough since the barrier is not strong enough for $G(r)$ to oscillate.

Mounds properties can also be studied from the function $G(r)$. The average mound height is calculated from $\sqrt{G(r=0)}$ and the average mound radius is the

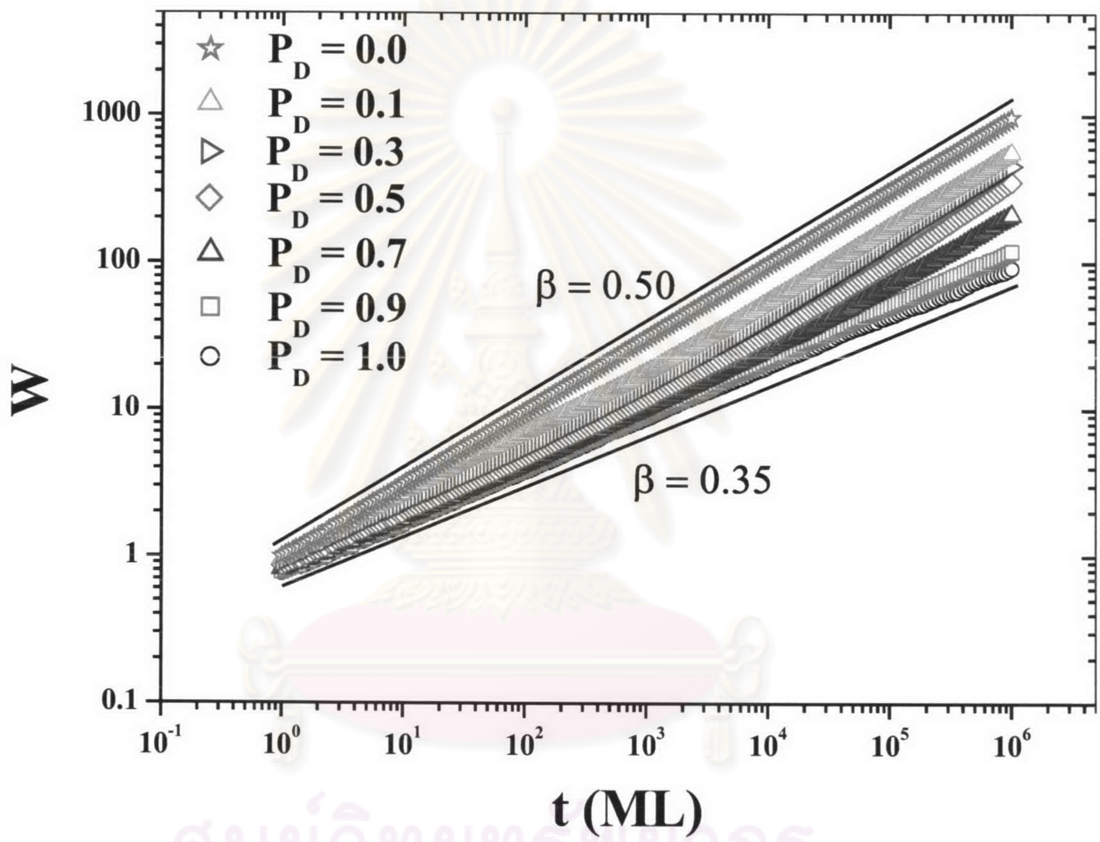

Figure 3.11: The surface width plot as a function of time in the system with $L =$ 1000. We fixed $P_U = 1.0$ and varies the values of $P_D = 0.0$, 0.1, 0.3, 0.5, 0.7, 0.9, and 1.0 from top to bottom.

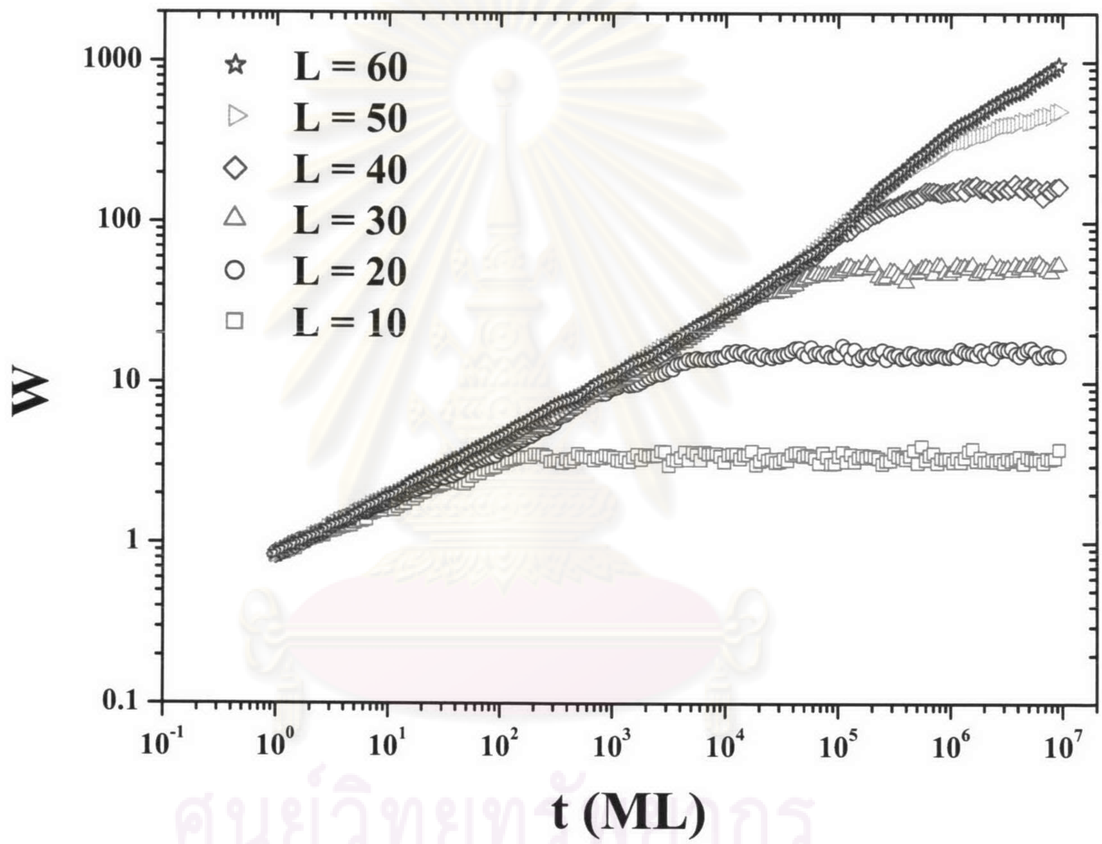

Figure 3.12: The W-t plot for our WV-ES model when we vary the substrate size $L = 10$, 20, 30, 40 and 50, $P_U = 1.0$ and $P_D = 0.5$.

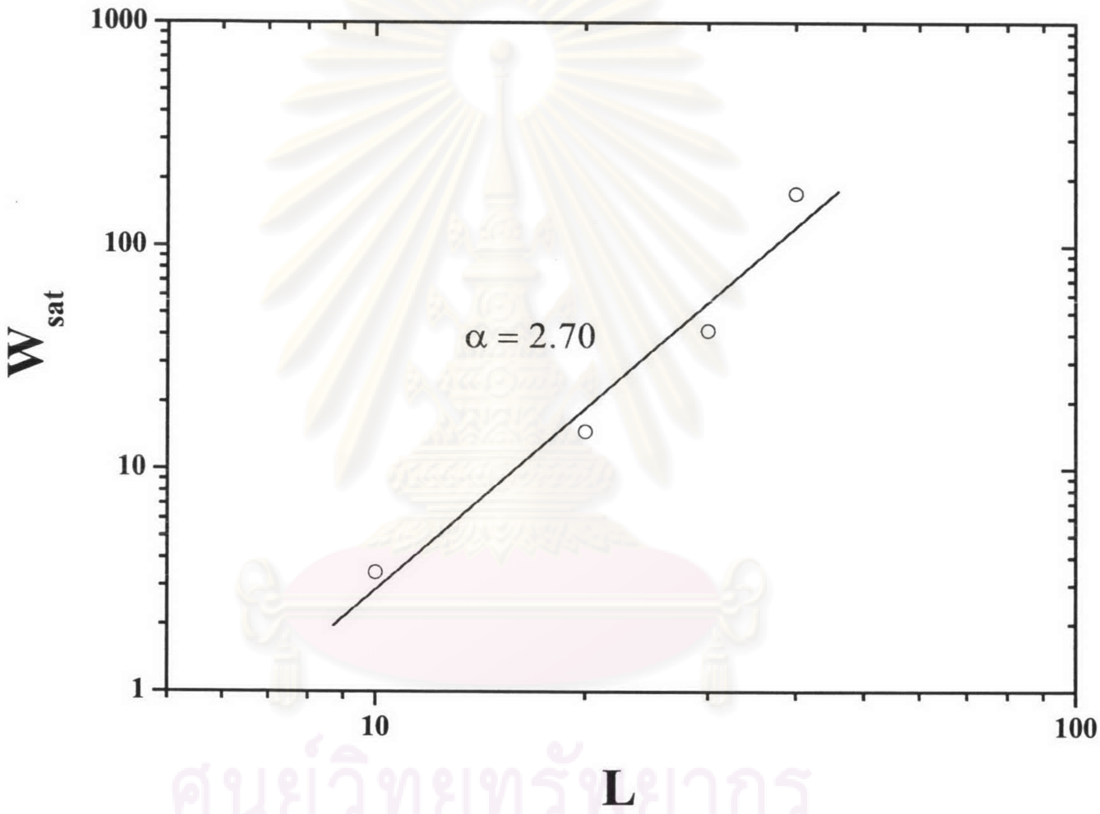

Figure 3.13: The calculation of the roughness exponent α in the WV-ES model. Here we obtained $\alpha \approx 2.70$.

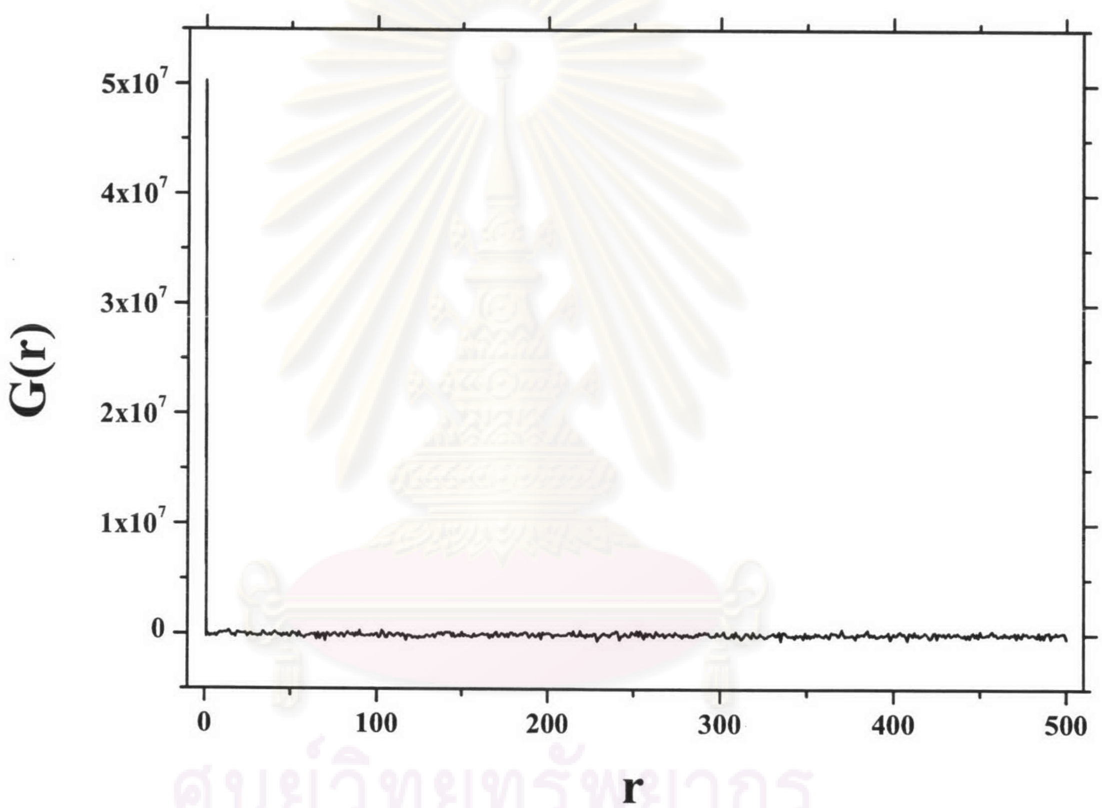

Figure 3.14: The correlation function of the RD model from the system of substrate size $L = 1000$ at time $t = 10^6$ ML.

distance of the first zero crossion of $G(r)$ as described in Chapter 1. From Fig. 3.16 we can see that the average mound height increases when P_D decreases while the average mound radius decreases when P_D decreases. This can be explained that the effect of a small value of P_D or a stronger barrier is to reduce the chance for a new adatom to hop down. Therefore, when a new adatom is deposited on top of each mound, it can diffuse only on each mound. The mound grows almost only in the vertical direction and becomes steeper with deeper grooves when P_D decreases. Furthermore, we can use $G(r)$ to detect the coarsening process by plotting $G(r)$ at different times. If the average mound radius calculated from the first zero crossing increases as the time increases, that means the coarsening still dominates in the growth process. However, when the average mound radius does not change in time, in another word, it remains constant as time increases, it means the coarsening process does not dominate in the growth process any more.

When we set the value of $P_U = P_D$ for all systems, the correlation function do not show any oscillation as in Fig. 3.17. Since the adatom has equals chance to hop in both directions, this is equivalent to no barrier in the system. So there is no mound formation on the surface in this case. In the cases of $P_U < P_D$, we do not see any oscillation either, see Fig. 3.18.

3.3 Particle Diffusion Current

In this section, we study the particle diffusion current [20] in the WV and WV-ES models in order to confirm whether these models belong to the EW universality class. As explained in Chapter 1, the particle diffusion current can help us determine the existence of the EW term, $\nabla^2 h$, in the continuum growth equation describing dynamic of the growth system.

Our results are summarized in Table 3.1 from a system of substrate size $L = 10^3$ and time $t = 10^6$ ML. The first result is the RD model. Since adatoms in this model are not allowed to diffuse, the particle current in this model is absolute

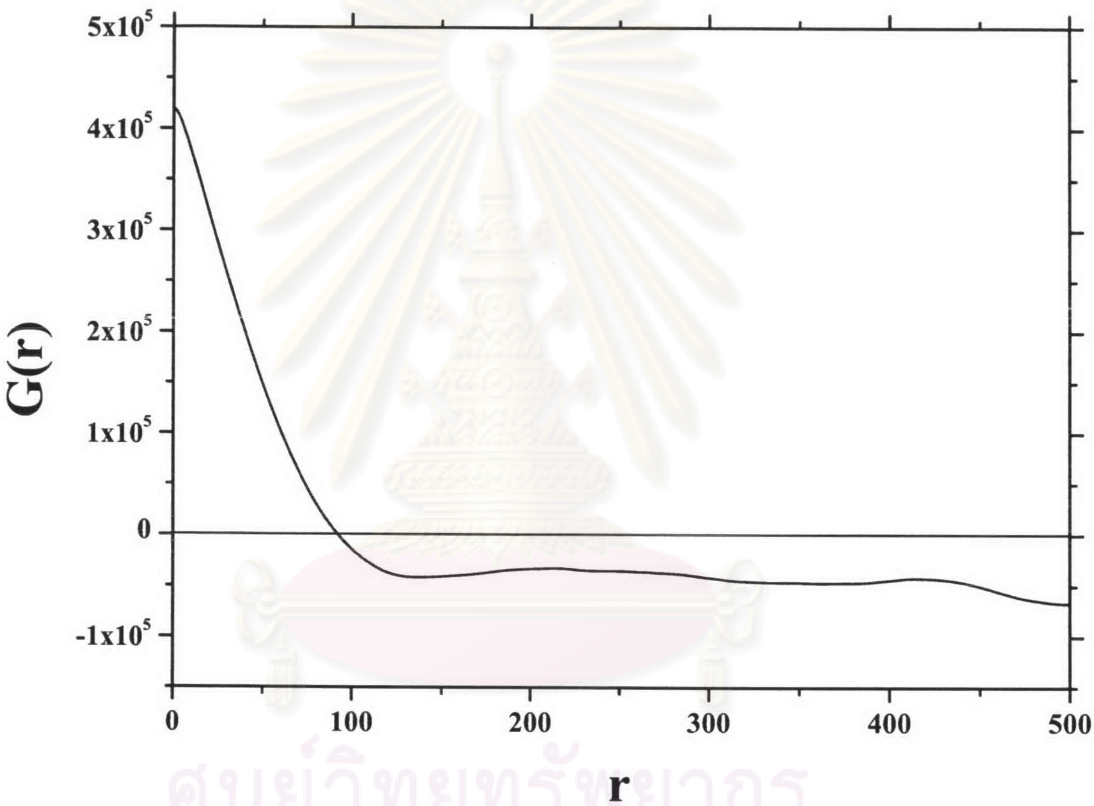

Figure 3.15: The correlation function of the WV model from the system of substrate size $L = 1000$ at time $t = 10^6$ ML.

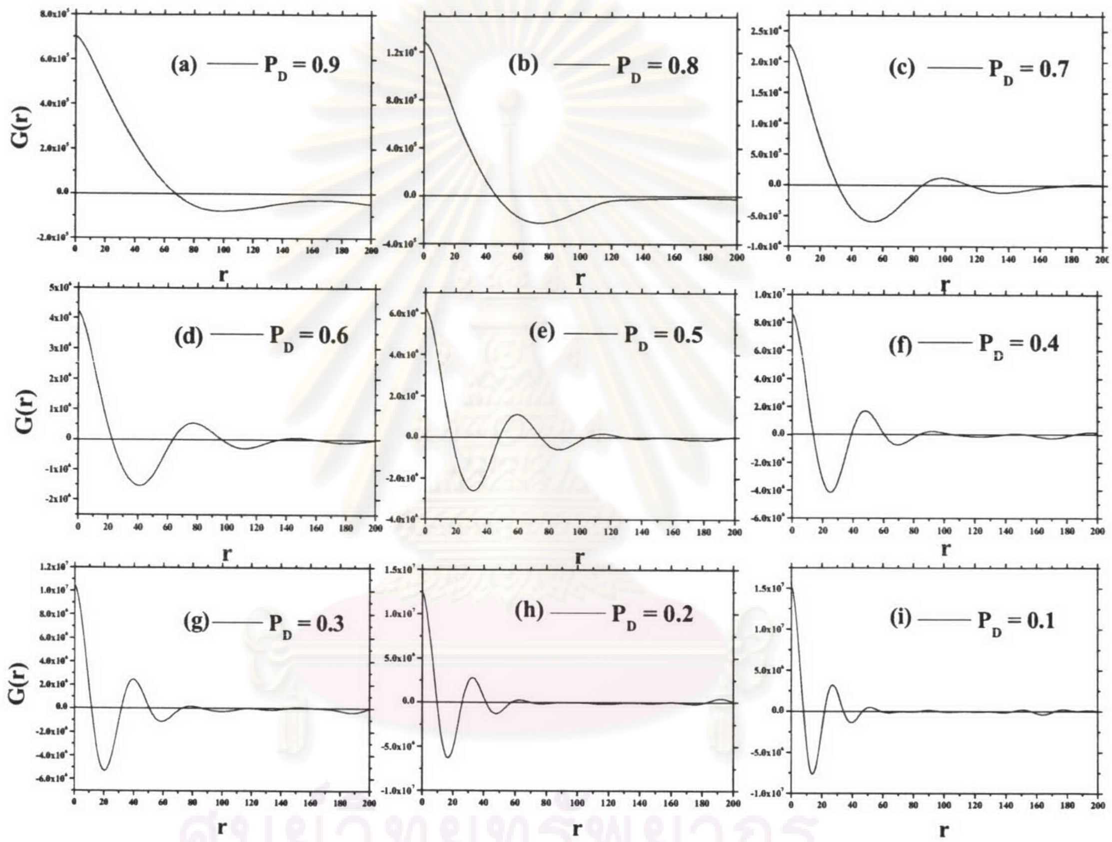

Figure 3.16: The correlation function of the WV-ES model from the system of substrate size $L = 1000$ at time $t = 10^6$ ML. We fix the value of $P_U = 1.0$ and vary the values of P_D from 0.9 to 0.1.

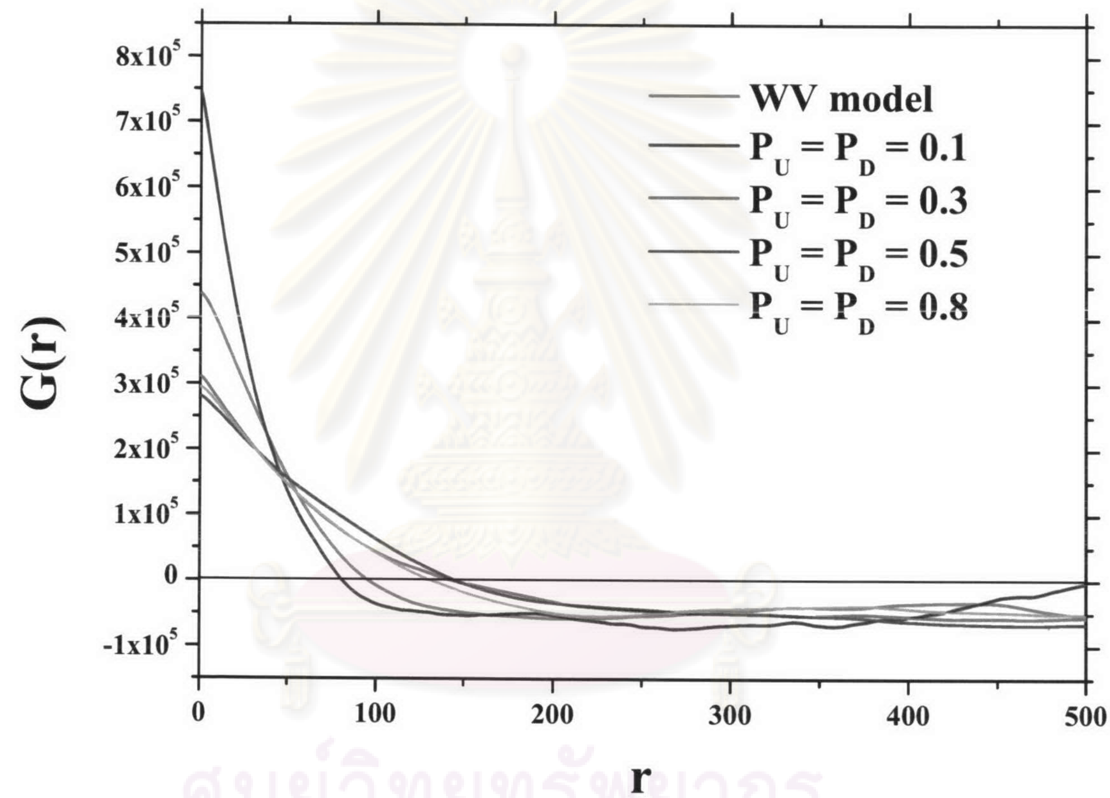

Figure 3.17: The correlation function of the WV-ES model in the case of $P_U = P_D$ from the system of substrate size $L = 1000$ at time $t = 10^6$ ML.

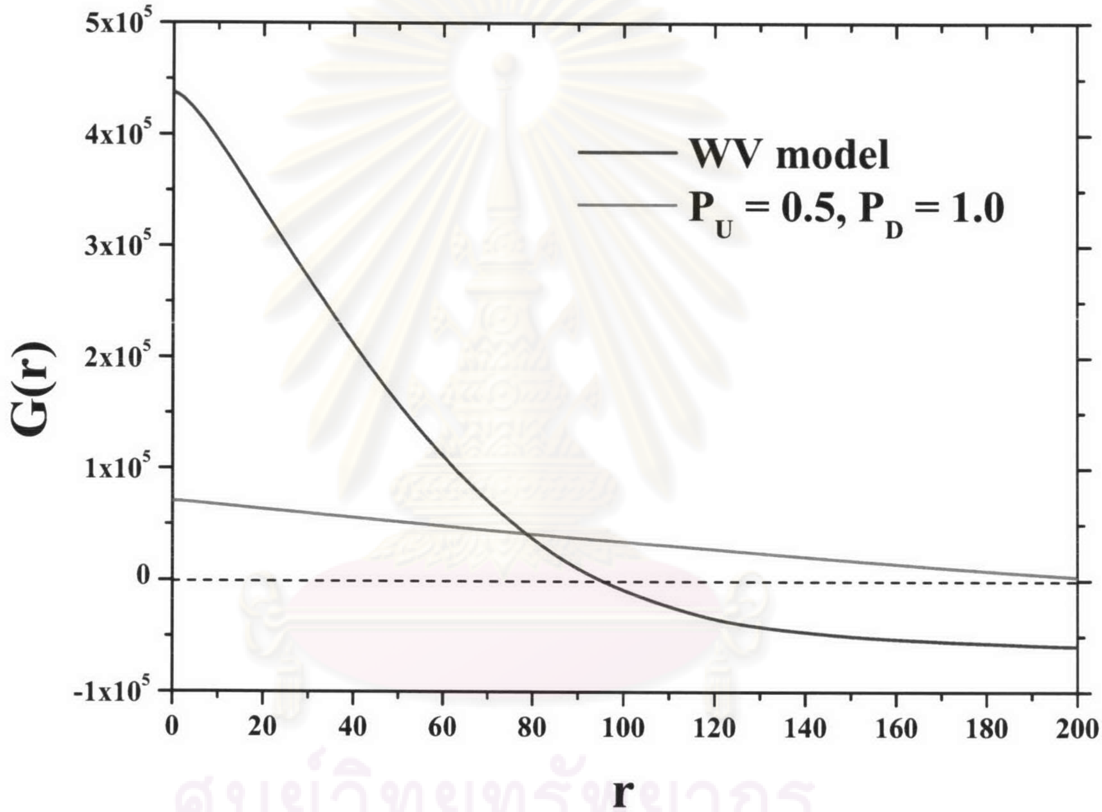

Figure 3.18: The correlation function of the WV-ES model in the cases of $P_U < P_D$ from the system of substrate size $L = 1000$ at time $t = 10^6$ ML.

zero, as shown in Fig 3.19. In the WV model, however, adatoms diffuse on the substrate and it is difficult to define "zero" current because the data fluctuates. To solve this problem, we study the WV model on a flat, i.e. untilt, substrate. The current obtained in this case is shown in Fig. 3.20. So we define "zero" current to be in the range between $\pm 5.0 \times 10^{-5}$. From the tilt substrate systems, the net current of the WV model is found to be *negative* or *downhill* as shown in Fig 3.21. This result confirms that WV model should follow the EW universality class asymptotically and it also implies that there is no mound formation on the WV surface. Our works agree with others [2, 20] that confirm the downhill current in 1+1 WV model.

Model	**current J at tan θ equals to**			
	2	1	0.5	0
RD	0	0	0	0
WV	-10^{-3}	-10^{-3}	-10^{-4}	$\pm 10^{-5}$
WV-ES ($P_D = 0.5$)	$+10^{-3}$	$+10^{-4}$	$+10^{-4}$	$\pm 10^{-5}$

Table 3.1: The particle diffusion current J of the discrete growth models.

For WV-ES model, we fixed $P_U = 1.0$ and then vary the values of P_D. We found that for $P_D = 1.0$ and 0.9, the net current is negative while for $P_D \leq 0.8$ the net current is positive as shown in Fig 3.22. This indicates that, at $P_D = 1.0$ and 0.9, the barrier is too weak to effect the system so the downhill current associating with the WV model has more influence on the system. The surface in this case is dynamical rough without mound formation. However, when $P_D \leq 0.8$ the ES barrier is strong and the uphill current associating with the ES barrier has more influence. In these cases we start to obtain mound formation on the surface (see Fig. 3.6 for the corresponding morphologies). But in the case of $P_D = 0.8$, we find the conflict between the correlation study and the particle current result, see Fig. 3.16 and Fig. 3.22. This may be because $P_D = 0.8$ is the boundary between mound formation surface and dynamical rough surface. So this value of P_D shows the conflict from the particle diffusion current and the correlation function.

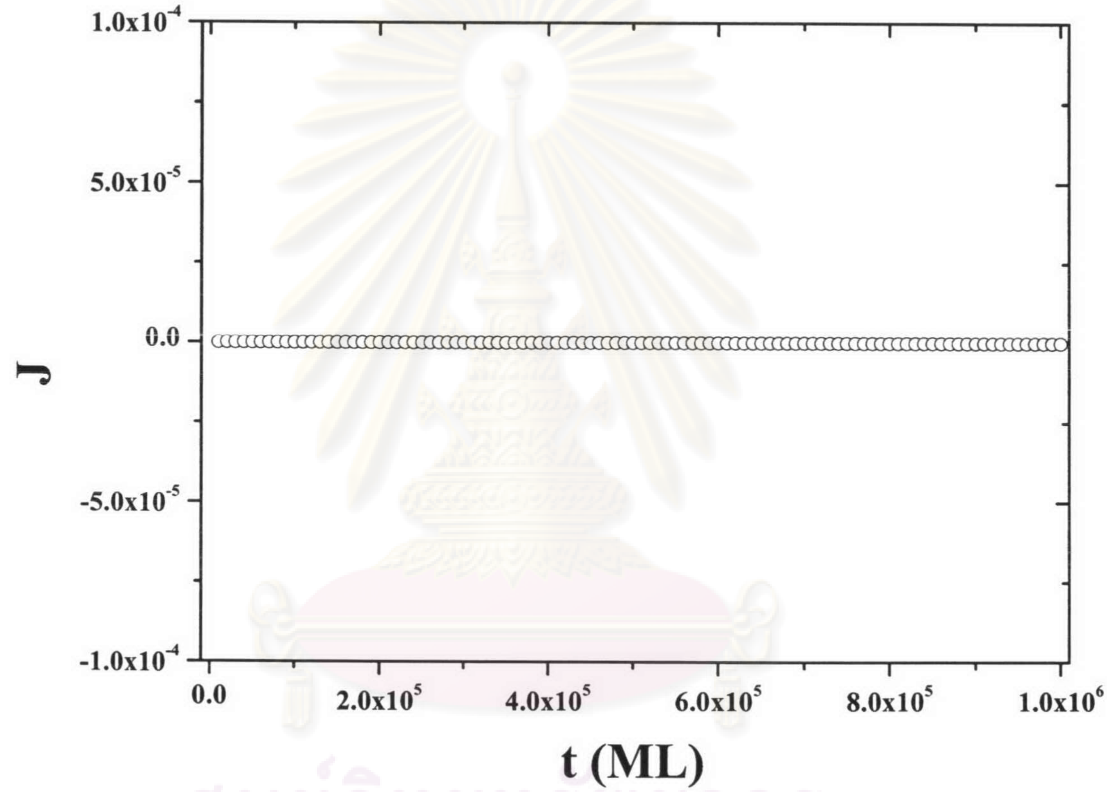

Figure 3.19: The particle diffusion current of the Random Deposition (RD) model. We obtained the zero current from the system of substrate size $L = 1000$ and $\tan\theta = 0.5$.

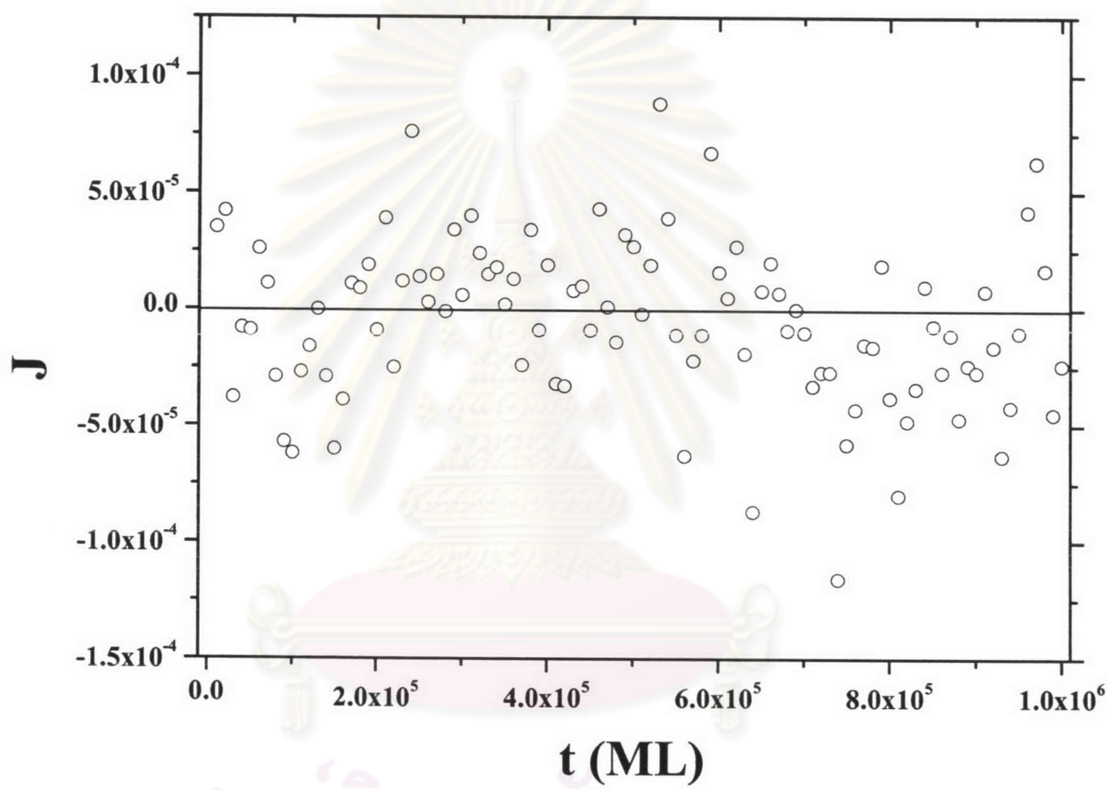

Figure 3.20: The particle diffusion current of the WV model with untilt substrate where we obtain the average zero current, $\pm 5.0 \times 10^{-5}$. This result comes from the system of substrate size $L = 1000$ and $\tan\theta = 0.5$.

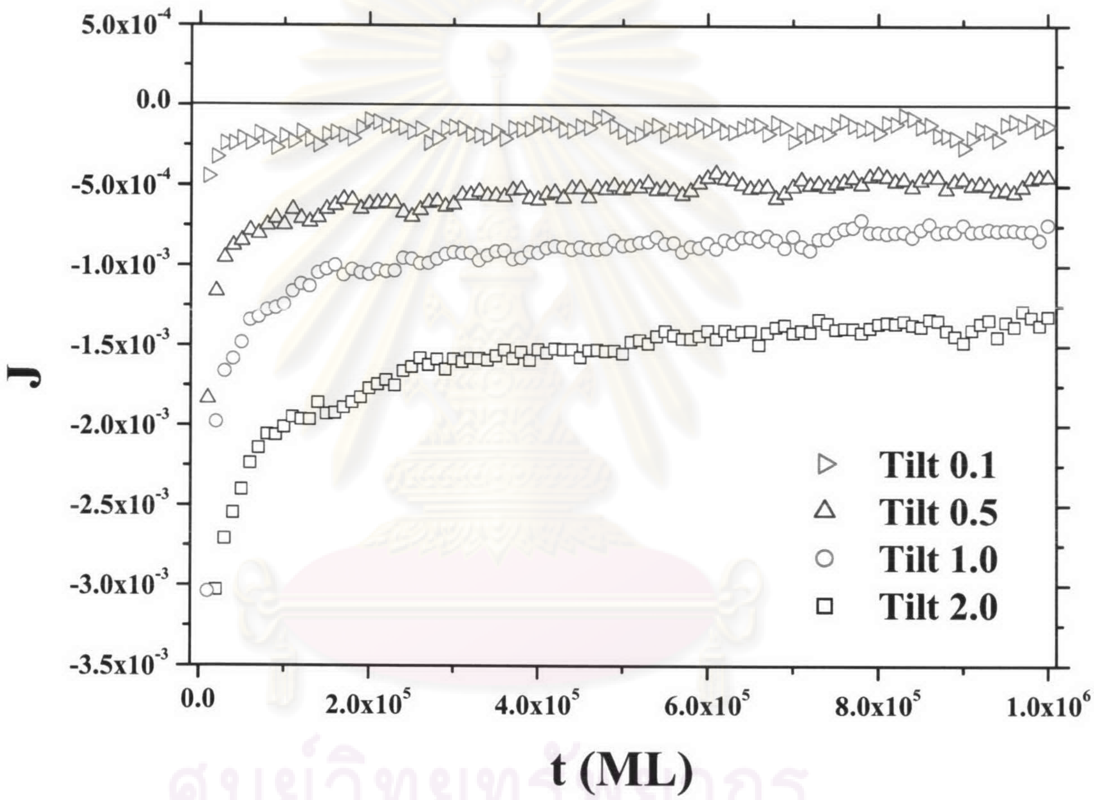

Figure 3.21: The particle diffusion current of the WV model with varying $\tan\theta$. We vary $\tan\theta = 0.1$, 0.5, 1.0, and 2.0 from top to bottom. Here $L = 1000$.

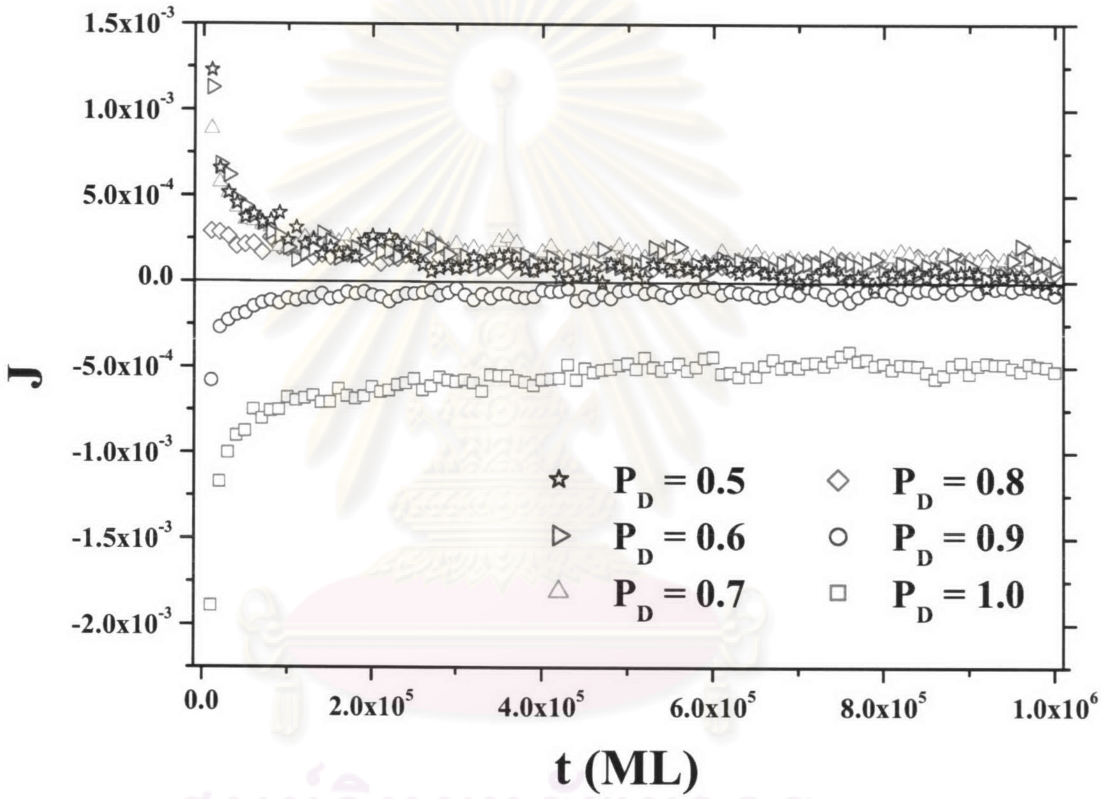

Figure 3.22: The particle diffusion current of the WV-ES model where we fix P_U = 1.0 and vary P_D = 0.5 to 1.0 with $\tan\theta = 0.5$. These results come from the systems of substrate size $L = 1000$.

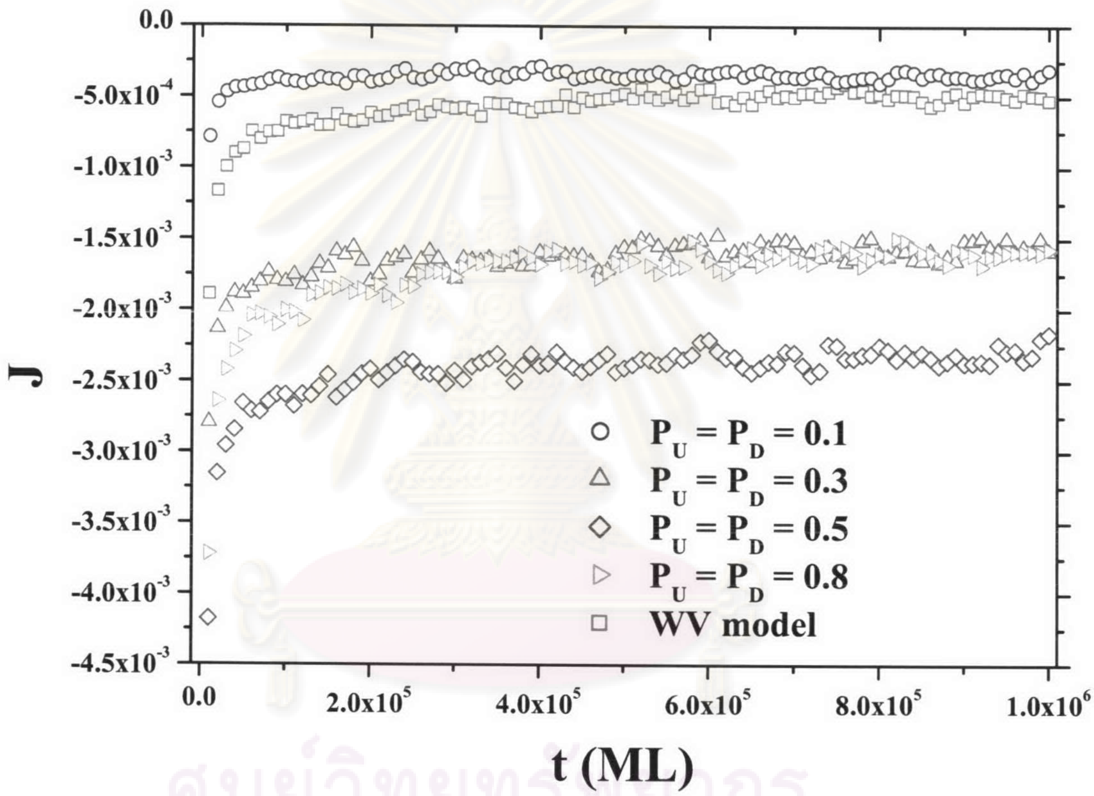

Figure 3.23: The particle diffusion current of the WV-ES model in the case of P_U = P_D with $\tan\theta = 0.5$. Here $L = 1000$.

In the case of $P_U = P_D$, we find the downhill current in every values of P_D as shown in Fig. 3.23. These current results agree with all our results (morphologies and surface width) and confirm that when $P_U = P_D$ the system behaves in the same way as the original WV model.

3.4 Growth Equation

Since all three exponents (α, β, z) from our simulation, the WV model in 1+1 dimensions seem to match the linear fourth order growth equation (Eq. (1.20)), so the linear fourth order term, $\nabla^4 h$, must be in the continuum growth equation. However, from the characteristic of the morphology, the up-down symmetry is broken [2, 3, 19] so a linear equation cannot describe the system and it seems the nonlinear fourth order term ($\nabla^2(\nabla h)^2$) is also presented in the continuum growth equation. Our particle diffusion current in the previous section shows a downhill current for the WV model which implies that the linear second order term (the EW term, $\nabla^2 h$) must be in the continuum growth equation too. So from all our results, the continuum growth equation describing the WV model in 1+1 dimensions should be in the form of

$$\frac{\partial h}{\partial t} = \nu_2 \nabla^2 h - \nu_4 \nabla^4 h + \lambda_{22} \nabla^2 (\nabla h)^2 + \eta(x, t). \tag{3.1}$$

With this equation, the WV simulation results should show statistical properties that belong to the $\nabla^4 h$ and $\nabla^2(\nabla h)^2$ terms and the eventual crossover to the behavior of the $\nabla^2 h$ term asymptotically. But due to the limit of computer resources and time constraints, we cannot carry out our simulations long enough to see this crossover. All our simulations still produce the critical exponents which belong to the MH equation, $\nabla^4 h$, as shown in Table 1.1. The only evidence of the $\nabla^2 h$ term is the downhill particle current in the previous section.

When we add the ES barrier into the WV model, all of our WV-ES model results do not agree with any universality class discussed in Chapter 1. The morphologies show mounds (or instability), the surface width has a crossover to

$\beta \rightarrow 0.5$, and the particle current is uphill. It is difficult to form a continuum equation to describe unstable growth like the WV-ES case. The only thing we can say is that the $\nabla^2 h$ term should be included in the equation with $\nu_2 < 0$ to reflect the instability.