Chapter II

Models

Due to the increase of interest in the kinetic surface roughening growth, there are many works that try to create atomistic (discrete) nonequilibrium models to describe the growth problem and also determine essential properties and asymptotic behavior of the problem. Our work started with the simplest model known as the *Random Deposition* (RD) model. Then we deal with a more complicated model, i.e. the *Wolf-Villain* (WV) model [3]. The WV model is a simple model with the dynamical diffusion/relaxation process which we are interested and focus on in our work.

Besides studying the model, we are also interested in studying mechanisms that make the surface rough during the diffusion/relaxation process. One of these mechanisms is a potential barrier that prevents diffusing adatoms from hopping down to lower terraces. This barrier is known as the *Ehrlich-Schwoebel* (ES) barrier [6, 7, 8]. We add the ES barrier into the WV model by modifying the diffusion rules of the original WV model in order to study effects of the ES barrier on the WV model. The computational method and the diffusion rules of the models are discussed in this chapter.

2.1 Discrete Growth Models

All models we study in this work are discrete, nonequilibrium and limited mobility growth models. We assume that the models obey *ideal* low temperature MBE growth conditions. This mean they are under the solid-on-solid (SOS) constraints (no desorption, no overhanging and no bulk vacancies formation on the growing surface). All of the deposited adatoms must become part of the growing film. The models are dynamical and the diffusion/relaxation process is instantaneous. In all models studied here, the deposition of an adatom is on a randomly chosen site on a one dimensional flat substrate (d = 1+1). An adatom diffuses instantaneously to a selected final site and sticks there permanently (no longer move). The diffusion of a diffusing adatom is in accordance with a set of well-defined rules characterizing each model. It was found [2, 19] that the diffusion length ℓ does not have much effect on the asymptotic behavior of the growth system, so here ℓ is fixed to be unity, i.e. nearest neighbor diffusion only. In our simulations, the time t is defined through the deposition rate. In our study, one second equals to an average growth of 1 monolayer (ML) which means the deposition rate is 1 ML per second. All our simulations are done with the periodic boundary condition on the substrate, i.e. if an adatom is deposited on the site $x = L$ (L is the substrate size) and wants to diffuse to the site $x = L + 1$ then the diffusing adatom will diffuse to the site $x = 1$ instead. This periodic boundary condition prevents finite size effects in the simulations. Processes of our simulations are summarized in the flow chart as shown in Fig. 2.1.

2.1.1 Random Deposition Model

The Random Deposition (RD) model is the simplest model among many growth models. An adatom is dropped randomly above a one dimensional flat substrate and then sticks instantaneously on the deposited site with no diffusion, see Fig 2.2. This means the lateral correlation length is $\ell = 0$ for RD model. In the simulation algorithm, we choose a random site x on a flat substrate size L and increase its height $h(x)$ by one. So the surface height of the RD model grows independently and the surface of the growing film is *uncorrelated*. Since the surface height are uncorrelated, the growth front can be describe by a *Poisson distribution* [1] and we can find the exact solution [1] for the growth exponent β to be 0.5. The RD model allows the surface width to grow indefinitely with time, thus the result is no saturation in W. In this case, the roughness exponent α is not defined (that is $\alpha \to \infty$ for the RD model from Eq. (1.5)). From Eq. (1.14), the dynamical exponent z is also not defined in this model.

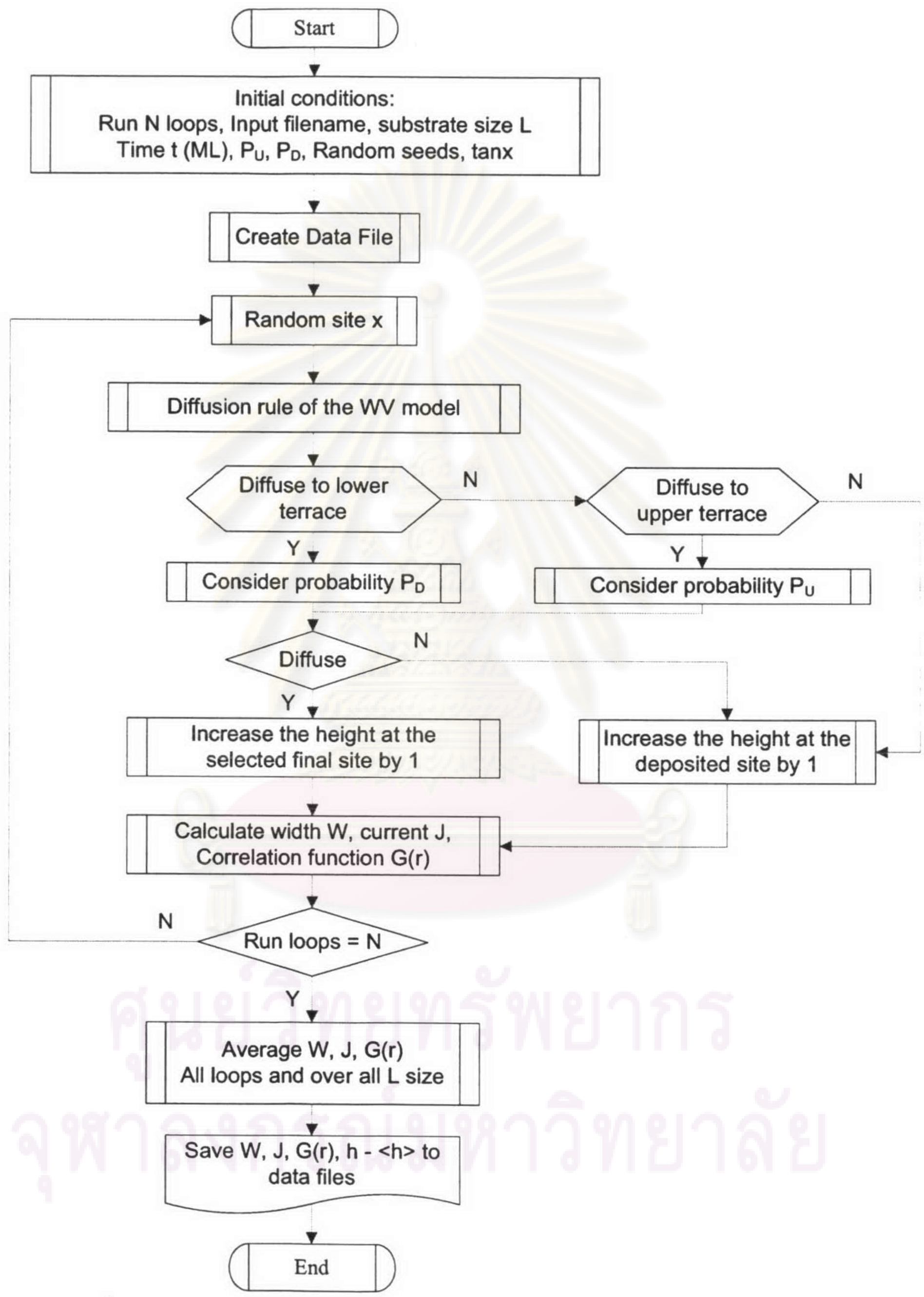

Figure 2.1: Flow chart of our simulation in all systems.

2.1.2 Wolf-Villain Model

Wolf-Villian (WV) model [3] is a simple model for kinetic surface roughening growth. It follows the MBE growth conditions and also under the SOS constraints. In the WV model, after an adatom is deposited on a randomly chosen site on a one dimensional flat substrate (d = 1+1), it diffuses instantaneously. In the diffusion process, the atom looks for a site within its diffusion length ℓ (for our study we set $\ell = 1$) that offers the strongest bindings. In another word, an adatom tries to increase its coordination number to the maximum value, see Fig 2.3. After an adatom finds its selected final site, it moves to that site and sticks there permanently. Then the next adatom is deposited and repeats the diffusion mechanism.

In the computational algorithm, we choose the site x randomly and then check the number of bonding at the nearest neighboring sites, $x \pm 1$, comparing with the number of bonding at the deposited site. If one of the nearest neighbor sites has higher number of bondings than at the deposited site, we increase the height at that site by one. If both nearest neighbors have higher bonding, the one with the highest coordination number is selected. If neither neighbor has larger number of bonding, we increase the height at x by one. Finally, if the number of bondings at both nearest neighboring sites (both $x \pm 1$ sites) are the same and it is more than at the deposited site, one of these sites is chosen by random (by using the random generator algorithm [24]).

2.2 Ehrlich-Schwoebel Barrier

While an adatom diffuses on the surface after being deposited on the surface, it may encounter an additional barrier called a *surface diffusion bias* [2, 20, 25]. A well known diffusion bias which leads to instability in the growing surface is the *Ehrlich-Schwoebel* (ES) barrier [6, 7, 8]. The ES barrier is a step edge potential barrier for an adatom diffusing over a step edge from upper to lower terraces, as

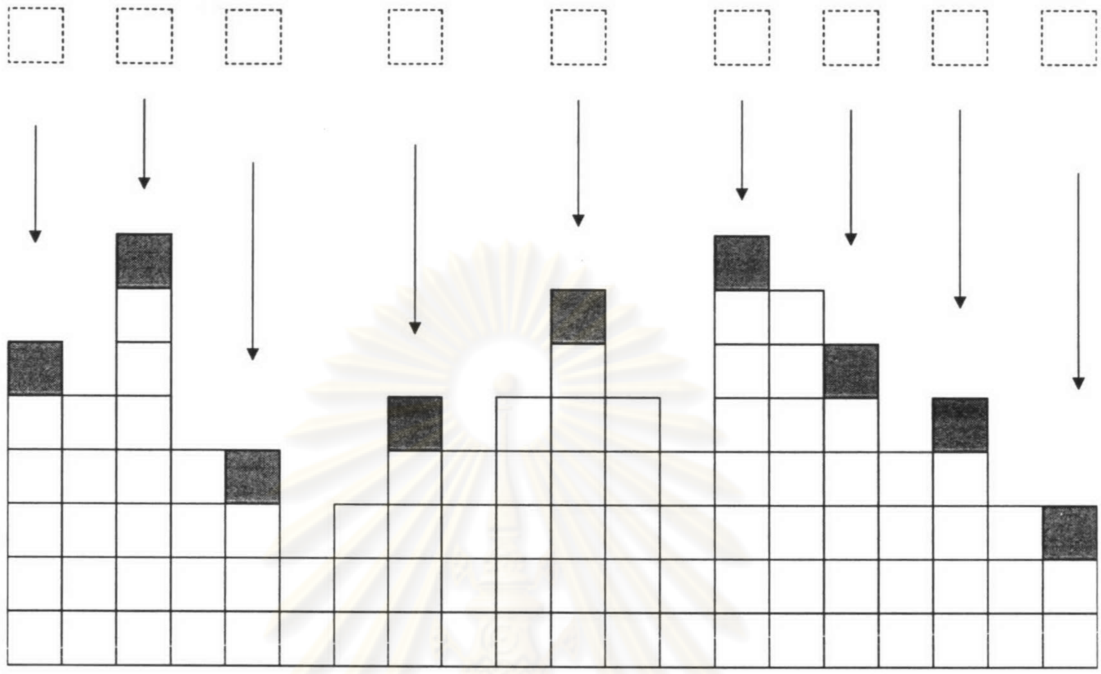

Figure 2.2: The Random Deposition (RD) model. The atoms are dropped randomly (the dash boxes) on top of the interface with no diffusion (the blue boxes).

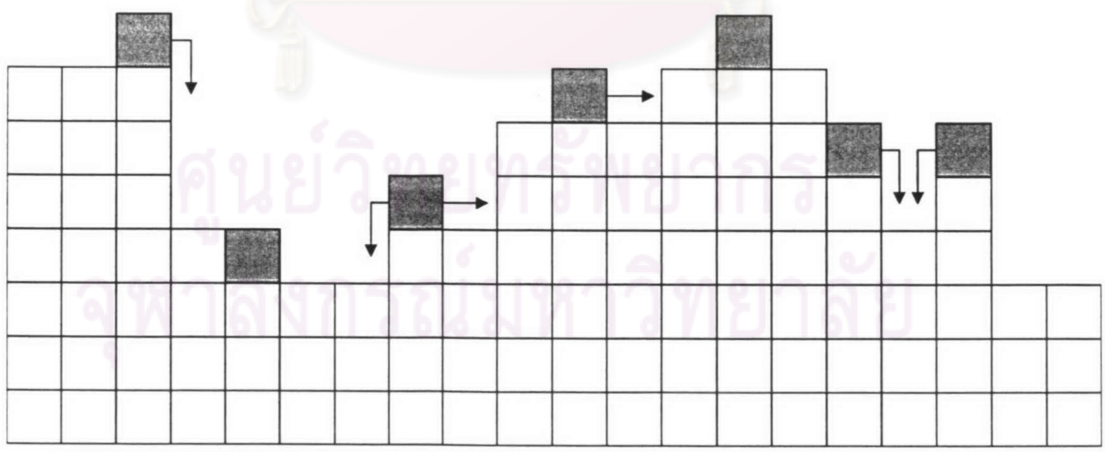

Figure 2.3: The diffusion rule of Wolf-Villain (WV) model. An adatom is deposited on a randomly chosen site on a one dimensional substrate (d = 1+1) and it diffuses instantaneously to increases its coordination number or its bondings.

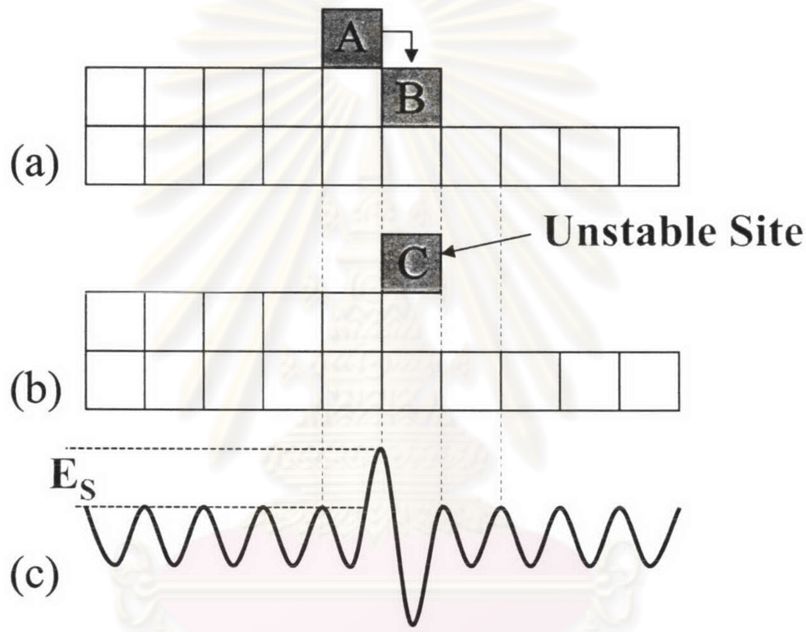

Figure 2.4: The Ehrlich-Schwoebel (ES) barrier. (a) An adatom at site A diffuses down to site B. (b) Adatom at site A must pass through an unstable site C before it arrives at site B. (c) A potential energy plot at the sites in the figures (a) and (b).

in Fig. 2.4. Since the ES barrier makes an atom more likely to attach itself to the upper terrace than the lower one, it leads to mound or pyramid type structures formation on the surface [2, 21, 22]. The mechanism of the ES barrier can be explained [1, 7, 25] as followed: While an adatom is diffusing from the upper to the lower terraces e.g. atom from site A going down to site B in Fig 2.4, it must pass through an unstable site C. At this site, there is only one bound with its next nearest neighboring site and so the atom will be very unstable at site C. This is equivalent to saying that the atom will have higher energy at site C compare to at other sites. An atom that does not have enough energy will not be able to go through site C in order to hop down to the lower terrace.

2.3 WV Model with ES Barrier

In our study, we are interested in studying effects of the ES barrier which leads to mound formation on the surface in the WV model. One of the reasons is because WV model is a good candidate [3] for studying ideal MBE growth systems and we want to understand effects of the ES barrier on the MBE growth process. Another reason is because the WV with ES barrier system possesses a conflict in the model itself. On one hand, we have the WV model which is known [3] to belong to the EW universality class. That means the system is stable with a downhill particle diffusion current [20]. On the other hand, the ES barrier is known to induce instability in a growth system [6, 7] and the particle current is uphill [20]. It is, therefore, an interesting question what type of behavior the WV model with the addition of the ES barrier will have.

In this section, we create a nonequilibrium atomistic growth model for ideal MBE growth under a surface diffusion bias (ES barrier) by implementing the ES barrier into the original WV model [3]. To add the ES barrier into the original WV model, we modified the diffusion rule of the original WV model. In Fig. 2.5, we show the modified WV model where we called WV-ES model. The diffusion rule of the WV-ES model are as follows:

1. An atom is deposited on a randomly chosen site (x) with the average rate of 1 ML per second.
2. The deposited atom looks for a better site according to the original WV diffusion rule.
3. The actual diffusion process is controlled by probabilities P_U and P_D in such a way that if the atom want to diffuse to the upper(lower) terrace, it faces the probability $P_U(P_D)$. If it cannot diffuse due to the probability, it sticks at the original deposition site.

The probabilities P_U and P_D are restricted by $0 \leq P_U, P_D \leq 1$. When $P_{U(D)} = 0$, no diffusion to the upper(lower) terrace is allowed. When $P_{U(D)} = 1$, there is no barrier in diffusion to the upper(lower) terraces. The ES barrier is implemented in our model by taking $P_D < P_U$ which makes it more likely for the adatom to attach to the upper terrace than the lower terrace. The strength of an ES barrier is controlled by the ratio P_U/P_D. If we set $P_D = P_U = 1$, our model is back to the original WV model [3]. The results of our numerical simulations, both for the WV and the WV-ES model, will be discussed in the next chapter.

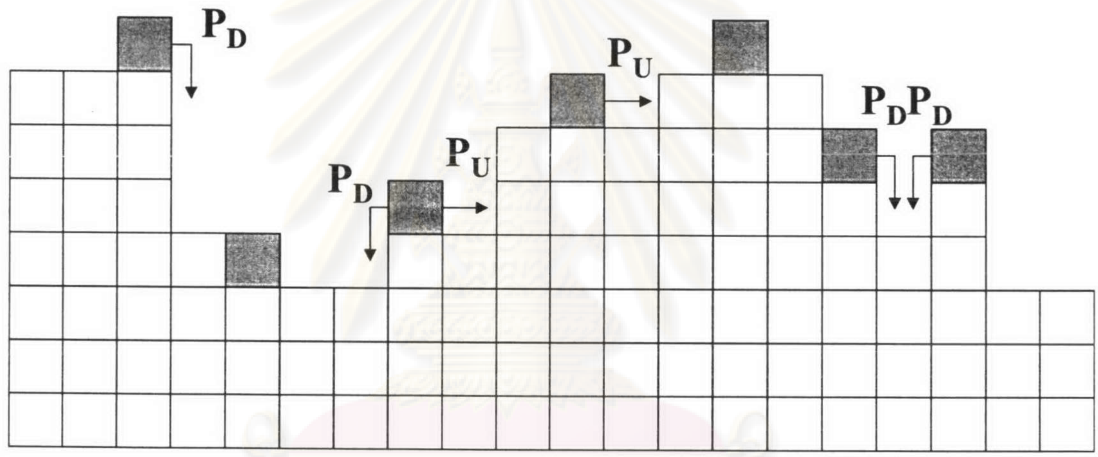

Figure 2.5: The diffusion rule of the WV-ES model. The adatom diffuses under the surface diffusion bias and it is controlled by the probabilities P_U and P_D. The ES barrier is implemented in the WV-ES model by taking the value of $P_D < P_U$.