Chapter IV

Conclusions

In our works, the results obtained from simple nonequilibrium growth model which is used to study the *ideal* molecular beam epitaxy (MBE) growth. Our study is based on 1+1 dimensional growth and under the solid-on-solid (SOS) constraints. The Wolf-Villain (WV) model [3] is the main model that we are interested in for the study of MBE growth. In real MBE growth, the existence of a potential barrier, known as the ES barrier [6, 7, 8], is seen experimentally. The barrier prevents an adatom from diffusing down to the lower terrace. Our main interest is to study the effects of the ES barrier on the WV model.

For the WV model, we start with the study of scaling properties. We find the growth exponent $\beta \approx 0.37$, the roughness exponent $\alpha \approx 1.40$ and the dynamical exponent $z = \alpha/\beta \approx 4$. These results agree with the Mullins-Herring (MH) universality class [14, 15]. However, the true asymptotic universality class of the WV model is the Edward-Wilkinson (EW) universality class [13]. In our simulations, we cannot reach the asymptotic time and find the asymptotic scaling properties of the WV model because of the limitation of our computer facilities. The downhill particle diffusion current is obtained for the WV model and confirms the EW behavior.

After we apply the ES barrier into the WV model (WV-ES model) by modify its diffusion rule. The ES barrier induces mound formation on the surface. In this situation, we confirm mound formation by using the particle diffusion current and the correlation function. The particle current is uphill and the correlation function oscillates from the WV-ES model. For the scaling properties of the WV-ES model, the growth exponent (β) in early time ($t \ll t_c \approx 10^3$ ML) approaches the same β as obtained from the original WV model. After $t \gg t_c$, β increases and approaches 0.5. This behavior does not depend on the strength of the ES barrier, which is defined by the ratio of P_U/P_D, as long as it is strong enough to induce mound. We find that when $P_D \geq 0.9$, the barrier is too weak and the effect of downhill current of the original WV model still influence the system and there is no mound formation. When $P_D = 1.0$, it corresponds with the original WV model. When $P_D \leq 0.7$ the particle diffusion current shows the uphill current and the correlation function oscillates. This implies that there are mound formation on the surface and their results are corresponding to each other. But when $P_D = 0.8$, there is a conflict between correlation function and the particle diffusion current. This may be due to at this value of P_D is the boundary between mound formation surface and dynamical rough surface. So at this value of P_D, it shows the confliction between these tools. Furthermore, the average mound height increases when the strength of the ES barrier increases (P_D decreases) while the average mound radius decreases when the barrier becomes stronger.

From our results, the continuum growth equation of the WV model in 1+1 dimensions is

$$\frac{\partial h}{\partial t} = \nu_2 \nabla^2 h - \nu_4 \nabla^4 h + \lambda_{22} \nabla^2 (\nabla h)^2 + \eta(x,t). \tag{4.1}$$

We should note here that the uphill current and the oscillatory correlation function can help us to detect mounds, but they cannot help us determine the cause of the mounded surface. Because there are other possible causes for mounds too [16, 31, 32]. So when seeing mounded surfaces, we should not rush to conclude that the ES barrier is the cause. But for our study, we can deduce that mound formations on the surface come from the effect of the ES barrier. In another word, the ES barrier is the cause of mound formation on the surface in our study.

For future work, we can make the model more realistic by studying growth on two dimensional substrates. Furthermore, we may relax the SOS constraints from the model. The effects of the substrate temperature can make each adatom hops more than once in the simulation. It will be very complicated if we apply all effects above into the model, and it will require more simulation time. But the modified model will be more realistic than the original WV model studied here.