A STUDY OF WOLF-VILLAIN MODEL WITH EHRLICH-SCHWOEBEL BARRIER

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ABSTRACT: Wolf-Villain (WV) model is a simple model used to study molecular beam epitaxy (MBE) growth. In this model, an adatom is deposited at a randomly chosen site on a flat substrate. The adatom then diffuses instantaneously within a finite diffusion length ℓ. In the WV model, the adatom tries to maximize its coordination number or its bondings. We study statistical properties of the morphology and interface width of thin films grown by this model. The morphology of WV model is kinetically rough and the growth exponent is $\beta \approx 0.375$. Then we study the effect of a potential barrier on the WV model. The potential barrier we are interested here is known as the *Ehrlich-Schwoebel* (ES) barrier. The ES barrier is introduced as an additional barrier for adatom diffusion over a step edge from upper to lower terraces. We found that the morphology is rough with mound/pyramid type structure formation on the surface. The growth exponent increases in this situation, with the value of β approaches 0.5.

KEYWORDS: Wolf-Villain (WV) model, MBE growth, Ehrlich-Schwoebel (ES) barrier

1. INTRODUCTION

Recently, there are many studies on the kinetic surface roughening growth (Wolf and Villain 1990; Das-Sarma and Tamborenea 1991; Tamborenea and Das-Sarma 1993; Family 1986; Punyindu 2000) because of the possible relevance to physical phenomena of growth dynamics in molecular beam epitaxy (MBE). There are many discrete growth models (Wolf and Villain 1990; Das-Sarma and Tamborenea 1991; Tamborenea and Das-Sarma 1993; Family 1986) used to describe MBE growth process via computer simulations. Among these many growth models, we are most interested in the model proposed by Wolf and Villain, known as Wolf-Villain (Wolf and Villain 1990) (WV) model. The WV model is a simple model used to study MBE growth. The model follows *ideal* low temperature MBE growth conditions and under *solid-on-solid* (SOS) constraint. This means the model does not allow overhangs and bulk vacancies in the growing film, and desorption process is not considered.

We study statistical properties of the morphology and interface width of thin films grown by this model. Its morphology is found to be kinetically rough and the *growth* exponent $\beta \approx 0.375$. The morphology of thin films obtained by this model depends on many kinetic processes such as deposition of adatoms and diffusion of an adatom. (Gerlach et al. 2001; Johnson et al. 1994). Our particular interest in this work is step edge diffusion of an adatom. In the step edge diffusion process, an adatom encounters a potential barrier, known as the *Ehrlich-Schwoebel* (Schwoebel and Shipsey 1966) (ES) barrier which is an additional barrier for adatom diffusion over a step edge from upper to lower terraces.

In this work we study effects of the ES barrier on the WV growth model. We found that the morphology of this new model is rough with mound/pyramid type structure formation on the surface. The growth exponent increase in this situation and the value of the growth exponent, β, approaches 0.5.

2. MODEL

Wolf-Villian (WV) model is a simple model which follows ideal MBE conditions and SOS constraint. In this model, there are deposition and diffusion processes. An adatom is deposited at a randomly chosen site on a flat substrate denoted by coordinate x. Then the adatom diffuses instantaneously under a finite diffusion length ℓ. In our study based on $\ell = 1$, the adatom can diffuse only to its nearest neighboring

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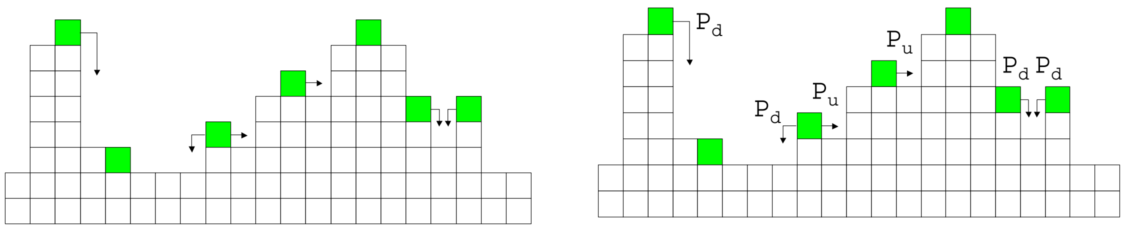
sites. Our work here is done in 1+1 dimensions which means the substrate is in one dimension plus another one dimension of the growth direction. After the diffusion process, the diffused adatom finds its final site and is incorporated permanently into the substrate. This means that the adatom can no longer move. Diffusion rule for the WV model is as following: the adatom tries to diffuse to the site that increases its coordination number to a *maximum* value. In other words, the adatom try to maximize its coordination number or its bondings, as Figure 1(a). In our simulation we define time t in a way that one second is equal to an average of one monolayer (ML) deposition of the growing film. We also use *periodic boundary conditions* to prevent finite size effect.



(a) (b)

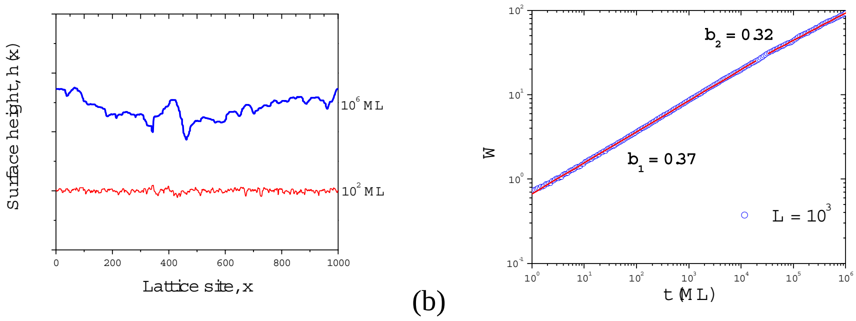
Figure 1. (a)The diffusion rule of the Wolf-Villain (WV) model. The adatom drop onto the substrate at x and try to maximize its coordination number or its bondings in the diffusion process. The adatom looks around among the nearest neighbor sites, x±1. It searches for the site that offers the strongest binding and moves to this site and sticks there. If there are as many bonds at x as at x±1, the adatom stay at x. If two sites next to x are equally preferable, one of them is chosen by random. (b)The configuration of the modified growth rule in 1+1 dimensions Wolf-Villain model. Here is the WV model with ES barrier. The probability $P_u(P_d)$ represents the chance of an adatom to diffuse to the upper(lower) terrace.

Next, we focus on the step edge diffusion process. The adatoms that tries to diffuse from the upper to lower terrace will encounter a potential barrier. The well known potential barrier we are interested in is the *Ehrlich-Schwoebel* (Schwoebel and Shipsey 1966) (ES) barrier. It is the step edge potential barrier which is known to cause mound/pyramid type structure formation on the surface. We apply the ES barrier to the WV model by modifying its diffusion process. The instantaneous relaxation process is now controlled by propabilities P_u and P_d ($0 \leqslant P_d, P_u \leqslant 1$) where P_d is the probability for adatom to diffuse down to the lower terrace and P_u is the same for diffusion to the upper terrace. In our growth model, the ES barrier is implemented by taking $P_u > P_d$ thus promoting diffusion on the same layer over a hop down to lower terrace. Once the atom selects the final site, it has to take probabilities P_u or P_d into account. These probabilities determine whether the atom hop to the selected final site or stick at the deposition site. The modified WV rule is shown in Figure 1(b).

3. RESULTS AND DISCUSSIONS

In our simulations, we study the model in 1+1 dimensions. The simulations were performed with a periodic boundary condition on a flat one dimensional substrate. Figure 2(a) shows morphology of the original WV model at 10^2 ML and 10^6 ML. In the figure, we see that surface of the film is not smooth but there is no mound/pyramid type structure formation on the surface either. This character of the morphology is called *dynamical rough* surface. The quantity we are interested is the *interface width* which characterizes *roughness* of the interface. The interface width is defined by the root mean square height fluctuation (Barabasi and Stanley 1995):

$$W = \sqrt{\langle h^2 \rangle - \langle h \rangle^2}. \tag{1}$$



(a) (b)

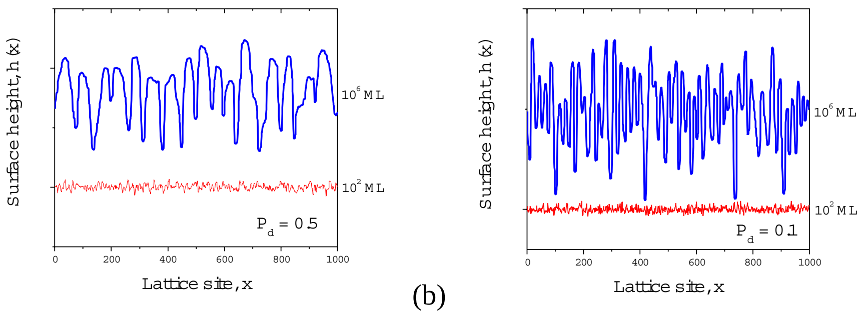
Figure 2. (a) Morphologies of the Wolf-Villain (WV) model in 1+1 dimensions by using substrate size L = 1000 lattice sites and time t = 10^2 **and** 10^6 **monolayer (ML). (b) The interface width W in the substrate size L =** 10^3 **system.**

In early time, the interface width increases as a power of time (Barabasi and Stanley 1995),

$$W \sim t^{\beta}, \qquad (2)$$

where the exponent β is known as the *growth exponent* which characterizes the time-dependent dynamics of the roughening process. Moreover, when we plot the interface width as a function of time we can find the growth exponent β. In this simulation, shown in Figure 2(b) using substrate size L = 10^3, we found that the growth exponent decreased from $\beta_1 \approx 0.37$ to $\beta_2 \approx 0.32$.

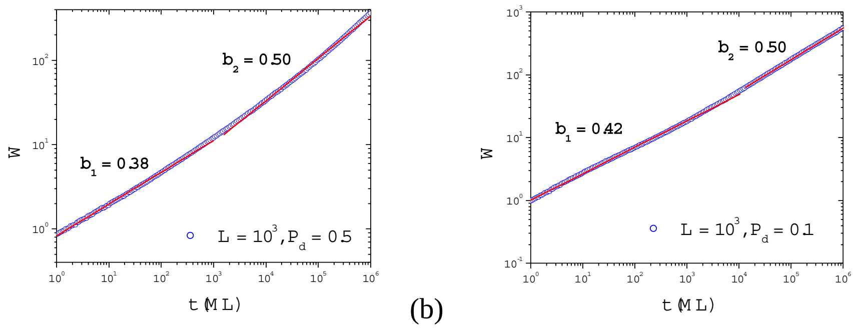
Next we add the ES barrier into the WV model. For this work we set $P_u = 1$ which means an adatom does not feel the barrier when it diffuses to the upper terrace. The value of P_d represents the strength of the ES barrier. In our simulation, we use two values of P_d: $P_d = 0.5$ and $P_d = 0.1$. The resulting morphologies are shown in Figure 3. It can be seen that there are mounds on the surface in both systems.



(a) (b)

Figure 3. Morphologies of the WV model with ES barrier in 1+1 dimensions showing the system with substrate size L = 10^3 **at** 10^2 **and** 10^6 **ML. The barrier strength, controlled by the value of** P_d**, is set at two different levels; i.e. (a)** $P_d = 0.5$ **and (b)** $P_d = 0.1$**.**

In Figure 4, we show our calculated interface width for both systems. For $P_d = 0.5$, the growth exponent changes from $\beta_1 \approx 0.38$ to $\beta_2 \approx 0.5$ while for $P_d = 0.1$ we found $\beta_1 \approx 0.42$ crossovers to $\beta_2 \approx 0.5$. We can explain (Das-Sarma and Punyindu 1999; Punyindu 2000) the crossover of β from comparatively small values to $\beta \approx 0.5$ in the following way. In the early time the whole substrate is connected and correlated. All growth exponent in the early time are similar to growth exponent obtained in the original WV model. After some time mounds are clearly developed and interact through the coarsening process. Later, mounds almost stop growing in the lateral size and the newly deposited adatoms are incorporated on top of existing mounds and make the mound steeper. The steepening process becomes dominant and there is little interaction between mounds at this time. Since the substrate is separated into pieces with no interaction to each other, the growth exponent β increases to the maximum possible value of 0.5.



(a) (b)

Figure 4. The interface width versus time plots. The system simulated with (a) P_d = 0.5 gives the $\beta_1 \approx 0.38$ to $\beta_2 \approx 0.5$ (b) P_d = 0.1 gives the $\beta_1 \approx 0.42$ to $\beta_2 \approx 0.5$.

4. CONCLUSIONS

In our simulation we first simulated the Wolf-Villain (WV) model. We found the dynamical rough surface. In the substrate size L = 10^3, the growth exponent change from $\beta_1 \approx 0.37$ to $\beta_2 \approx 0.32$. When we applied the Ehrlich-Schwoebel (ES) barrier into the WV growth model, there are mounds on the surface in both P_d = 0.5 and P_d = 0.1 systems. In the early time, all growth exponent are similar to growth exponent obtained in the original WV model. After some time mounds are developed and almost stop growing in the latteral size. The newly deposited adatoms are incorporated on top of existing mounds and make the mound steeper. There is little interaction between mounds and the substrate is separated into pieces with no interaction to each other. The growth exponent β increases to $\beta \approx 0.5$.

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