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Kinetic Monte Carlo simulation of the flux dependence of semiconductor quantum dot growth

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Abstract. Performing an event-based continuous kinetic Monte Carlo (KMC) simulation, all the important kinetic behaviors take place during the growth of the semiconductor material in the molecular beam epitaxy (MBE) system such as deposition, diffusion, desorption, and nucleation are considered, we investigate the effects of the growth conditions which are important to form semiconductor quantum dot (QD) in MBE system. The simulation results provide a detailed characterization of the atomic kinetic effects. The KMC simulation is also used to explore the effects of anisotropy effects to the epitaxy growth of QD. We find that the flux plays an important role in determining the size of the QD. The agreement between our simulation and experiment indicates that this KMC simulation is useful to study the growth mode and the atomic kinetics during the growth of the semiconductor QDs in MBE system.

Introduction

Self-assemlbed QDs in semi-conductor heterostructures are of great interest because of their discrete atom-like energy levels, good optical properties, and promising device applications such as QD lasers and photodetectors [1-3]. A number of experiments have been performed in order to achieve the QDs of high optical quality and size-ordering, and these studies show that the growth mode is very complex and sensitive to the growth conditions [4-6]. Excited by experimental interest, some theoretical approaches have been developed to address the mechanisms determining the size and distribution of the QDs. Computer simulation is one of the theoretical methods, which can give some detailed information about the growth of QDs.

An event-based KMC simulation has been successful in reproducing growth process in MBE system [7, 8]. Such a simulation study is useful not only for investigating the kinetic of MBE growth but also for analyzing the growth mode and surface morphology during the growth.

In this paper we develop such a Monte Carlo simulation for strained semiconductor systems. First we simulate the flux dependence of the InAs QD grown by MBE machine on GaAs (100) substrate. Some aspects of atomic kinetic during MBE growth are discussed. Then the KMC simulation is also used to explore the anisotropy effects on the substrate to the epitaxy growth of semiconductor QD. The simulation results are in excellent qualitative agreement with the experimental results.

Kinetic Monte Carlo model and Discussion

Our KMC simulation is based on the solid-on-solid model. Deposition and diffusion are considered the main relevant processes during the growth of the semiconductor materials, this is particularly fitting for the MBE system, because it is known that deposition, diffusion, desorption, and nucleation will all take place during the growth of the semiconductor material in the MBE system. While in order to inhibit the atom desorption, some factors such as the low temperature and high pressure of as are normally adopted in the experiment. The atoms can still diffuse after nucleation unless their eight neighboring positions are all occupied by other atoms. The hopping rate for a single atom is given by Arrhenius' law:

$$P = V_O \exp\left[-\left(E_S + E_N + E_{DB} + E_{AD}\right)/k_B T\right] \tag{1}$$

$$E_N = \left(n + \beta m\right)E_n - \varepsilon\left(n' + \beta m'\right)E_n \tag{2}$$

$$E_{DB} = -A^* E_{db} + \varepsilon^* B^* E_{db} \tag{3}$$

Here the attempt frequency $V_o = 10^{13}s^{-1}$. E_S is the atomic binding energy to the surface, E_{AD} represents the energy barrier effect of anisotropic diffusion. E_n is the atomic binding energy to a single nearest neighbor atom, and in order to include the contribution of the next nearest neighbor atom, we multiply E_n by β, the value of which is $1/\sqrt{2}$. A coupling constant ε of 0.2 is used in Eq. (2), which describes a weak coupling between the two adjacent lattice sites. The integers n and m are the numbers of the nearest and next nearest neighbor atoms, while n′ and m′ have the same meaning but correspond to the site to which the atom will hop (destination site). Because of the existence of dangling bond of the adatom, a additional item E_{db} is considered in our model which represents the contribution of one dangling bond to the hopping rate of the adatom. In our simulation it is 0.01 eV. A is the number of the dangling bond of the adatom, and B has the same meaning as a but corresponds to the destination site. Now all the important physical procedures which affect the diffusion of an atom are considered. The next task is to define a very little time interval corresponding to one Monte Carlo step during which there is only one atom that can diffuse. We compute the time interval by $\Delta t=1/\sum p_i$. The most efficient search method developed to date is the binary tree process which is used in our simulation to locate an atom to diffuse in every time interval. Some parameters used in the simulation are typical for a variety of semiconductor materials: E_s = 1.3eV, E_n =0.3 eV, ε =0.2, $\beta=1/\sqrt{2}$, and k_B is the Boltzmann constant. In this simulation we only focus on a submonolayer heteroepitaxy growth. It is sufficient because we assume that the two-dimension inlands can be the nucleation sites and during the 2D/3D transition, the QDs formed on these 2D inlands. In simulation after all the atoms have been deposited on the substrate the system is allowed to equilibrate by a growth interruption.

We restrict in our simulation on a 200*200 grid (in units of lattice constant). Firstly, we study the growth flux dependence during the growth of InAs QDs in MBE system. Since normally most semiconductor InAs QDs are grown on the GaAs (001) substrate which means there isn't any anisotropy to the deposited atom, so under this condition E_{AD} is set to 0 in the simulation. We can see our program can easily be applied to an anisotropic or isotropy system by changing the value of E_{AD}.

Fig. 1(a), (b) and (c) show the growth flux dependence of InAs QDs on GaAs(100) substrate in simulation, and the other parameters are the same except the growth flux, the growth temperature T=723K, growth interruption=20s.

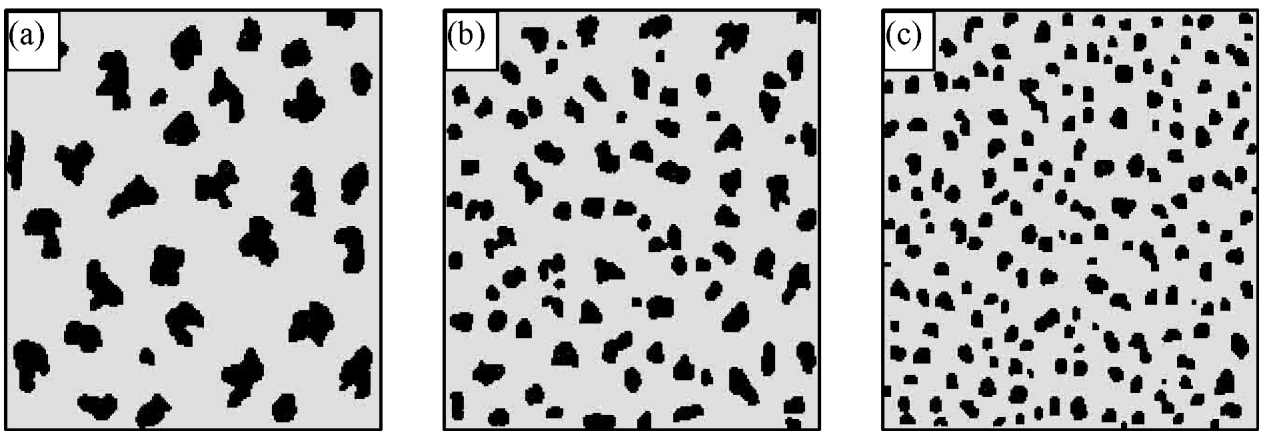

Figure 1. (a) t = 18s, flux = 0.01 ML/s (b) t = 1.8s, flux =0.1 ML/s (c) t = 0.18 s, flux = 1.0 ML/s. The other parameters are: T = 723 K, growth interruption = 20 s.

In order to give a more apparent simulation results to show the growth flux dependence of the QDs. We simulate a number of different growth flux dependence of the QDs' growth and plot the dependence as a curve in Fig. 2(the growth rate changes from 0.03 to 3 ML/s, it covers most of the range of growth rate in the MBE machine).

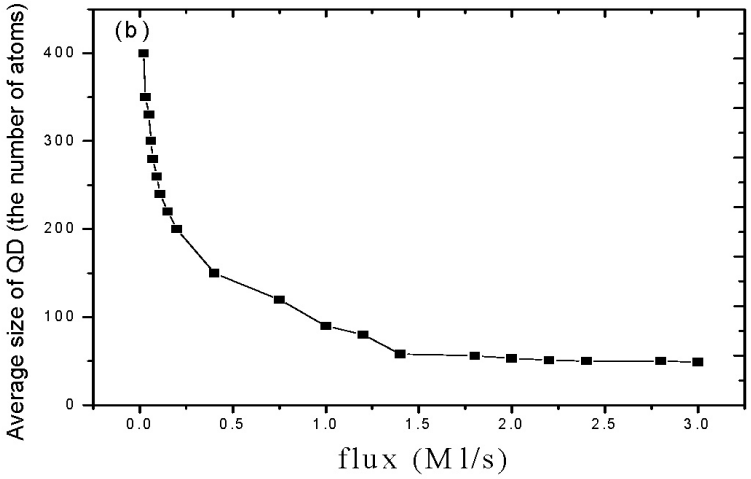

Figure.2 Average size of QD VS growth flux

We can find that the lower the growth flux is, the larger will be the QD. It can be understand that at low flux, the deposit atom will have more time to attempt a diffusion, and hence the adatoms have a large diffusion constant. As a result each island will on average collect adatoms from a circular area of a larger radius of the mean free path of a single adatom. So this will result in a larger QDs. The same effects have been observed in experiments [9]. It should be noted that this is a purely kinetic effect, the moment research is mainly a investigation about the kinetic effects during the growth of semiconductor QDs, the simulation results are reasonable in some moderate experimental conditions, and in some other extreme conditions such as very high temperature and very large or small growth flux, the thermodynamic effects must be considered in the theoretical simulation. This will be studied in our further research.

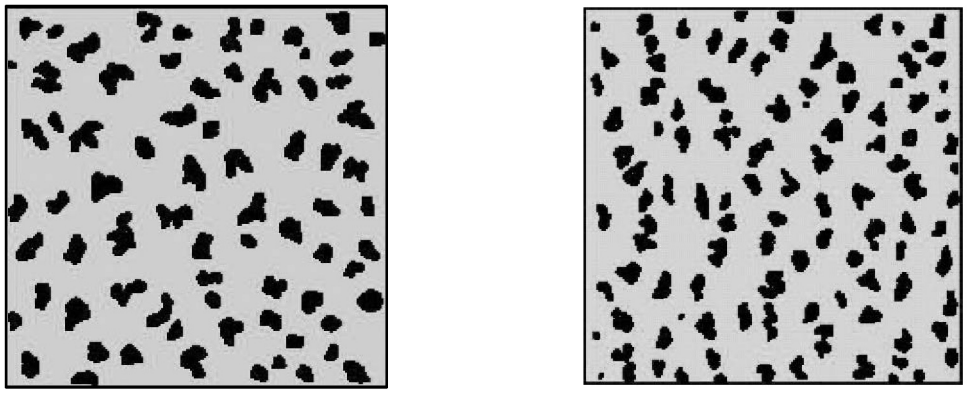

Figure 3. Spatial distribution of atoms, the gray area represents the substrate, the black represents the QD. Simulation parameters are T=723 K, f=0.06 ML/s, growth time=3s, growth interruption =50 s. (a) without E_{AD} (b) with E_{AD}.

Secondly, we investigate the anisotropy effect of the substrate to the growth of the semiconductor QDs, for example the InAs QDs' growth on GaAs (100) substrate. In order to simulate this condition, we firstly simulate the anisotropy effect by setting the E_{AD} =0.1 eV (Eq.1), and the other parameters are same in the simulation. Fig. 3 shows the difference without (Fig. 3a) and with (Fig. 3b) the anisotropy effect on the substrate, we can easily find that when the QDs are grown on the isotropy substrate (Fig. 3a), the two dimensional islands distribute randomly on the subsurface because

everywhere on it is same to the deposited atom. After E_{AD} is considered (Fig. 3b), the islands become elongated. The same phenomenon has been observed in the experiment [10].

Summary

B In brief summary, we investigate the flux dependence of the semiconductor QD growth by a KMC simulation and found that the lower the growth flux is, the larger will be the QD, also some aspects of atomic kinetic during MBE growth are discussed. And the KMC model is also used to explore the anisotropy effects on the substrate to the epitaxy growth of semiconductor QD. It is found that the anisotropy on the substrate will result in a elongated QDs, however will not get a ordered QDs' distribution. The simulation results are in well qualitative agreement with experiments. So this simulation approach is useful to study the growth mode and atomic kinetic during the growth of semiconductor quantum dots.

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