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The kinetic process of non-smooth substrate thin film growth via parallel Monte Carlo method

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ABSTRACT

A Monte Carlo simulation model of thin film growth based on parallel algorithm is presented. Non-smooth substrate with special defect mode is introduced in such a model. The method of regionalizing is used to divide the substrate into sub-regions. This method is supposed to be modulated according to the defect mode. The effects of surface defect mode and substrate temperature, such as the nucleation ratio and the average island size, are studied through parallel Monte Carlo method. The kinetic process of thin film growth in the defect mode is also discussed. Results show that surface defect mode contributes to crystal nucleation. Analyzing parallel simulation results we find that density defect points, substrate temperature and the number of processors contribute decisively to the parallel efficiency and speedup. According to defect mode we can obtain large grain size more feasibly and the parallel algorithm of this model can guide the non-smooth substrate simulation work.

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1. Introduction

Thin film plays an important role in modern industry due to its unique optical, electrical and mechanical properties. Computer simulation technology can be applied to efficiently simulate thin film growth and study the mechanism of film formation [1]. Molecule dynamics and kinetic Monte Carlo method (KMC) are two common ways of simulating thin film growth by computer [2,3]. The KMC method, which is based on energy calculation and widely used as an atom simulation method, is appropriate for simulating dynamics evolution processes such as depositing thin film through PVD [4]. A considerable amount of research on simulation of thin film growth based on KMC has been published, including studies of surface nucleation [5–7], porous columnar growth [8–10], grain growth and grain boundary diffusion [11–13], and other processes of thin film growth [14,15].

Thin film growth simulation has been paying close attention to thin film growth with different structures on the smooth substrate [16,17]. In real thin film growth, it is necessary to study the kinetic process on defect substrate since the substrate cannot be of ideal smoothness. The defect substrate has an effect on the thin film morphology (such as grain size and surface roughness) and performance (such as mechanical properties and scatter). Meanwhile, certain defect modes can be considered as special structure substrates, which can be made into unique devices, such as sculpture thin films with pre-construct substrate or low dimensional systems (quantum wells and quantum wires) [18].

Simulation programs require higher computational efficiency as the simulation growth model becomes more complicated and more factors are taken into consideration, especially at a high substrate temperature or in a large simulation area, which costs much computational time and memory. Parallel kinetic Monte Carlo method can make full use of the processor's capability, saving computational time and simulating a large scale of thin film growth [19]. The adaptation between parallel algorithm and simulation model must be taken into account—it requires sub-region division as well as appropriate strategies for facilitating communication between neighboring processors [20,21]. When we consider the non-smooth substrate, a parallel simulation model can simulate thin film growth more accurately and make more discussions of the parameters' relationship available.

This paper begins by establishing a parallel kinetic Monte Carlo model of thin film growth on a non-smooth substrate with defect mode. The model adopts parallel calculation with sub-region division and is able to modulate the scope of sub-regions according to its defect mode. Then the kinetic process and film-formation quality under the influence of defect energy and substrate temperature are discussed. We find that defect density, substrate temperature and the number of processors influence the parallel efficiency as a whole.

2. Simulation model

The simulation model is shown in Fig. 1 and is described in what follows. Thin film growth is simulated on a tetragonal lattice whose

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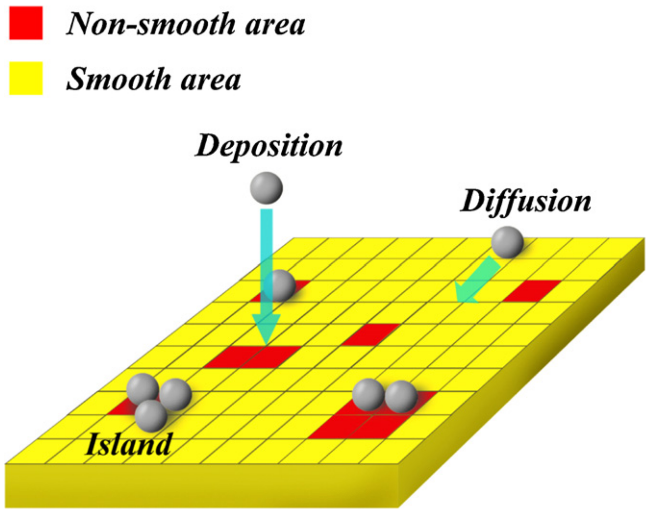

Fig. 1. Illustration of simulation model.

area is $L \times L$ with its periodical boundary. The procedure of thin film growth in this model is as follows:

(i) Defect points are generated on the substrate according to different defect modes. The defect mode on the substrate is one of the key points in this paper. There are two cases in this step: the random defect point and the pre-construct defect point. In the case of the random defect point, the program generates defect points when it starts (the number of defect points can be chosen). We can save the defect points' information as a static array and mark each of the defect points' sites. The defect energy of defect points can be set according to the substrate material. In the case of the pre-construct defect point, some defect points, which are of a certain order, are generated, such as point defect, line defect and plane defect.

(ii) Particles deposit on the substrate randomly. (If they settle down on the defect site, it will have the defect energy, which the system will mark and calculate.) The deposition rate in this model is L^2F and the time increment in deposition is $1/(L^2F)$. F is the vertical deposition rate in ML/S. In the process of deposition, a lattice site is randomly selected for deposition, and each site can only accommodate one particle—the arrival of any other particles is prohibited.

(iii) Particles diffuse on the substrate and some gather into islands. The defect site must be considered and particles can only move to the vacant site. According to kinetic Monte Carlo method, particles select a transition path out of a certain probability. The probability is equal to V, the hopping rate along such a transition path. V is determined by Arrhenius rate equation:

$$V_i = E_0 \exp(-E_{ij}/k_BT) \tag{1}$$

Here $E_0 = 2k_BT/h$, k_B is the Boltzmann's constant. T is the substrate temperature and h is Planck's constant. E_{ij} is the energy barrier from the origin site i to the final site j. E_{ij} in this model is determined by

$$E_{ij} = E_s + aE_d + \Delta E_{ij} \tag{2}$$

E_s is the energy of substrate contributing to particles. E_d stands for defect energy; here α is defect mode factor, changing from 0 to1. ΔE_{ij} is the interaction energy between atoms and can be obtained from two body Morse potential functions.

The time increment of this step is ΔT, which is given by

$$\Delta T = (-\ln R)/V_i \tag{3}$$

where R is a random number between 0 and 1.

(iv) If simulation time is long enough for particles to carry diffusion again, the procedure goes back to (iii), if not backs to (ii).

Thin film growth simulation requires a large arithmetical scale. The simulation program will be time-consuming and difficult to carry out smoothly if: (1) there is a high substrate temperature ($T > 600$ K); (2) there is a large simulation area; or (3) a complicated simulation model such as defect mode substrate is employed. Parallel algorithm is applied to our model to improve calculation efficiency. Here a parallel model based on Shim and Amar [22] and Merrick and Fichthorn [23] is developed to cater to our defect mode setting. There are many different ways to employ parallel technology. Our work draws on the MPI database.

According to the parallel algorithm, the substrate is divided into N regions; here N is the number of processors and each region has the same area. If ΔE_{ij} in formula (2) is concerned with two regions in the charge of two processors, then the neighboring regions will communicate with each other and transfer messages back and forth. When there are a large number of defect points in the boundary, the resulting heavy communication will waste much time and memory. Given that our defect mode setting is not standard, we change the parallel method correspondingly. Here we propose the method of regionalizing to improve parallel calculation. In our model, we divide the parallel area into sub-regions of different sizes according to defect mode. This results in a different number of particles depositing in each sub-region, but guarantees that every processor can get generally the same computation, which then reduces the average computational time.

3. Result and discussion

We simulate Al film, which grows on defect substrate SiO_2. The simulation area is 200×200 ($L = 200$) with a coverage rate of 30%. In this paper the random defect point is considered as the defect type because we want to research the particles' behavior on a common defect substrate first. Moreover, we also consider the pre-construct defect point and it will be discussed in other research. In this model, the substrate contribution is mostly determined by the substrate material so here we assign 0.75 eV to E_s, which is the energy of the SiO2 substrate contribution according to Ref [24]. When referring to Ref. [25], we assume $\Delta E_{ij} = 0.37$ eV for $\Delta E_{ij}/E_s = 0.5$. Since there are no experimental or theoretical data for the defect energy E_d, we assume $E_d = 0.25$ eV for $E_d/E_s = 0.3$. We study the change of the average island size and the nucleation ratio at a substrate temperature from 500 K to 700 K with a density from 5% to 30% of defect points of the substrate area. The program is run several times using different numbers of processors (one, two, four or eight) to compare and test parallel efficiency.

According to Ref. [22], here we used a strip decomposition, because we think it is more feasible to obtain and can reduce the communication time. In our model, the width of ghost region is $L_{ghost} = 0.1L_{processor}$; the $L_{processor}$ stands for the width of each processor's region. For example, if the simulation region is divided into 4 sub-regions, the $L_{processor} = L/4 = 50$, then $L_{ghost} = 5$. If there are many defect points in the boundary, the value of $L_{processor}$ will increase and L_{ghost} will not change. The cycle time is described here as $t = 1/(L^2F)$, which is equal to the deposition rate, because we consider the deposition time interval as the two particles reach the substrate.

Fig. 2 displays the relationship among substrate temperature, density of defect points (D) and nucleation ratio; here nucleation ratio is the percentage of the nucleation number in depositing particles. At each substrate temperature level, the nucleation ratio tends to be of the same fluctuation inspite of the change of defect points. When defect points increase on the substrate, the nucleation

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