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Visual simulation of GaInP thin film growth

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ABSTRACT

Metal organic chemical vapor deposition (MOCVD) technology is a very efficient way to uniformly grow multi-chip, multilayer and a big area thin film. Kinetic Monte Carlo (KMC) method is one of the important research tools that carry out dynamic simulation of atomic thin films growth. Based on the method of KMC, this paper proposes an algorithm of the process of GaInP thin film grown by MOCVD. KMC simulation and the visualization emulation of GaInP thin film growth in MOCVD reactor are realized. The results of simulation and visualization truly and intuitively displayed process of GaInP thin film growth in MOCVD reactor. The simulation results with this paper's algorithm well coincide with experimental results. This visualization results provide the optimizations of processing parameters which grow GaInP thin film by MOCVD with theoretical basis.

1. Introduction

Nowadays high-efficiency multi-junction solar cells (GaAs basic series multi-junction solar cells) are the most competitive in the new generation solar cells in the world, and they are high-performance and long-life space main electrical sources which aerospace craft urgently require. The most familiar three junctions solar cells are GaInP/GaAs/Ge tandem cells, which can improve photoelectric conversion efficiency of solar cell. Among all the methods of developing GaAs Solar Cells, MOCVD technology can grow various complex apparatus' structures, making the study and scale-production of multi-junction stack cells possible [1–3]. The principle of MOCVD technology is to take the organic compounds of III and II group (such metallic organic compounds as $Ga(CH_3)_3$, $Al(CH_3)_3$, $Zn(C_2H_5)_2$) and the hydrides of V and VI group (PH_3, AsH_3, H_2Se, etc.) as the raw materials of crystal growth, and carry out vapor deposition on substrate by means of thermal decomposition, and grow the compound semiconductors of III–V and II–VI group and thin film single crystal materials of their ternary and quaternary compound semiconductors. To grow high quality thin film material is to ensure uniformity of the thickness and component of epitaxial layer. GaInP is ideal lattice-matched material of top cell with GaAs. At present GaInP/GaAs/Ge tandem solar cell made of it has achieved more than photovoltaic conversion efficiency of 30% [4]. Kurtz et al. [5] carefully studied the relationship between band gap energy of $Ga_{0.5}In_{0.5}P$ and growth temperature and growth rate. Wang et al. [6] used a low pressure metal organic chemical vapor deposition (LP-MOCVD) system to grow the GaAs tunnel junction of $GaInP_2$/GaAs/Ge tandem solar cells and studied the design principle of tunnel junction. However, nowadays all the studies at home and abroad have been paid attention to technical characteristics of this kind of tandem solar cells, optimization of process and structural parameters at the macroscopic level, so as to improve conversion efficiency. Its film growth mechanism has little attention at the microscopic level.

The growth of thin films is a process of surface dynamics. It represents a series of atomic process in the thin film surface such as atom bonding, diffusion and re-evaporation. Among these processes, diffusion decides core formation and core

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growth. Accurate description of these processes at an atomic level is considerable valuable for improving growth techniques of thin films and making excellent performance thin films. With the development of surface analytic technology, especially the occurrence of Scanning Tunneling Microscopy (STM), Atomic Force Microscopy (AFM), we can directly watch surface morphology of thin films taking on resolution capability at the atomic level. However, because at present it is impossible to trace all the physical processes about atomic deposition and thin films growth in experiment, computer simulation has already become one of important ways that research atomic processes of thin films growth. The computer simulation methods mainly have first principle, molecular dynamics (MD), monte carlo (MC) and finite element method, etc [7]. Among these methods, Kinetic Monte Carlo (KMC) method combining MD with MC is one of important research tools that carry out dynamic simulation of atomic thin films growth [8].

Sung et al. [9] used a three-dimensional (3D) MC simulation model to study grain growth in a binary Pt–Co system. They used two methods—random nucleation and film growth to simulate the grain growth of the single disordered phase. The results showed that the number and distribution of the nuclei of the ordered phase played an important role in grain size and grain morphology. Rahman et al. [10] applied KMC technique to the diffusion of two-dimensional (2D) Cu clusters on Cu(111). The results showed interesting trends in the diffusion rate and in the frequencies of the microscopic mechanisms. Cho et al. [11] implemented KMC method on an atomic scale that incorporates the effect of surface diffusion as well as the interplay between surface topography and the changing vapor incidence angle, and simulated film growth by physical vapor deposition on rotating substrates. Fu et al. [12] combined the computational fluid dynamics and KMC method and presented a multiscale modeling of fluid dynamics, thermodynamics, and MD to study the chemical and physical growth process of GaN in a standard MOCVD reactor. The theoretical model provided us with a fundamental guideline for optimizing GaN MOCVD growth at the microscopic level. Zhang et al. [13] developed a three-dimensional KMC technique for simulating growth of thin Cu films. The results showed that there exists an optimum growth temperature at a given deposition rate which made surface roughness minimize and the relative density saturate. Yu et al. [14] developed a new model for simulation of the growth of $PbTiO_3$ thin film basing on KMC method. The simulation results showed that the deposition rate and the substrate temperature play a very important role in the initial process of growth of $PbTiO_3$ thin films. Yu et al. [15] applied KMC simulation to the study of film epitaxial growth. Wang et al. [16] introduced the classical MC model of grain growth and stated the limitation of the model and modified algorithms both at home and aboard in recent years. They indicated that combination of MC method and practical process is the main direction for future study. However, Refs. [9–16] mainly applied MC or KMC method to study on mechanisms of grain or thin growth. These studies exist two main disadvantages that are quite limited display capacity and poorer man-machine interactive capacity. Virtual reality (VR) has the intuition and interactive properties making up deficiency of computer simulation so as to make simulation results take on effect of 3D stereo display [17–19]. Qin et al. [20] applied Monte Carlo Potts method to 3D modeling for single phase polycrystalline organization, thus realizing 3D visualization, and building digital and nearly actual 3D microstructure model. Chen and Wang [21] proposed a method for 3D simulation and visualization of polycrystalline grain's shape based on virtual reality modeling language (VRML), and realized the real-time and interactive 3D-visualization of simulation results in the browser. However, Refs. [20,21] only applied VR technology to visualization study on polycrystalline grain, being deficient in visualization study on grain growth of multiple compound.

In this paper, an algorithm of the process of GaInP thin film grown by MOCVD on the basis of KMC has been proposed. Compared with the reported works which mostly suppose the atom randomly was absorbed on substrate surface, in this paper, in the absorption event, the atomic coordination of Ga, In and P has come from the results of optimization on MOCVD reactor with CFD simulation. With the background of growing GaInP thin film by MOCVD technology, the paper uses combination of KMC simulation and VR technology to carry out visualization research on GaInP thin film growth process. By research, process of GaInP thin film growth in MOCVD reactor is truly and intuitively displayed. In addition, the rule that different process parameters such as simulation time, substrate temperature and deposition rate affect thin film growth is acquired, providing theoretical basis for optimizing filming process.

2. KMC simulation of GaInP thin film growth

2.1. KMC lattice model

Because GaInP is of face-centered cubic (FCC) crystal series blende structure, the Monte Carlo Lattice is confirmed to be made of $N \times N \times H$ small cube whose length equals to the average atomic diameters of Ga, In and P atoms, i.e. 0.292 nm. N and H are length (width) and height, respectively. In this model, N is selected as 200, H is decided by the number of simulation objects and computing quantity. Fig. 1 is KMC simulation domain under space coordinates system, in the Fig. 1, x, y and z coordinate axes represent length, width and height direction, respectively.

2.2. KMC event

In the process of thin film growth, suppose three kinds of events occur: (1) incident atoms are adsorbed on the substrate surface; (2) adsorbed atoms are diffused on the substrate surface; (3) adsorbed atoms are evaporated. In this Model, the KMC events are made of adsorption, diffusion and evaporation events. They are respectively described as follows.