Superlattices and Microstructures 97 (2016) 132–139

Contents lists available at ScienceDirect

Superlattices and Microstructures

journal homepage: www.elsevier.com/locate/superlattices

A binary phase field crystal study for liquid phase heteroepitaxial growth

Yanli Lu**, Yingying Peng*, Zheng Chen

State Key Lab of Solidification Processing, Northwestern Polytechnical University, 710072, Xi'an, PR China

ARTICLE INFO

Article history:
Received 25 March 2016
Accepted 26 May 2016
Available online 11 June 2016

Keywords:
Liquid phase heteroepitaxial growth
Binary PFC
Substrate vicinal angles

ABSTRACT

The liquid phase heteroepitaxial growth on predefined crystalline substrate is studied with binary phase field crystal (PFC) model. The purpose of this paper focuses on changes of the morphology of epitaxial films, influences of substrate vicinal angles on epitaxial growth, characteristics of islands growth on both sides of the substrate as well. It is found that the morphology of epitaxial films undergoes the following transitions: layer-by-layer growth, islands formation, mismatch dislocations nucleation and climb towards the film-substrate interface. Meanwhile, the density of steps and islands has obviously direct ratio relations with the vicinal angles. Also, preferential regions are found when islands grow on both sides of the substrate. For thinner substrate, the arrangement of islands is more orderly and the appearance of preferential growth is more obvious than that of thicker substrate. Also, the existing of preferential regions is much more valid for small substrate vicinal angles in contrast for big substrate vicinal angles.

1. Introduction

Due to its unique optical and electronic properties, thin film material is widely used in optoelectronics and semiconductor devices [1–3], especially in the design and production of Large Scale Integrated circuit and precision components. Therefore, the fabrication technology of films plays an increasingly important role. In its practical application, the properties of thin film material is strongly dependent on the microstructure of the film, especially the defects in crystal lattice [4]. Hence, it is necessary to deeply explore the growth mechanism of thin film and the theory of defects formation, which is helpful to control the formation of defects and get high-quality thin film materials.

Liquid phase epitaxy [5]is a near-equilibrium process, in which the solid phase grows on a predefined crystalline substrate surrounding liquid phase, it has become one of the most important techniques in manufacturing and processing nanoscale materials. The difference of lattice constant between the deposited material and substrate results in mismatch strain. Morphological instability induced by the strain leads to rough surfaces and defects in the film, as known as the Asaro-Tiller-Grinfeld instability [6,7]. This phenomenon has been studied using fully continuum models [8]and hybrid discrete-continuous step-flow or island dynamics models [9]. Motivated by some experiments on the heteroepitaxy of SiGe islands on Si nanomembranes [10] and strained InGaAs layers on InP substrates [11], many scholars have paid attentions to simulations of heteroepitaxy. Chen Cheng [12] employed the phase-field crystal in pure materials to study the influences of the

* Corresponding author.
** Corresponding author.
E-mail addresses: luyanli@nwpu.edu.cn (Y. Lu), pyingying@189.cn (Y. Peng).

http://dx.doi.org/10.1016/j.spmi.2016.05.039
0749-6036/

substrate vicinal angles and the lattice mismatch on the shape transition of strained islands in heteroepitaxy; Pinku Nath [13] presented a new modification of the solid-on-solid heteroepitaxial KMC model combined with the ball and spring model allowing for efficient simulation of SK heteroepitaxy; M. Klawtanong [14]studied the effects of deposition flux, lattice mismatch, and growth temperature on the morphology of film surfaces in fast kinetic Monte Carlo simulations.

Although, many researches have made significant progresses these years, most of them mainly concentrated on pure materials [15,16]. Also, these initial works proposed that the morphological instability of pure film results in buckling or roughening of substrate and dislocations nucleate at the film surface. However, less reports known have investigated the influences of composition of alloy on epitaxial thin films. In this paper, the two-dimensional binary alloy liquid phase epitaxial growth is examined using a recently developed binary phase-filed crystal model [17,18]. The morphology changes of epitaxial films growth on a planar substrate, influences of substrate vicinal angles on the epitaxial growth and islands growth on both sides of substrate are investigated.

2. Simulation method

2.1. Model

The growth of epitaxial layer on substrate typically occurs on timescales much larger than phonon timescales and involves the nucleation of single dislocation that are of the size of the atomic spacing. Binary phase field crystal model has its unique advantages to examine this phenomenon, not only for its ability to primly incorporate elasticity and plasticity on atomic length and diffusive timescales, even multiple crystal orientations caused by the periodic oscillations of the crystal lattice, the periodic oscillations have been observed [19], but also for its capacity to involve the solidification, phase segregation, solute diffusion and other important features.

For a binary alloy made up of A and B atoms, the total number density is defined $\rho = \rho_A + \rho_B$. To simplify calculations, it is convenient to fist introduce the following dimensionless fields: $n_A \equiv (\rho_A - \overline{\rho}_A)/\overline{\rho}$, $n_B \equiv (\rho_B - \overline{\rho}_B)/\overline{\rho}$. Also, it indicates the atomic number density field n and the concentration field δN (To show the atomic density difference, it can be approximated as the concentration field), which gives

$$\begin{aligned} n &= n_A + n_B = (\rho - \overline{\rho})/\overline{\rho} \\ \delta N &= (n_B - n_A) + (\overline{\rho}_B - \overline{\rho}_A)/\overline{\rho} = (\rho_B - \rho_A)/\overline{\rho} \end{aligned} \tag{1}$$

where F is the free energy functional given by

$$F = \int d\overline{x} \left(\begin{array}{c} \frac{n}{2}\left[\left(B_0^l n + B_2^l)\delta N\right)^2 + B_0^s(2)R_0 + R_1(\delta N)\right)^2 + \left(R_0 + R_1(\delta N)\right)^4\right]n \\ -\frac{t}{3}n^3 + \frac{v}{4}n^4 + \gamma(\delta N) + \frac{w}{2}(\delta N)^2 + \frac{u}{4}(\delta N)^4 + \frac{L^2}{2}\left|\overrightarrow{\nabla}(\delta N)^2\right| \end{array} \right) \tag{2}$$

Briefly outlining the physical meaning of the model parameters as follows: the B_0^l, B_2^l, B_0^S, t , v, w, L, γ, R_0, R_1 and u are constants, whose values depend on the material parameters. t, γ and v are determined by the low order terms of a local expansion of the classical density functional theory description of the material. The length scale of phase separation is decided by the interplay of u, L and w. B_2^l determines liquid volume modulus with the changing of atomic concentration field. B_0^l is the liquid temperature. B_0^S is associated with the solid phase of the elastic constants. $\Delta B = B_0^l - B_0^s$ corresponds to temperature characterized the initial driving force of crystallization, which can be enhanced by lowering ΔB. The interatomic distance may be tuned via parameters R_0 and R_1. $R = R_0 + R_1(\delta N)$ expresses the interatomic distance, for further simplification, we suppose that R and δN have a linear correlation, R has another expression like $R = R_0(1 + \alpha(\delta N))$, α represents the solute diffusion factor. Besides, in the spirit of keeping calculations as simple as possible without losing the basic physics contained in the model, $\gamma = 0$ in the free energy. Minimizing the free energy, $n = A[1/2\cos(2qy/\sqrt{3}) - \cos(qx)\cos(qy/\sqrt{3})]$ willbe used. Substituting this expression into (2) and minimizing with respect to q and A, recalling that δN is assumed constant over the scale that n varies, getting $q_{eq} = \sqrt{3}/(2R)$ and $A_{\min} = 4(t + \sqrt{t^2 - 15v\Delta B})/(15v)$.

Assuming a substitutional diffusion between species A and B, that the same M mobility applies for the two species, furthermore, considering that the mobility coefficient is a constant, the dynamics of the fields n and δN decouple, the respective equations of motions have the form:

$$\frac{\partial n}{\partial t} = M\nabla^2\frac{\delta F}{\delta n} \tag{3}$$

$$\frac{\partial(\delta N)}{\partial t} = M\nabla^2\frac{\delta F}{\delta(\delta N)} \tag{4}$$

The numerical discretization of Eq. (3) and Eq. (4) is solved using the mixed explicit-implicit Fourier transformations and operator splitting by G. Tegze [20].