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A Monte Carlo investigation of growth and characterization of heteroepitaxial thin films

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ABSTRACT

We investigate the growth of mismatched thin films by a kinetic Monte Carlo computer simulation and including a local photoemission model with reflection high-energy electron diffraction (RHEED) intensity for comparison. The strain is introduced through an elastic energy term based on a valence force field approximation. We describe an atomistic mechanism for dislocation nucleation during first stage of GaSb/GaAs (001) growth and in situ variations of photoemission current (PE) and RHEED intensity are reported. We have shown the formation of grooves corresponding to (111) facets, a precursor to the formation of misfit defects. The surface roughening and facetting by creation of grooves explain the absence of photoemission and RHEED oscillations in accordance with experimental observations [J.J. Zinck and D.H. Chow, J. Cryst. Growth, 175/176 (1997) 323, J.J. Zinck and D.H Chow, Appl. Phys. Lett. 66 (1995) 3524].

1. Introduction

The heteroepitaxial growth of lattice mismatched materials has been extensively investigated during recent years, both on theoretical and experimental grounds. The reason is that large strain energies develop in the layer from the first stages of the growth. The relaxation of the strain energy combined with the kinetics of atomic motions on the surface then leads to the various morphologies observed experimentally. An atomistic understanding of the processes controlling the quality of the interface formed under MBE growth conditions is of extreme importance. The Solid On Solid model [3], was the guideline for the first simulations during the past decades. In an effort to develop this approach, Madhukar and Ghaisas [4] have introduced, in the eighties, the essential features by introducing atomic surface reactivity and studying the influence of the local configurations on the growth rate incorporation.

The simulations presented in this paper differ from the previous models in two very important aspects. The first involves the interactions between atoms in interstitial sites, considered as intermediate configurations for interlayer migrations, leading to the faceting behaviour. The second aspect takes into account the deformation of structures and their effects: strains generated at the interface, their relaxation and the creation of point defects. The interesting example presented here is the GaSb/GaAs (001) growth presenting a large lattice mismatch of 8% and characterized by large island formation [5] with the presence of stacking faults associated with dislocations [5,6] in most of them.

To study in situ, the dynamic MBE growth of GaSb on GaAs, we have used our theoretical model of photoemission oscillations (PE) [7,8] and reflection high-energy electron diffraction (RHEED) intensity. Experimentally, the effect of lattice mismatch parameter on the oscillations of photoemission current was studied by Zinck and Chow [1] in the case of the quantum well AlSb/GaSb/AlSb deposited on (001) GaAs and InAs substrates. As seen on Fig. 1, the oscillations of photoemission current are absent during growth of the quantum well on GaAs substrate (Fig. 1a), but quite clear during growth on InAs substrate (Fig. 1b). The authors also showed a roughness front profile of films deposited on GaAs compared with those deposited on InAs substrate. These observations are attributed to the presence of dislocations and of defects in the interface between GaSb and GaAs due to the important mismatch between GaSb and GaAs (8%) compared with that between GaSb and InAs that is of 1%.

The purpose of this paper is to display the effect of lattice mismatch parameter on the oscillations of photoemission current and to study the first stage of GaSb/GaAs (001) growth to describe the

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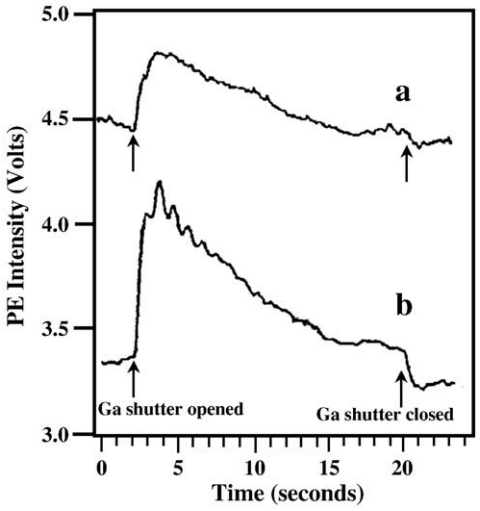

Fig. 1. Measurements of photoemission current [1] during growth of single quantum well AlSb/GaSb/AlSb on (a) (001) GaAs substrate and (b) (001) InAs substrate. The figure shows the effect of lattice mismatch parameter on photoemission oscillations.

dislocations generation. The model is described in section 2 and the results are presented and discussed in section 3.

2. Model

The general simulation technique has been described in detail previously [7–10]. A Monte Carlo process is associated to a valence force field (VFF) energetic model [11], in order to describe strain effects, due to the different nature of the deposited material and the substrate. The Kinetic Monte Carlo (KMC) method is based on a set of elementary atomic mechanisms. Their determination is certainly one of the key points of KMC simulation as a significant set of events is necessary to describe the correct behaviour of the film growth. The original aspect of our model concerns the introduction of two new concepts into the simulations in addition to classical events used in most epitaxy simulations: adsorption on the surface, desorption from the surface and intralayer migrations.

1. The first concept deals with the interlayer migrations, which is performed through an intermediate interstitial position [10]. This intermediate configuration allows migrations over several steps by successive jumps from interstitial to interstitial positions.
2. The second concept concerns the interaction between atoms in interstitial positions [12]. The result is the introduction of atoms in suspended positions with only one bond directed toward the substrate and a second bond with an atom in an upper layer. This atomic position is of first importance for observation of defects like vacancies or dislocations.

Next, when an event occurs, the structure needs to be relaxed in order to minimize the strain energy. We use the VFF semi-empirical potential in order to describe the elastic part of the total energy. We have used the formulation of Martin [11] for the stretching term and the model of Stillinger and Weber for the bending term [13]:

$$E_{\text{stress}} = \frac{k_r}{r_0^2}\sum_{\text{bonds}}(\Delta r)^2 + \frac{9}{8}k_\theta \sum_{\text{bond.angles}}\left(\frac{1}{3} + \cos\theta\right)^2 \quad (1)$$

The coefficients k_r and k_θ are calculated from the elastic constants [11] of the materials so that no adjustable parameter is used in our simulation, r_0 is the perfect crystal bond length, Δr is the bond length variation, while θ is the angle between two adjacent bonds. By the fact that in usual semiconductors, the value of k_r is 20 to 50 times larger than k_θ, showing the much greater difficulty to distort bond lengths rather than angles, we have assumed that the bond lengths are those of the GaAs and GaSb, while the bond angles are determined to minimize the bending term.

This VFF energetic model presents several advantages: (i) it is well adapted to non compact semiconductor structures, (ii) it is simple enough to execute the multi-million minimizations needed to simulate the growth, (iii) activation energies, depending on the local strain, can be simply defined.

The Monte Carlo procedure is based on the attribution of a time to each elementary event involving a single atom in the deposited layer. We follow a Poisson scheme, using an Arrhenius law combined with activation energy barriers.

$$\lambda_i = \nu \exp\left(-\frac{\Delta E_i}{kT}\right) \quad (2)$$

where $\Delta E_i = n\Phi + E_{\text{stress}}$ is the activation energy. The chemical binding energy Φ is deduced from the cohesive energy of the material and including the first and the second nearest neighbors interactions. n denoted the number of bonds to break in order to execute the move. T is the growth temperature and $\nu = 10^{12}$ s^{-1} is the vibrational frequency for atomic motions. With these assumptions, activation energy and a hopping rate is calculated for each possible event on the surface. The Monte Carlo time also includes a random part. The event associated with the lowest time is executed and a new cycle begins.

Concerning the photoemission current and RHEED intensity models, the sensibility of both RHEED and photoemission oscillations to the growth conditions [2] supports the hypothesis that both phenomena occur by mechanism related to the fluctuation of step density on the surface. Therefore, we have calculated the RHEED intensity within a kinematics theory, which is acceptable for incidence angles leading to destructive interference between adjacent (001) molecular planes [14]. To explain the photoemission oscillations, we have assumed that the photoemission properties depend on the chemical nature of the adsorbed atoms and to be proportional to the number of dangling bonds of group III atoms.

3. Results and discussion

The material under study is GaSb presenting 8% lattice mismatch with GaAs. To illustrate the effect of lattice mismatch parameter on the dynamic of growth, we present for comparison the case of GaSb deposited on InAs substrate presenting a misfit of 1%. The interaction energies are [15]: $\Phi_{\text{Gasb}} = 0.75$ eV, $\Phi_{\text{Ga–Ga}} = 0.17$ eV and $\Phi_{\text{Sb–Sb}} = 0.18$ eV, $\Phi_{\text{In–As}} = 0.7$ eV, $\Phi_{\text{In–In}} = 0.16$ eV, $\Phi_{\text{As–As}} = 0.2$ eV and elastic constant $k_\theta = 1.1$ eV. Simulations have been performed to deposit eight atomic layers on a 60×60 atoms flat substrate with periodic boundary conditions in the lateral directions. The growth temperature is set to 700 K with a deposition rate fixed to 0.35 monolayers (ML) per second.

As shown in Fig. 2a and b, we have analysed during growth, the dynamic behaviour of surface roughness as well as RHEED and photoemission oscillations for GaSb deposited respectively on GaAs and InAs substrates versus time.

In the case of GaSb on InAs growth (Fig. 2a), the RHEED and photoemission oscillations present regular amplitude interpreted by a layer by layer growth mode in agreement with experience. On the one hand, we explain this by the nearest chemical binding energies between deposited and substrate atoms and on the other hand by nearly lattice-match of GaSb and InAs (misfit of 1%) so that internal strain is negligible. However, the inter-layers migrations of atoms are done preferentially toward the down layers where they are more stable identically to homoepitaxial growth [7,8].

We note for GaSb deposited on GaAs, as it is clearly represented on Fig. 2b, a marked roughness (higher than one monolayer) and a low oscillations amplitudes even absent of RHEED and photoemission