Atomic scale simulation of epitaxial growth: Cases of GaAs/GaAs and CdTe/GaAs

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We present a kinetic Monte Carlo model describing the growth by molecular beam epitaxy (MBE) of semiconductor compounds and including a local photoemission model with reflection high-energy electron diffraction (RHEED) intensity for comparison. We investigate the cases of both homoepitaxial and heteroepitaxial growth. The valence force field approximation is used for the strain energy calculations in mismatched thin films In homoepitaxial growth of GaAs, we have study the variations of photoemission current and RHEED intensity and examined the GaAs morphology. In high lattice mismatch heteroepitaxial growth (CdTe/GaAs), we have shown the formation of grooves corresponding to (111) facets, precursor to the formation of misfit defects.

Keywords: Simulation; Interface structure, Photoemission current; Reflection high-energy electron diffraction; crystal defects

1. INTRODUCTION

An atomistic understanding of the processes controlling the quality interface formed under MBE growth is of extreme importance and simulation is a perfect tool for the understanding of strain and stress effects during growth and for the description of defects nucleation mechanisms. During last years, the solid on solid (SOS) model have been employed for large materials but the point and extended defects are inherently absent. This is due to the basic principle of the model, which excludes vacancies and overhangs from the beginning [1,2]. Our model presented here, goes beyond this approximation in the sense that it contains a mechanism which is derived from one type of interlayer migration over two atomic layers [3,4] and leading to vacancies and overhangs.

In this work, we study the growth of GaAs/GaAs and CdTe/GaAs with 14,6% lattice mismatch. In section II, we present the basic atomic events used in our model and the simplified VFF approximation used to express the strain energy. Section III is dedicated to present and discuss results of simulation growth, in particular the growth mode examined via the variations of photoemission current (PE) and reflection high-energy electron diffraction (RHEED) intensity and formation of grooves with (111) facets.

II. DESCRIPTION OF THE MODEL

The model deals with heteroepitaxial growth. Briefly, a Monte Carlo technique has been associated to an energy model to investigate the kinetics of the surface evolution. The elementary events describing the kinetic processes are deposition, evaporation, surface migration involving substitutional positions and interlayer migrations involving interstitial positions of the crystal [3]. The deposition site is defined randomly on an empty substitutional position on the surface and the random interval time is calculated considering the predefined deposition rate.

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

$$\lambda_i = \nu \exp(-\frac{\Delta E_i}{kT}) \qquad (1)$$

Where $\Delta E_i = n\gamma + E_s$ is the activation energy. For the strain energy E_s, the empirical valence force field (VFF) approximation [5] is used as it is perfectly adapted to zinc-blend lattices. The chemical binding energy is deduced from the cohesive energy of the material and including the first and the second nearest neighbours 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. A Monte Carlo time can be determined including a random part, and the event associated with the lowest time is executed and a new Monte Carlo cycle time is performed.

III. RESULTS AND DISCUSSION

Simulations of thin films growth on a (001) oriented substrate have been carried out. The

substrate surface has been assumed to be perfect and unreconstructed. The simulations were performed on square substrate sizes varied from (20x20) to (50x50) atoms with periodic boundary conditions to avoid edge effects. The thickness of the deposited films is up to 10 atomic layers.

3.1. Homoepitaxial growth of GaAs

In our Monte Carlo simulations the arsenic is provided as As_2 molecules as has been observed experimentally [6,7] in MBE growth of GaAs. The molecules are then physisorbed on the surface and migrate until they arrive at active Ga sites where they will be decomposed with two As atoms being incorporated. The RHEED intensity was calculated within a kinematics theory, which is acceptable for incidence angles leading to destructive interference between adjacent (001) molecular planes [8]. 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 which control the dynamic process of growth [9].

For high As_2 pressure, Ga flux fixed to deliver 1ML/s and substrate temperature fixed to 580°C, we have examined as shown in figure1 the dynamic behaviour of RHEED intensity and photoemission current versus diatomic deposited layers. It is seen that the period of each type of oscillations coincides exactly with addition to the bilayer (Ga+As). The oscillatory behaviour of photoemission current and RHEED intensity is a consequence of the formation, during growth, of clusters which leads to a change in the step density distribution as that observed experimentally [10]. This result display that RHEED intensity and photoemission current are complementary and substantiated their correlation with the dynamic of the growth front morphology. The first (RHEED) inform us upon the roughness of the surface and the second (PE) upon its composition. Note also regular amplitude for both RHEED and PE oscillations indicating a layer-by-layer mode growth conditions.

3.2. Heteroepitaxial growth

A lattice mismatch of 14.6% corresponding to CdTe/GaAs, has been used. A cross-section of the growing films on the plane (011) is carried out. Figure 2 shows the cross section of (011) plane of the growing film. It can be seen that the deposited films are not flat, but present grooves with identical facets. The facets are oriented (111), in agreement with experimental observations [11,12,13,14].

The groove is formed from the multiplication of vacancies in the successive deposited atomic layers. In fact, the appearance of a vacancy in the first layer directly involves 2 vacancies in the next layer, then 4 in the following one, then 8 vacancies etc. This is due to the zincblende structure and the strain that prevents the definite incorporation of the atom in the bottom of the groove. The reason of the formation of this defect is that as the strain increases in the deposited film, the lattice position becomes more and more unstable.

Next, when we have introduced reactions, which present collective incorporation of atoms, growth is performed by completing top layers of islands delimited by V-grooves. Thus after a certain time there is no stable position available for incoming atoms, leading to narrowing grooves filling by interstitial atoms, with no chance of individual incorporation. The result of these interactions is then collective incorporation of these atoms in stable crystal sites. Consequently, the 'suspended' configuration with only one bond toward the substrate and one upward appears and marks creation of defects (figure 2). And single vacancies (V in figure 2) or cluster vacancies are now possible and are observed in our simulation. The majority of point defects created are grouped causing a segmented dislocation line.

VI. CONCLUSION

We have presented some results of homoepitaxial and heteroepitaxial growth of thin films, with particular reference to the cases of GaAs/GaAs and CdTe/GaAs respectively. We have combined a Monte Carlo technique with the VFF approximation to determine the strain and the stress by energy minimization. In homoepitaxial growth, we have shown the relationship between RHEED intensity, photoemission current and growth front profile. In heteroepitaxial growth, we have observed that grooves showing (111) facets with unstable bottoms are formed during the early stages of growth using enhanced interlayer migrations, interstitial multiplication, and reaction allowing the narrowing of valley facets to form a dislocation.

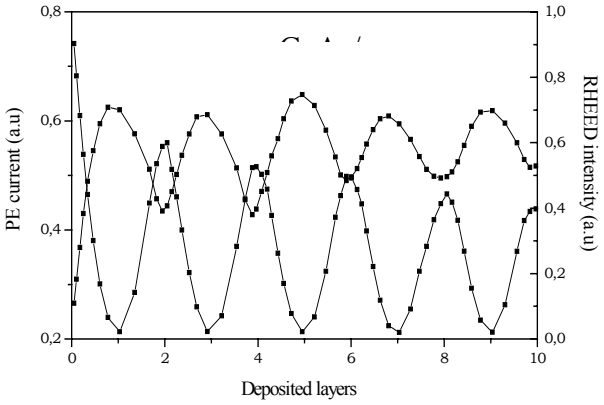

Figure 1: Oscillatory behaviour of RHEED intensity and photoemission current at T=580°C and deposition rate of 1ML/s.

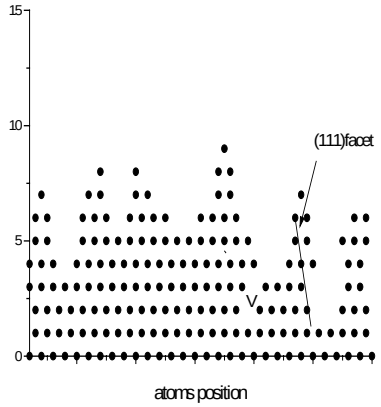

Figure 2: Projection on a (011) plane of a portion of growing film showing vacant sites(V) and growth on (111) facet.

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